

APBS
3.0.0

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Chapter 1

APBS Programmers Guide

APBS was written by Nathan A. Baker.
Additional contributing authors listed in the code documentation.

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1.2 License

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This documentation provides information about the programming interface provided by the APBS software and a general guide to linking to the APBS libraries. Information about installation, configuration, and general usage can be found in the [User's Guide](#).

1.3 Programming Style

APBS was developed following the [Clean OO C](#) style of Mike Holst. In short, Clean OO C code is written in a object-oriented, ISO C-compliant fashion, and can be compiled with either a C or C++ compiler.

Following this formalism, all public data is enclosed in structures which resemble C++ classes. These structures and member functions are then declared in a public header file which provides a concise description of the interface for the class. Private functions and data are included in private header files (or simply the source code files themselves) which are not distributed. When using the library, the end-user only sees the public header file and the compiled library and is therefore (hopefully) oblivious to the private members and functions. Each class is also equipped with a constructor and destructor function which is responsible for allocating and freeing any memory required by the instantiated objects. As mentioned above, public data members are enclosed in C structures which are visible to the end-user. Public member functions are generated by mangling the class and function names *and* passing a pointer to the object on which the member function is supposed to act. For example, a public member function with the C++ declaration

```
public double Foo::bar(int i, double d)
```

would be declared as

```
VEXTERNC double Foo_bar(Foo *thee, int i, double d)
```

where `VEXTERNC` is a compiler-dependent macro, the underscore `_` replaces the C++ double-colon `::`, and `thee` replaces the `this` variable implicit in all C++ classes. Since they do not appear in public header files, private functions could be declared in any format pleasing to the user, however, the above declaration convention should generally be used for both public and private functions. Within the source code, the public and private function declarations/definitions are prefaced by the macros `VPUBLIC` and `VPRIVATE`, respectively. These are macros which reduce global name pollution, similar to encapsulating private data within C++ classes.

The only C++ functions not explicitly covered by the above declaration scheme are the constructors (used to allocate and initialize class data members) and destructors (used to free allocated memory). These are declared in the following fashion: a constructor with the C++ declaration

```
public void Foo::Foo(int i, double d)
```

would be declared as

```
VEXTERNC Foo* Foo_ctor(int i, double d)
```

which returns a pointer to the newly constructed `Foo` object. Likewise, a destructor declared as

```
public void Foo::~~Foo()
```

in C++ would be

```
VEXTERNC void Foo_dtor(Foo **thee)
```

in Clean OO C.

Finally, inline functions in C++ are simply treated as macros in Clean OO C and declared/defined using `define` statements in the public header file.

See any of the APBS header files for more information on Clean OO C programming styles.

1.4 Application programming interface documentation

The API documentation for this code was generated by [doxygen](#). You can either view the API documentation by using the links at the top of this page, or the slight re-worded/re-interpreted list below:

- [Class overview](#)
- [Class declarations](#)
- [Class members](#)
- [Class methods](#)

Chapter 2

Bug List

Global **Bmat_printHB** (Bmat *thee, char *fname)

Hardwired to only handle the single block symmetric case.

Global **energyFE** (NOsh *nosh, int icalc, Vfetk *fetk[NOSH_MAXCALC], int *nenergy, double *totEnergy, double *qfEnergy, double *qmEnergy, double *dielEnergy)

"calcenergy 2" does not work

Global **initFE** (int icalc, NOsh *nosh, FEMparm *feparm, PBEparm *pbeparm, Vpbe *pbe[NOSH_MAXCALC], Valist *alist[NOSH_MAXMOL], Vfetk *fetk[NOSH_MAXCALC])

THIS FUNCTION IS HARD-CODED TO SOLVE LRPBE

THIS FUNCTION IS HARD-CODED TO SOLVE LRPBE

Class **sVpmgp**

Value ipcon does not currently allow for preconditioning in PMG

Global **Vacc_fastMolAcc** (Vacc *thee, double center[VAPBS_DIM], double radius)

This routine has a slight bug which can generate very small internal regions of high dielectric (thanks to John Mongan and Jess Swanson for finding this)

Global **Vacc_molAcc** (Vacc *thee, double center[VAPBS_DIM], double radius)

This routine has a slight bug which can generate very small internal regions of high dielectric (thanks to John Mongan and Jess Swanson for finding this)

Global **Vfetk_dumpLocalVar** ()

This function is not thread-safe

Global **Vfetk_externalUpdateFunction** (SS **simps, int num)

This function is not thread-safe.

Global **Vfetk_fillArray** (Vfetk *thee, Bvec *vec, Vdata_Type type)

Several values of type are not implemented

Global **Vfetk_PDE_ctor** (Vfetk *fetk)

Not thread-safe

Global **Vfetk_PDE_ctor2** (PDE *thee, Vfetk *fetk)

Not thread-safe

Global **Vfetk_PDE_delta** (PDE *thee, int type, int chart, double txq[], void *user, double F[])

This function is not thread-safe

Global **Vfetk_PDE_DFu_wv** (PDE *thee, int key, double W[], double dW[][VAPBS_DIM], double V[], double dV[][VAPBS_DIM])

This function is not thread-safe

Global **Vfetk_PDE_Fu** (PDE *thee, int key, double F[])

This function is not thread-safe

This function is not implemented (sets error to zero)

Global **Vfetk_PDE_Fu_v** (PDE *thee, int key, double V[], double dV[][VAPBS_DIM])

This function is not thread-safe

Global **Vfetk_PDE_initElement** (PDE *thee, int elementType, int chart, double tvx[][VAPBS_DIM], void *data)

This function is not thread-safe

Global **Vfetk_PDE_initFace** (PDE *thee, int faceType, int chart, double tnvect[])

This function is not thread-safe

Global **Vfetk_PDE_initPoint** (PDE *thee, int pointType, int chart, double txq[], double tU[], double tdU[][VAPBS_DIM])

This function is not thread-safe

This function uses pre-defined boundary definitions for the molecular surface.

Global **Vfetk_PDE_Ju** (PDE *thee, int key)

This function is not thread-safe.

Global **Vfetk_PDE_markSimplex** (int dim, int dimll, int simplexType, int faceType[VAPBS_NVS], int vertexType[VAPBS_NVS], int chart[], double vx[][VAPBS_DIM], void *simplex)

This function is not thread-safe

Global **Vfetk_PDE_u_D** (PDE *thee, int type, int chart, double txq[], double F[])

This function is hard-coded to call only multiple-sphere Debye-Hückel functions.

This function is not thread-safe.

Global **Vfetk_PDE_u_T** (PDE *thee, int type, int chart, double txq[], double F[])

This function is not thread-safe.

Global **Vfetk_write** (Vfetk *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, Bvec *vec, Vdata_Format format)

Some values of format are not implemented

Global **Vgreen_helmholtz** (Vgreen *thee, int npos, double *x, double *y, double *z, double *val, double kappa)

Not implemented yet

Global **Vgreen_helmholtzD** (Vgreen *thee, int npos, double *x, double *y, double *z, double *gradx, double *grady, double *gradz, double kappa)

Not implemented yet

Global **Vgrid_writeUHBD** (Vgrid *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, char *title, double *pvec)

This routine does not respect partition information

Global **Vpackmg** (int *iparm, double *rparm, size_t *nrwk, int *niwk, int *nx, int *ny, int *nz, int *nlev, int *nu1, int *nu2, int *mgkey, int *itmax, int *istop, int *ipcon, int *nonlin, int *mgsmoo, int *mgprol, int *mgcoar, int *mgsolv, int *mgdisc, int *iinfo, double *errtol, int *ipkey, double *omegal, double *omegan, int *irite, int *iperf)

Can this path variable be replaced with a Vio socket?

Global **Vpbe_ctor2** (Vpbe *thee, Valist *alist, int ionNum, double *ionConc, double *ionRadii, double *ionQ, double T, double soluteDiel, double solventDiel, double solventRadius, int focusFlag, double sdens, double z_mem, double L, double membraneDiel, double V)

The focusing flag is currently not used!!

Global **Vpee_markRefine** (Vpee *thee, AM *am, int level, int akey, int rcol, double etol, int bkey)

This function is no longer up-to-date with FEtk and may not function properly

Global **Vpmg_fillco** (Vpmg *thee, Vsurf_Meth surfMeth, double splineWin, Vchrg_Meth chargeMeth, int useDielXMap, Vgrid *dielXMap, int useDielYMap, Vgrid *dielYMap, int useDielZMap, Vgrid *dielZMap, int useKappaMap, Vgrid *kappaMap, int usePotMap, Vgrid *potMap, int useChargeMap, Vgrid *chargeMap)

useDielMap could only be passed once, not three times, to this function - why not just once? that's what the call in [routines.c](#) ends up doing - just passing useDielMap three times. - P. Ellis 11/3/11

Global **Vpmg_printColComp** (Vpmg *thee, char path[72], char title[72], char mxtype[3], int flag)

Can this path variable be replaced with a Vio socket?

Chapter 3

Deprecated List

Global [sMGparm::nlev](#)

Just ignored now

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Chapter 7

Module Documentation

7.1 dependencies

7.2 Vcsm class

A charge-simplex map for evaluating integrals of delta functions in a finite element setting.

Files

- file [vcsm.c](#)
Class Vcsm methods.
- file [vcsm.h](#)
Contains declarations for the Vcsm class.

Data Structures

- struct [sVcsm](#)
Charge-simplex map class.

Typedefs

- typedef struct [sVcsm](#) [Vcsm](#)
Declaration of the Vcsm class as the Vcsm structure.

Functions

- VEXTERNC void [Gem_setExternalUpdateFunction](#) ([Gem](#) *thee, void(*externalUpdate)(SS **simps, int num))
External function for FEtk Gem class to use during mesh refinement.
- VEXTERNC [Valist](#) * [Vcsm_getValist](#) ([Vcsm](#) *thee)
Get atom list.
- VEXTERNC int [Vcsm_getNumberAtoms](#) ([Vcsm](#) *thee, int isimp)
Get number of atoms associated with a simplex.
- VEXTERNC [Vatom](#) * [Vcsm_getAtom](#) ([Vcsm](#) *thee, int iatom, int isimp)
Get particular atom associated with a simplex.
- VEXTERNC int [Vcsm_getAtomIndex](#) ([Vcsm](#) *thee, int iatom, int isimp)
Get ID of particular atom in a simplex.
- VEXTERNC int [Vcsm_getNumberSimplices](#) ([Vcsm](#) *thee, int iatom)

Get number of simplices associated with an atom.

- VEXTERNC SS * [Vcsm_getSimplex](#) ([Vcsm](#) *thee, int isimp, int iatom)

Get particular simplex associated with an atom.

- VEXTERNC int [Vcsm_getSimplexIndex](#) ([Vcsm](#) *thee, int isimp, int iatom)

Get index particular simplex associated with an atom.

- VEXTERNC unsigned long int [Vcsm_memChk](#) ([Vcsm](#) *thee)

Return the memory used by this structure (and its contents) in bytes.

- VEXTERNC [Vcsm](#) * [Vcsm_ctor](#) ([Valist](#) *alist, [Gem](#) *gm)

Construct Vcsm object.

- VEXTERNC int [Vcsm_ctor2](#) ([Vcsm](#) *thee, [Valist](#) *alist, [Gem](#) *gm)

FORTTRAN stub to construct Vcsm object.

- VEXTERNC void [Vcsm_dtor](#) ([Vcsm](#) **thee)

Destroy Vcsm object.

- VEXTERNC void [Vcsm_dtor2](#) ([Vcsm](#) *thee)

FORTTRAN stub to destroy Vcsm object.

- VEXTERNC void [Vcsm_init](#) ([Vcsm](#) *thee)

Initialize charge-simplex map with mesh and atom data.

- VEXTERNC int [Vcsm_update](#) ([Vcsm](#) *thee, SS **simps, int num)

Update the charge-simplex and simplex-charge maps after refinement.

7.2.1 Detailed Description

A charge-simplex map for evaluating integrals of delta functions in a finite element setting.

7.2.2 Typedef Documentation

7.2.2.1 Vcsm

```
typedef struct sVcsm Vcsm
```

Declaration of the Vcsm class as the Vcsm structure.

Definition at line 122 of file [vcsm.h](#).

7.2.3 Function Documentation

7.2.3.1 Gem_setExternalUpdateFunction()

```
VEXTERNC void Gem_setExternalUpdateFunction (
    Gem * thee,
    void(*) (SS **simps, int num) externalUpdate )
```

External function for FEtk Gem class to use during mesh refinement.

Author

Nathan Baker

Parameters

<i>thee</i>	The FEtk geometry manager
<i>externalUpdate</i>	Function pointer for call during mesh refinement

7.2.3.2 Vcsm_ctor()

```
VEXTERNC Vcsm * Vcsm_ctor (
    Valist * alist,
    Gem * gm )
```

Construct Vcsm object.

Author

Nathan Baker

Note

- The initial mesh must be sufficiently coarse for the assignment procedures to be efficient
- The map is not built until Vcsm_init is called

Returns

Pointer to newly allocated Vcsm object

Parameters

<i>alist</i>	List of atoms
<i>gm</i>	FEtk geometry manager defining the mesh

Definition at line 136 of file [vcsm.c](#).

7.2.3.3 Vcsm_ctor2()

```
VEXTERNC int Vcsm_ctor2 (
    Vcsm * thee,
    Valist * alist,
    Gem * gm )
```

FORTTRAN stub to construct Vcsm object.

Author

Nathan Baker

Note

- The initial mesh must be sufficiently coarse for the assignment procedures to be efficient
- The map is not built until Vcsm_init is called

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	The Vcsm object
<i>alist</i>	The list of atoms
<i>gm</i>	The FEtk geometry manager defining the mesh

Definition at line 147 of file [vcsn.c](#).

7.2.3.4 Vcsn_dtor()

```
VEXTERNC void Vcsn_dtor (
    Vcsn ** thee )
```

Destroy Vcsn object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location for Vcsn object
-------------	--

Definition at line 292 of file [vcsn.c](#).

7.2.3.5 Vcsn_dtor2()

```
VEXTERNC void Vcsn_dtor2 (
    Vcsn * thee )
```

FORTTRAN stub to destroy Vcsn object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to Vcsn object
-------------	------------------------

Definition at line 300 of file [vcsn.c](#).

7.2.3.6 Vcsn_getAtom()

```
VEXTERNC Vatom * Vcsn_getAtom (
    Vcsn * thee,
    int iatom,
    int isimp )
```

Get particular atom associated with a simplex.

Author

Nathan Baker

Returns

Array of atoms associated with a simplex

Parameters

<i>thee</i>	The Vcsm object
<i>iatom</i>	Index of atom in Vcsm list ofr this simplex
<i>isimp</i>	Simplex ID

Definition at line 77 of file [vcsm.c](#).

7.2.3.7 Vcsm_getAtomIndex()

```
VEXTERNC int Vcsm_getAtomIndex (
    Vcsm * thee,
    int iatom,
    int isimp )
```

Get ID of particular atom in a simplex.

Author

Nathan Baker

Returns

Index of atom in Valist object

Parameters

<i>thee</i>	The Vcsm object
<i>iatom</i>	Index of atom in Vcsm list for this simplex
<i>isimp</i>	Simplex ID

Definition at line 88 of file [vcsm.c](#).

7.2.3.8 Vcsm_getNumberAtoms()

```
VEXTERNC int Vcsm_getNumberAtoms (
    Vcsm * thee,
    int isimp )
```

Get number of atoms associated with a simplex.

Author

Nathan Baker

Returns

Number of atoms associated with a simplex

Parameters

<i>thee</i>	The Vcsm object
<i>isimp</i>	Simplex ID

Definition at line 69 of file [vcsn.c](#).

7.2.3.9 Vcsn_getNumberSimplices()

```
VEXTERNC int Vcsn_getNumberSimplices (
    Vcsn * thee,
    int iatom )
```

Get number of simplices associated with an atom.

Author

Nathan Baker

Returns

Number of simplices associated with an atom

Parameters

<i>thee</i>	The Vcsn object
<i>iatom</i>	The Valist atom index

Definition at line 99 of file [vcsn.c](#).

7.2.3.10 Vcsn_getSimplex()

```
VEXTERNC SS * Vcsn_getSimplex (
    Vcsn * thee,
    int isimp,
    int iatom )
```

Get particular simplex associated with an atom.

Author

Nathan Baker

Returns

Pointer to simplex object

Parameters

<i>thee</i>	The Vcsn object
<i>isimp</i>	Index of simplex in Vcsn list
<i>iatom</i>	Valist atom index

Definition at line 109 of file [vcsn.c](#).

7.2.3.11 Vcsn_getSimplexIndex()

```
VEXTERNC int Vcsn_getSimplexIndex (
```

```
Vcsm * thee,  
int isimp,  
int iatom )
```

Get index particular simplex associated with an atom.

Author

Nathan Baker

Returns

Gem index of specified simplex

Parameters

<i>thee</i>	The Vcsm object
<i>isimp</i>	Index of simplex in Vcsm list
<i>iatom</i>	Index of atom in Valist

Definition at line 119 of file [vcsm.c](#).

7.2.3.12 Vcsm_getValist()

```
VEXTERNC Valist * Vcsm_getValist (  
    Vcsm * thee )
```

Get atom list.

Author

Nathan Baker

Returns

Pointer to Valist atom list

Parameters

<i>thee</i>	The Vcsm object
-------------	-----------------

Definition at line 62 of file [vcsm.c](#).

7.2.3.13 Vcsm_init()

```
VEXTERNC void Vcsm_init (  
    Vcsm * thee )
```

Initialize charge-simplex map with mesh and atom data.

Author

Nathan Baker

Note

The initial mesh must be sufficiently coarse for the assignment procedures to be efficient

Parameters

<i>thee</i>	The Vcsm object
-------------	-----------------

Definition at line 170 of file [vcsm.c](#).

7.2.3.14 Vcsm_memChk()

```

VEXTERNC unsigned long int Vcsm_memChk (
    Vcsm * thee )

```

Return the memory used by this structure (and its contents) in bytes.

Author

Nathan Baker

Returns

The memory used by this structure and its contents in bytes

Parameters

<i>thee</i>	The Vcsm object
-------------	-----------------

Definition at line 129 of file [vcsm.c](#).

7.2.3.15 Vcsm_update()

```

VEXTERNC int Vcsm_update (
    Vcsm * thee,
    SS ** simps,
    int num )

```

Update the charge-simplex and simplex-charge maps after refinement.

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	The Vcsm object
<i>simps</i>	List of pointer to newly created (by refinement) simplex objects. The first simplex is expected to be derived from the parent simplex and therefore have the same ID. The remaining simplices are the children and should represent new entries in the charge-simplex map.
<i>num</i>	Number of simplices in simps list

Definition at line 326 of file [vcsn.c](#).

7.3 Vfetk class

FETk master class (interface between FETk and APBS)

Files

- file [vfetk.c](#)
Class Vfetk methods.
- file [vfetk.h](#)
Contains declarations for class Vfetk.

Data Structures

- struct [sVfetk](#)
Contains public data members for Vfetk class/module.
- struct [sVfetk_LocalVar](#)
Vfetk LocalVar subclass.

Macros

- #define [VRINGMAX](#) 1000
Maximum number of simplices in a simplex ring.
- #define [VATOMMAX](#) 1000000
Maximum number of atoms associated with a vertex.

Typedefs

- typedef enum [eVfetk_LsolvType](#) [Vfetk_LsolvType](#)
Declare FEMparm_LsolvType type.
- typedef enum [eVfetk_MeshLoad](#) [Vfetk_MeshLoad](#)
Declare FEMparm_GuessType type.
- typedef enum [eVfetk_NsolvType](#) [Vfetk_NsolvType](#)
Declare FEMparm_NsolvType type.
- typedef enum [eVfetk_GuessType](#) [Vfetk_GuessType](#)
Declare FEMparm_GuessType type.
- typedef enum [eVfetk_PrecType](#) [Vfetk_PrecType](#)
Declare FEMparm_GuessType type.
- typedef struct [sVfetk_LocalVar](#) [Vfetk_LocalVar](#)
Declaration of the Vfetk_LocalVar subclass as the Vfetk_LocalVar structure.
- typedef struct [sVfetk](#) [Vfetk](#)
Declaration of the Vfetk class as the Vfetk structure.

Enumerations

- enum `eVfetk_LsolvType` { `VLT_SLU` =0 , `VLT_MG` =1 , `VLT_CG` =2 , `VLT_BCG` =3 }
Linear solver type.
- enum `eVfetk_MeshLoad` { `VML_DIRICUBE` , `VML_NEUMCUBE` , `VML_EXTERNAL` }
Mesh loading operation.
- enum `eVfetk_NsolvType` { `VNT_NEW` =0 , `VNT_INC` =1 , `VNT_ARC` =2 }
Non-linear solver type.
- enum `eVfetk_GuessType` { `VGT_ZERO` =0 , `VGT_DIRI` =1 , `VGT_PREV` =2 }
Initial guess type.
- enum `eVfetk_PrecType` { `VPT_IDEN` =0 , `VPT_DIAG` =1 , `VPT_MG` =2 }
Preconditioner type.

Functions

- VPUBLIC double `Vfetk_energy` (`Vfetk *thee`, int color, int nonlin)
Return the total electrostatic energy.
- VEXTERNNC Gem * `Vfetk_getGem` (`Vfetk *thee`)
Get a pointer to the Gem (grid manager) object.
- VEXTERNNC AM * `Vfetk_getAM` (`Vfetk *thee`)
Get a pointer to the AM (algebra manager) object.
- VEXTERNNC `Vpbe` * `Vfetk_getVpbe` (`Vfetk *thee`)
Get a pointer to the Vpbe (PBE manager) object.
- VEXTERNNC `Vcsm` * `Vfetk_getVcsm` (`Vfetk *thee`)
Get a pointer to the Vcsm (charge-simplex map) object.
- VEXTERNNC int `Vfetk_getAtomColor` (`Vfetk *thee`, int iatom)
Get the partition information for a particular atom.
- VEXTERNNC `Vfetk` * `Vfetk_ctor` (`Vpbe *pbe`, `Vhal_PBEType` type)
Constructor for Vfetk object.
- VEXTERNNC int `Vfetk_ctor2` (`Vfetk *thee`, `Vpbe *pbe`, `Vhal_PBEType` type)
FORTTRAN stub constructor for Vfetk object.
- VEXTERNNC void `Vfetk_dtor` (`Vfetk **thee`)
Object destructor.
- VEXTERNNC void `Vfetk_dtor2` (`Vfetk *thee`)
FORTTRAN stub object destructor.
- VEXTERNNC double * `Vfetk_getSolution` (`Vfetk *thee`, int *length)
Create an array containing the solution (electrostatic potential in units of $k_B T/e$) at the finest mesh level.
- VEXTERNNC void `Vfetk_setParameters` (`Vfetk *thee`, `PBEparm *pbeparm`, `FEMparm *feparm`)
Set the parameter objects.
- VEXTERNNC double `Vfetk_dqmEnergy` (`Vfetk *thee`, int color)
Get the "mobile charge" and "polarization" contributions to the electrostatic energy.
- VEXTERNNC double `Vfetk_qfEnergy` (`Vfetk *thee`, int color)
Get the "fixed charge" contribution to the electrostatic energy.
- VEXTERNNC unsigned long int `Vfetk_memChk` (`Vfetk *thee`)
Return the memory used by this structure (and its contents) in bytes.
- VEXTERNNC void `Vfetk_setAtomColors` (`Vfetk *thee`)
Transfer color (partition ID) information frmo a partitioned mesh to the atoms.
- VEXTERNNC void `Bmat_printHB` (`Bmat *thee`, char *fname)

- Writes a Bmat to disk in Harwell-Boeing sparse matrix format.*
- VEXTERNC Vrc_Codes Vfetc_genCube (Vfetc *thee, double center[3], double length[3], Vfetc_MeshLoad meshType)
- Construct a rectangular mesh (in the current Vfetc object)*
- VEXTERNC Vrc_Codes Vfetc_loadMesh (Vfetc *thee, double center[3], double length[3], Vfetc_MeshLoad meshType, Vio *sock)
- Loads a mesh into the Vfetc (and associated) object(s).*
- VEXTERNC PDE * Vfetc_PDE_ctor (Vfetc *fetc)
- Constructs the FEtk PDE object.*
- VEXTERNC int Vfetc_PDE_ctor2 (PDE *thee, Vfetc *fetc)
- Initializes the FEtk PDE object.*
- VEXTERNC void Vfetc_PDE_dtor (PDE **thee)
- Destroys FEtk PDE object.*
- VEXTERNC void Vfetc_PDE_dtor2 (PDE *thee)
- FORTTRAN stub: destroys FEtk PDE object.*
- VEXTERNC void Vfetc_PDE_initAssemble (PDE *thee, int ip[], double rp[])
- Do once-per-assembly initialization.*
- VEXTERNC void Vfetc_PDE_initElement (PDE *thee, int elementType, int chart, double txq[VAPBS_DIM], void *data)
- Do once-per-element initialization.*
- VEXTERNC void Vfetc_PDE_initFace (PDE *thee, int faceType, int chart, double tvec[])
- Do once-per-face initialization.*
- VEXTERNC void Vfetc_PDE_initPoint (PDE *thee, int pointType, int chart, double txq[], double tU[], double tdU[VAPBS_DIM])
- Do once-per-point initialization.*
- VEXTERNC void Vfetc_PDE_Fu (PDE *thee, int key, double F[])
- Evaluate strong form of PBE. For interior points, this is:*
- VEXTERNC double Vfetc_PDE_Fu_v (PDE *thee, int key, double V[], double dV[VAPBS_DIM])
- This is the weak form of the PBE; i.e. the strong form integrated with a test function to give:*
- VEXTERNC double Vfetc_PDE_DFu_wv (PDE *thee, int key, double W[], double dW[VAPBS_DIM], double V[], double dV[VAPBS_DIM])
- This is the linearization of the weak form of the PBE; e.g., for use in a Newton iteration. This is the functional linearization of the strong form integrated with a test function to give:*
- VEXTERNC void Vfetc_PDE_delta (PDE *thee, int type, int chart, double txq[], void *user, double F[])
- Evaluate a (discretized) delta function source term at the given point.*
- VEXTERNC void Vfetc_PDE_u_D (PDE *thee, int type, int chart, double txq[], double F[])
- Evaluate the Dirichlet boundary condition at the given point.*
- VEXTERNC void Vfetc_PDE_u_T (PDE *thee, int type, int chart, double txq[], double F[])
- Evaluate the "true solution" at the given point for comparison with the numerical solution.*
- VEXTERNC void Vfetc_PDE_bisectEdge (int dim, int dimII, int edgeType, int chart[], double vx[VAPBS_DIM])
- Define the way manifold edges are bisected.*
- VEXTERNC void Vfetc_PDE_mapBoundary (int dim, int dimII, int vertexType, int chart, double vx[VAPBS_DIM])
- Map a boundary point to some pre-defined shape.*
- VEXTERNC int Vfetc_PDE_markSimplex (int dim, int dimII, int simplexType, int faceType[VAPBS_NVS], int vertexType[VAPBS_NVS], int chart[], double vx[VAPBS_DIM], void *simplex)
- User-defined error estimator – in our case, a geometry-based refinement method; forcing simplex refinement at the dielectric boundary and (for non-regularized PBE) the charges.*
- VEXTERNC void Vfetc_PDE_oneChart (int dim, int dimII, int objType, int chart[], double vx[VAPBS_DIM], int dimV)

- Unify the chart for different coordinate systems – a no-op for us.*

 - VEXTERNC double [Vfetc_PDE_Ju](#) (PDE *thee, int key)

Energy functional. This returns the energy (less delta function terms) in the form:
- VEXTERNC void [Vfetc_externalUpdateFunction](#) (SS **simps, int num)

External hook to simplex subdivision routines in Gem. Called each time a simplex is subdivided (we use it to update the charge-simplex map)
- VEXTERNC int [Vfetc_PDE_simplexBasisInit](#) (int key, int dim, int comp, int *ndof, int dof[])

Initialize the bases for the trial or the test space, for a particular component of the system, at all quadrature points on the master simplex element.
- VEXTERNC void [Vfetc_PDE_simplexBasisForm](#) (int key, int dim, int comp, int pdkey, double xq[], double basis[])

Evaluate the bases for the trial or test space, for a particular component of the system, at all quadrature points on the master simplex element.
- VEXTERNC void [Vfetc_readMesh](#) (Vfetc *thee, int skey, Vio *sock)

Read in mesh and initialize associated internal structures.
- VEXTERNC void [Vfetc_dumpLocalVar](#) ()

Debugging routine to print out local variables used by PDE object.
- VEXTERNC int [Vfetc_fillArray](#) (Vfetc *thee, Bvec *vec, [Vdata_Type](#) type)

Fill an array with the specified data.
- VEXTERNC int [Vfetc_write](#) (Vfetc *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, Bvec *vec, [Vdata_Format](#) format)

Write out data.
- VEXTERNC Vrc_Codes [Vfetc_loadGem](#) (Vfetc *thee, Gem *gm)

Load a Gem geometry manager object into Vfetc.

7.3.1 Detailed Description

FEtk master class (interface between FEtk and APBS)

7.3.2 Macro Definition Documentation

7.3.2.1 VATOMMAX

```
#define VATOMMAX 1000000
```

Maximum number of atoms associated with a vertex.

Definition at line 1779 of file [vfetc.c](#).

7.3.2.2 VRINGMAX

```
#define VRINGMAX 1000
```

Maximum number of simplices in a simplex ring.

Definition at line 1776 of file [vfetc.c](#).

7.3.3 Typedef Documentation

7.3.3.1 Vfetk

Vfetk

Declaration of the Vfetk class as the Vfetk structure.

Definition at line 207 of file [vfetk.h](#).

7.3.3.2 Vfetk_GuessType

```
typedef enum eVfetk_GuessType Vfetk_GuessType
```

Declare FEMparm_GuessType type.

Definition at line 148 of file [vfetk.h](#).

7.3.3.3 Vfetk_LocalVar

```
typedef struct sVfetk_LocalVar Vfetk_LocalVar
```

Declaration of the Vfetk_LocalVar subclass as the Vfetk_LocalVar structure.

Definition at line 259 of file [vfetk.h](#).

7.3.3.4 Vfetk_LsolvType

```
typedef enum eVfetk_LsolvType Vfetk_LsolvType
```

Declare FEMparm_LsolvType type.

Definition at line 97 of file [vfetk.h](#).

7.3.3.5 Vfetk_MeshLoad

```
typedef enum eVfetk_MeshLoad Vfetk_MeshLoad
```

Declare FEMparm_GuessType type.

Definition at line 114 of file [vfetk.h](#).

7.3.3.6 Vfetk_NsolvType

```
typedef enum eVfetk_NsolvType Vfetk_NsolvType
```

Declare FEMparm_NsolvType type.

Definition at line 131 of file [vfetk.h](#).

7.3.3.7 Vfetk_PrecType

```
typedef enum eVfetk_PrecType Vfetk_PrecType
```

Declare FEMparm_GuessType type.

Definition at line 165 of file [vfetk.h](#).

7.3.4 Enumeration Type Documentation

7.3.4.1 eVfetk_GuessType

```
enum eVfetk_GuessType
```

Initial guess type.

Note

Do not change these values; they correspond to settings in FEtk

Enumerator

VGT_ZERO	Zero initial guess
VGT_DIRI	Dirichlet boundary condition initial guess
VGT_PREV	Previous level initial guess

Definition at line 138 of file [vfetk.h](#).

7.3.4.2 eVfetk_LsolvType

enum [eVfetk_LsolvType](#)

Linear solver type.

Note

Do not change these values; they correspond to settings in FEtk

Enumerator

VLT_SLU	SuperLU direct solve
VLT_MG	Multigrid
VLT_CG	Conjugate gradient
VLT_BCG	BiCGStab

Definition at line 86 of file [vfetk.h](#).

7.3.4.3 eVfetk_MeshLoad

enum [eVfetk_MeshLoad](#)

Mesh loading operation.

Enumerator

VML_DIRICUBE	Dirichlet cube
VML_NEUMCUBE	Neumann cube
VML_EXTERNAL	External mesh (from socket)

Definition at line 104 of file [vfetk.h](#).

7.3.4.4 eVfetk_NsolvType

enum [eVfetk_NsolvType](#)

Non-linear solver type.

Note

Do not change these values; they correspond to settings in FEtk

Enumerator

VNT_NEW	Newton solver
VNT_INC	Incremental
VNT_ARC	Psuedo-arclength

Definition at line 121 of file [vfetk.h](#).

7.3.4.5 eVfetk_PrecType

```
enum eVfetk_PrecType
```

Preconditioner type.

Note

Do not change these values; they correspond to settings in FEtk

Enumerator

VPT_IDEN	Identity matrix
VPT_DIAG	Diagonal scaling
VPT_MG	Multigrid

Definition at line 155 of file [vfetk.h](#).

7.3.5 Function Documentation**7.3.5.1 Bmat_printHB()**

```
VEXTERNC void Bmat_printHB (
    Bmat * thee,
    char * fname )
```

Writes a Bmat to disk in Harwell-Boeing sparse matrix format.

Author

Stephen Bond

Note

This is a friend function of Bmat

Bug Hardwired to only handle the single block symmetric case.

Parameters

<i>thee</i>	The matrix to write
<i>fname</i>	Filename for output

Definition at line 1026 of file [vfetk.c](#).

7.3.5.2 Vfetk_ctor()

```
VEXTERNC Vfetk * Vfetk_ctor (
    Vpbe * pbe,
    Vhal_PBEType type )
```

Constructor for Vfetk object.

Author

Nathan Baker

Returns

Pointer to newly allocated Vfetk object

Note

This sets up the Gem, AM, and Aprx FEtk objects but does not create a mesh. The easiest way to create a mesh is to then call Vfetk_genCube

Parameters

<i>pbe</i>	Vpbe (PBE manager object)
<i>type</i>	Version of PBE to solve

Definition at line 532 of file [vfetk.c](#).

7.3.5.3 Vfetk_ctor2()

```
VEXTERNC int Vfetk_ctor2 (
    Vfetk * thee,
    Vpbe * pbe,
    Vhal_PBEType type )
```

FORTTRAN stub constructor for Vfetk object.

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Note

This sets up the Gem, AM, and Aprx FEtk objects but does not create a mesh. The easiest way to create a mesh is to then call Vfetk_genCube

Parameters

<i>thee</i>	Vfetk object memory
<i>pbe</i>	PBE manager object
<i>type</i>	Version of PBE to solve

Definition at line 545 of file [vfetk.c](#).

7.3.5.4 Vfetk_dqmEnergy()

```
VEXTERNC double Vfetk_dqmEnergy (
    Vfetk * thee,
    int color )
```

Get the "mobile charge" and "polarization" contributions to the electrostatic energy.

Using the solution at the finest mesh level, get the electrostatic energy due to the interaction of the mobile charges with the potential and polarization of the dielectric medium:

$$G = \frac{1}{4I_s} \sum_i c_i q_i^2 \int \bar{\kappa}^2(x) e^{-q_i u(x)} dx + \frac{1}{2} \int \epsilon (\nabla u)^2 dx$$

for the NPBE and

$$G = \frac{1}{2} \int \bar{\kappa}^2(x) u^2(x) dx + \frac{1}{2} \int \epsilon (\nabla u)^2 dx$$

for the LPBE. Here i denotes the counterion species, I_s is the bulk ionic strength, $\bar{\kappa}^2(x)$ is the modified Debye-Huckel parameter, c_i is the concentration of species i , q_i is the charge of species i , ϵ is the dielectric function, and $u(x)$ is the dimensionless electrostatic potential. The energy is scaled to units of $k_B T$.

Author

Nathan Baker

Parameters

<i>thee</i>	Vfetk object
<i>color</i>	Partition restriction for energy evaluation, only used if non-negative

Returns

The "mobile charge" and "polarization" contributions to the electrostatic energy in units of $k_B T$.

Parameters

<i>thee</i>	The Vfetk object
<i>color</i>	Partition restriction for energy calculation; if non-negative, energy calculation is restricted to the specified partition (indexed by simplex and atom colors)

Definition at line 842 of file [vfetk.c](#).

7.3.5.5 Vfetk_dtor()

```
VEXTERNC void Vfetk_dtor (
    Vfetk ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of Vfetk object
-------------	--

Definition at line 625 of file [vfetk.c](#).

7.3.5.6 Vfetk_dtor2()

```
VEXTERNC void Vfetk_dtor2 (
    Vfetk * thee )
```

FORTTRAN stub object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to Vfetk object to be destroyed
-------------	---

Definition at line 633 of file [vfetk.c](#).

7.3.5.7 Vfetk_dumpLocalVar()

```
VEXTERNC void Vfetk_dumpLocalVar ( )
```

Debugging routine to print out local variables used by PDE object.

Author

Nathan Baker

Bug This function is not thread-safe

Definition at line 2255 of file [vfetk.c](#).

7.3.5.8 Vfetk_energy()

```
VEXTERNC double Vfetk_energy (
    Vfetk * thee,
    int color,
    int nonlin )
```

Return the total electrostatic energy.

Using the solution at the finest mesh level, get the electrostatic energy using the free energy functional for the Poisson-Boltzmann equation without removing any self-interaction terms (i.e., removing the reference state of isolated charges present in an infinite dielectric continuum with the same relative permittivity as the interior of the protein) and return the result in units of $k_B T$. The argument *color* allows the user to control the partition on which this energy is calculated; if (*color* == -1) no restrictions are used. The solution is obtained from the finest level of the passed AM object, but atomic data from the Vfetk object is used to calculate the energy.

Author

Nathan Baker

Returns

Total electrostatic energy in units of $k_B T$.

Using the solution at the finest mesh level, get the electrostatic energy using the free energy functional for the Poisson-Boltzmann equation without removing any self-interaction terms (i.e., removing the reference state of isolated charges present in an infinite dielectric continuum with the same relative permittivity as the interior of the protein) and return the result in units of $k_B T$. The argument *color* allows the user to control the partition on which this energy is calculated; if (*color* == -1) no restrictions are used. The solution is obtained from the finest level of the passed AM object, but atomic data from the Vfetc object is used to calculate the energy.

Author

Nathan Baker

Returns

Total electrostatic energy in units of $k_B T$.

< Total energy

<

<

Parameters

<i>thee</i>	The Vfetc object
<i>color</i>	Partition restriction for energy calculation; if non-negative, energy calculation is restricted to the specified partition (indexed by simplex and atom colors)
<i>nonlin</i>	If 1, the NPBE energy functional is used; otherwise, the LPBE energy functional is used. If -2, SMPBE is used.

Definition at line 693 of file [vfetc.c](#).

7.3.5.9 Vfetc_externalUpdateFunction()

```

VEXTERNC void Vfetc_externalUpdateFunction (
    SS ** simps,
    int num )

```

External hook to simplex subdivision routines in Gem. Called each time a simplex is subdivided (we use it to update the charge-simplex map)

Author

Nathan Baker

Bug This function is not thread-safe.

Parameters

<i>simps</i>	List of parent (<i>simps</i> [0]) and children (remainder) simplices
<i>num</i>	Number of simplices in list

Definition at line 2078 of file [vfetc.c](#).

7.3.5.10 Vfetk_fillArray()

```

VEXTERNC int Vfetk_fillArray (
    Vfetk * thee,
    Bvec * vec,
    Vdata_Type type )

```

Fill an array with the specified data.

Author

Nathan Baker

Note

This function is thread-safe

Bug Several values of type are not implemented

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	The Vfetk object with the data
<i>vec</i>	The vector to hold the data
<i>type</i>	The type of data to write

Definition at line 2299 of file [vfetk.c](#).

7.3.5.11 Vfetk_genCube()

```

VEXTERNC Vrc_Codes Vfetk_genCube (
    Vfetk * thee,
    double center[3],
    double length[3],
    Vfetk_MeshLoad meshType )

```

Construct a rectangular mesh (in the current Vfetk object)

Author

Nathan Baker

Generates a new cube mesh within the provided Vfetk object based on the specified mesh type. Creates a new copy of the mesh based on the global variables at the top of the file and the mesh type, then recenters the mesh based on the center and length variables provided to the function.

Parameters

<i>thee</i>	Vfetk object
<i>center</i>	Center for mesh, which the new mesh will adjust to
<i>length</i>	Mesh lengths, which the new mesh will adjust to
<i>meshType</i>	Mesh boundary conditions

Definition at line 885 of file [vfetk.c](#).

7.3.5.12 Vfetk_getAM()

```
VEXTERNC AM * Vfetk_getAM (
    Vfetk * thee )
```

Get a pointer to the AM (algebra manager) object.

Author

Nathan Baker

Returns

Pointer to the AM (algebra manager) object

Parameters

<i>thee</i>	The Vfetk object
-------------	------------------

Definition at line 497 of file [vfetk.c](#).

7.3.5.13 Vfetk_getAtomColor()

```
VEXTERNC int Vfetk_getAtomColor (
    Vfetk * thee,
    int iatom )
```

Get the partition information for a particular atom.

Author

Nathan Baker

Note

Friend function of Vatom

Returns

Partition ID

Parameters

<i>thee</i>	The Vfetk object
<i>iatom</i>	Valist atom index

Definition at line 517 of file [vfetk.c](#).

7.3.5.14 Vfetk_getGem()

```
VEXTERNC Gem * Vfetk_getGem (
    Vfetk * thee )
```

Get a pointer to the Gem (grid manager) object.

Author

Nathan Baker

Returns

Pointer to the Gem (grid manager) object

Parameters

<i>thee</i>	Vfetk object
-------------	--------------

Definition at line 490 of file [vfetk.c](#).

7.3.5.15 Vfetk_getSolution()

```

VEXTERNC double * Vfetk_getSolution (
    Vfetk * thee,
    int * length )

```

Create an array containing the solution (electrostatic potential in units of $k_B T/e$) at the finest mesh level.

Author

Nathan Baker and Michael Holst

Note

The user is responsible for destroying the newly created array

Returns

Newly created array of length "length" (see above); the user is responsible for destruction

Parameters

<i>thee</i>	Vfetk object with solution
<i>length</i>	Ste to length of the newly created solution array

Definition at line 641 of file [vfetk.c](#).

7.3.5.16 Vfetk_getVcsm()

```

VEXTERNC Vcsm * Vfetk_getVcsm (
    Vfetk * thee )

```

Get a pointer to the Vcsm (charge-simplex map) object.

Author

Nathan Baker

Returns

Pointer to the Vcsm (charge-simplex map) object

Parameters

<i>thee</i>	The Vfetk object
-------------	------------------

Definition at line 510 of file [vfetk.c](#).

7.3.5.17 Vfetk_getVpbe()

```
VEEXTERNC Vpbe * Vfetk_getVpbe (
    Vfetk * thee )
```

Get a pointer to the Vpbe (PBE manager) object.

Author

Nathan Baker

Returns

Pointer to the Vpbe (PBE manager) object

Parameters

<i>thee</i>	The Vfetk object
-------------	------------------

Definition at line 503 of file [vfetk.c](#).

7.3.5.18 Vfetk_loadGem()

```
VEEXTERNC Vrc_Codes Vfetk_loadGem (
    Vfetk * thee,
    Gem * gm )
```

Load a Gem geometry manager object into Vfetk.

Author

Nathan Baker

Parameters

<i>thee</i>	Destination
<i>gm</i>	Geometry manager source

7.3.5.19 Vfetk_loadMesh()

```
VEEXTERNC Vrc_Codes Vfetk_loadMesh (
    Vfetk * thee,
```

```

double center[3],
double length[3],
Vfetk_MeshLoad meshType,
Vio * sock )

```

Loads a mesh into the Vfetk (and associated) object(s).

Author

Nathan Baker

If we have an external mesh, load that external mesh from the provided socket. If we specify a non-external mesh type, we generate a new mesh cube based on templates. We then create and store a new Vcsm object in our Vfetk structure, which will carry the mesh data.

Parameters

<i>thee</i>	Vfetk object to load into
<i>center</i>	Center for mesh (if constructed)
<i>length</i>	Mesh lengths (if constructed)
<i>meshType</i>	Type of mesh to load
<i>sock</i>	Socket for external mesh data (NULL otherwise)

Definition at line 980 of file [vfetk.c](#).

7.3.5.20 Vfetk_memChk()

```

VEXTERNC unsigned long int Vfetk_memChk (
    Vfetk * thee )

```

Return the memory used by this structure (and its contents) in bytes.

Author

Nathan Baker

Returns

The memory used by this structure and its contents in bytes

Parameters

<i>thee</i>	THe Vfetk object
-------------	------------------

Definition at line 867 of file [vfetk.c](#).

7.3.5.21 Vfetk_PDE_bisectEdge()

```

VEXTERNC void Vfetk_PDE_bisectEdge (
    int dim,
    int dimII,
    int edgeType,
    int chart[],
    double vx[][VAPBS_DIM] )

```

Define the way manifold edges are bisected.

Author

Nathan Baker and Mike Holst

Note

This function is thread-safe.

Parameters

<i>dim</i>	Intrinsic dimension of manifold
<i>dimII</i>	Embedding dimension of manifold
<i>edgeType</i>	Type of edge being refined
<i>chart</i>	Chart for edge vertices, used here as accessibility bitfields
<i>vx</i>	Edge vertex coordinates

7.3.5.22 Vfetk_PDE_ctor()

```
VEXTERNC PDE * Vfetk_PDE_ctor (
    Vfetk * fetk )
```

Constructs the FEtk PDE object.

Author

Nathan Baker

Returns

Newly-allocated PDE object

Bug Not thread-safe

Parameters

<i>fetk</i>	The Vfetk object
-------------	------------------

Definition at line 1176 of file [vfetk.c](#).

7.3.5.23 Vfetk_PDE_ctor2()

```
VEXTERNC int Vfetk_PDE_ctor2 (
    PDE * thee,
    Vfetk * fetk )
```

Initializes the FEtk PDE object.

Author

Nathan Baker (with code by Mike Holst)

Returns

1 if successful, 0 otherwise

Bug Not thread-safe

Parameters

<i>thee</i>	The newly-allocated PDE object
<i>fetk</i>	The parent Vfetk object

Definition at line 1187 of file [vfetk.c](#).

7.3.5.24 Vfetk_PDE_delta()

```

VEXTERNC void Vfetk_PDE_delta (
    PDE * thee,
    int type,
    int chart,
    double txq[],
    void * user,
    double F[] )

```

Evaluate a (discretized) delta function source term at the given point.

Author

Nathan Baker

Bug This function is not thread-safe

Parameters

<i>thee</i>	PDE object
<i>type</i>	Vertex type
<i>chart</i>	Chart for point coordinates
<i>txq</i>	Point coordinates
<i>user</i>	Vertex object pointer
<i>F</i>	Set to delta function value

Definition at line 1780 of file [vfetk.c](#).

7.3.5.25 Vfetk_PDE_DFu_wv()

```

VEXTERNC double Vfetk_PDE_DFu_wv (
    PDE * thee,
    int key,
    double W[],
    double dW[][VAPBS_DIM],
    double V[],
    double dV[][VAPBS_DIM] )

```

This is the linearization of the weak form of the PBE; e.g., for use in a Newton iteration. This is the functional linearization

of the strong form integrated with a test function to give:

$$\int_{\Omega} [\epsilon \nabla w \cdot \nabla v + b'(u) w v - f v] dx$$

where $b'(u)$ denotes the functional derivation of the mobile ion term.

Author

Nathan Baker and Mike Holst

Returns

Integrand value

Bug This function is not thread-safe

Parameters

<i>thee</i>	The PDE object
<i>key</i>	Integrand to evaluate (0 = interior weak form, 1 = boundary weak form)
<i>W</i>	Trial function value at current point
<i>dW</i>	Trial function gradient at current point
<i>V</i>	Test function value at current point
<i>dV</i>	Test function gradient

7.3.5.26 Vfetk_PDE_dtor()

```

VEXTERNC void Vfetk_PDE_dtor (
    PDE ** thee )

```

Destroys FETk PDE object.

Author

Nathan Baker

Note

Thread-safe

Parameters

<i>thee</i>	Pointer to PDE object memory
-------------	------------------------------

Definition at line 1231 of file [vfetk.c](#).

7.3.5.27 Vfetk_PDE_dtor2()

```

VEXTERNC void Vfetk_PDE_dtor2 (
    PDE * thee )

```

FORTTRAN stub: destroys FETk PDE object.

Author

Nathan Baker

Note

Thread-safe

Parameters

<i>thee</i>	PDE object memory
-------------	-------------------

Definition at line 1246 of file [vfetk.c](#).**7.3.5.28 Vfetk_PDE_Fu()**

```

VEXTERNC void Vfetk_PDE_Fu (
    PDE * thee,
    int key,
    double F[ ] )

```

Evaluate strong form of PBE. For interior points, this is:

$$-\nabla \cdot \epsilon \nabla u + b(u) - f$$

where $b(u)$ is the (possibly nonlinear) mobile ion term and f is the source charge distribution term (for PBE) or the induced surface charge distribution (for RPBE). For an interior-boundary (simplex face) point, this is:

$$[\epsilon(x) \nabla u(x) \cdot n(x)]_{x=0^+} - [\epsilon(x) \nabla u(x) \cdot n(x)]_{x=0^-}$$

where $n(x)$ is the normal to the simplex face and the term represents the jump in dielectric displacement across the face. There is no outer-boundary contribution for this problem.

Author

Nathan Baker

Bug This function is not thread-safe

This function is not implemented (sets error to zero)

Parameters

<i>thee</i>	The PDE object
<i>key</i>	Type of point (0 = interior, 1 = boundary, 2 = interior boundary)
<i>F</i>	Set to value of residual

Definition at line 1695 of file [vfetk.c](#).**7.3.5.29 Vfetk_PDE_Fu_v()**

```

VEXTERNC double Vfetk_PDE_Fu_v (
    PDE * thee,
    int key,

```



```
double V[ ],
double dV[ ][VAPBS_DIM] )
```

This is the weak form of the PBE; i.e. the strong form integrated with a test function to give:

$$\int_{\Omega} [\epsilon \nabla u \cdot \nabla v + b(u)v - fv] dx$$

where $b(u)$ denotes the mobile ion term.

Author

Nathan Baker and Mike Holst

Returns

Integrand value

Bug This function is not thread-safe

Parameters

<i>thee</i>	The PDE object
<i>key</i>	Integrand to evaluate (0 = interior weak form, 1 = boundary weak form)
<i>V</i>	Test function at current point
<i>dV</i>	Test function derivative at current point

Definition at line 1703 of file [vfetk.c](#).

7.3.5.30 Vfetk_PDE_initAssemble()

```
EXTERN void Vfetk_PDE_initAssemble (
    PDE * thee,
    int ip[],
    double rp[] )
```

Do once-per-assembly initialization.

Author

Nathan Baker and Mike Holst

Note

Thread-safe

Parameters

<i>thee</i>	PDE object
<i>ip</i>	Integer parameter array (not used)
<i>rp</i>	Double parameter array (not used)

Definition at line 1508 of file [vfetk.c](#).

7.3.5.31 Vfetk_PDE_initElement()

```

VEXTERNC void Vfetk_PDE_initElement (
    PDE * thee,
    int elementType,
    int chart,
    double tvx[ ][VAPBS_DIM],
    void * data )

```

Do once-per-element initialization.

Author

Nathan Baker and Mike Holst

Bug This function is not thread-safe

Parameters

<i>thee</i>	PDE object
<i>elementType</i>	Material type (not used)
<i>chart</i>	Chart in which the vertex coordinates are provided, used here as a bitfield to store molecular accessibility
<i>tvx</i>	Vertex coordinates
<i>data</i>	Simplex pointer (hack)

7.3.5.32 Vfetk_PDE_initFace()

```

VEXTERNC void Vfetk_PDE_initFace (
    PDE * thee,
    int faceType,
    int chart,
    double tnvec[ ] )

```

Do once-per-face initialization.

Author

Nathan Baker and Mike Holst

Bug This function is not thread-safe

Parameters

<i>thee</i>	THE PDE object
<i>faceType</i>	Simplex face type (interior or various boundary types)
<i>chart</i>	Chart in which the vertex coordinates are provided, used here as a bitfield for molecular accessibility
<i>tnvec</i>	Coordinates of outward normal vector for face

Definition at line 1559 of file [vfetk.c](#).

7.3.5.33 Vfetk_PDE_initPoint()

```

VEXTERNC void Vfetk_PDE_initPoint (
    PDE * thee,
    int pointType,
    int chart,
    double txq[],
    double tU[],
    double tdU[][VAPBS_DIM] )

```

Do once-per-point initialization.

Author

Nathan Baker

Bug This function is not thread-safe

This function uses pre-defined boudnary definitions for the molecular surface.

Parameters

<i>thee</i>	The PDE object
<i>pointType</i>	The type of point – interior or various faces
<i>chart</i>	The chart in which the point coordinates are provided, used here as bitfield for molecular accessibility
<i>txq</i>	Point coordinates
<i>tU</i>	Solution value at point
<i>tdU</i>	Solution derivative at point

7.3.5.34 Vfetk_PDE_Ju()

```

VEXTERNC double Vfetk_PDE_Ju (
    PDE * thee,
    int key )

```

Energy functional. This returns the energy (less delta function terms) in the form:

$$c^{-1}/2 \int (\epsilon(\nabla u)^2 + \kappa^2(\cosh u - 1)) dx$$

for a 1:1 electrolyte where *c* is the output from Vpbe_getZmagic.

Author

Nathan Baker

Returns

Energy value (in kT)

Bug This function is not thread-safe.

Parameters

<i>thee</i>	The PDE object
<i>key</i>	What to evaluate: interior (0) or boundary (1)?

Definition at line 2003 of file [vfetk.c](#).

7.3.5.35 Vfetk_PDE_mapBoundary()

```
VEXTERNC void Vfetk_PDE_mapBoundary (
    int dim,
    int dimII,
    int vertexType,
    int chart,
    double vx[VAPBS_DIM] )
```

Map a boundary point to some pre-defined shape.

Author

Nathan Baker and Mike Holst

Note

This function is thread-safe and is a no-op

Parameters

<i>dim</i>	Intrinsic dimension of manifold
<i>dimII</i>	Embedding dimension of manifold
<i>vertexType</i>	Type of vertex
<i>chart</i>	Chart for vertex coordinates
<i>vx</i>	Vertex coordinates

7.3.5.36 Vfetk_PDE_markSimplex()

```
VEXTERNC int Vfetk_PDE_markSimplex (
    int dim,
    int dimII,
    int simplexType,
    int faceType[VAPBS_NVS],
    int vertexType[VAPBS_NVS],
    int chart[],
    double vx[][VAPBS_DIM],
    void * simplex )
```

User-defined error estimator – in our case, a geometry-based refinement method; forcing simplex refinement at the dielectric boundary and (for non-regularized PBE) the charges.

Author

Nathan Baker

Returns

1 if mark simplex for refinement, 0 otherwise

Bug This function is not thread-safe

Parameters

<i>dim</i>	Intrinsic manifold dimension
<i>dimII</i>	Embedding manifold dimension
<i>simplexType</i>	Type of simplex being refined
<i>faceType</i>	Types of faces in simplex
<i>vertexType</i>	Types of vertices in simplex
<i>chart</i>	Charts for vertex coordinates
<i>vx</i>	Vertex coordinates
<i>simplex</i>	Simplex pointer

7.3.5.37 Vfetk_PDE_oneChart()

```

VEXTERNC void Vfetk_PDE_oneChart (
    int dim,
    int dimII,
    int objType,
    int chart[],
    double vx[][VAPBS_DIM],
    int dimV )

```

Unify the chart for different coordinate systems – a no-op for us.

Author

Nathan Baker

Note

Thread-safe; a no-op

Parameters

<i>dim</i>	Intrinsic manifold dimension
<i>dimII</i>	Embedding manifold dimension
<i>objType</i>	???
<i>chart</i>	Charts of vertices' coordinates
<i>vx</i>	Vertices' coordinates
<i>dimV</i>	Number of vertices

7.3.5.38 Vfetk_PDE_simplexBasisForm()

```

VEXTERNC void Vfetk_PDE_simplexBasisForm (
    int key,
    int dim,
    int comp,
    int pdkey,
    double xq[],
    double basis[] )

```

Evaluate the bases for the trial or test space, for a particular component of the system, at all quadrature points on the master simplex element.

Author

Mike Holst

Parameters

<i>key</i>	Basis type to evaluate (0 = trial, 1 = test, 2 = trialB, 3 = testB)
<i>dim</i>	Spatial dimension
<i>comp</i>	Which component of elliptic system to produce basis for
<i>pdkey</i>	Basis partial differential equation evaluation key: <ul style="list-style-type: none"> • 0 = evaluate basis(x,y,z) • 1 = evaluate basis_x(x,y,z) • 2 = evaluate basis_y(x,y,z) • 3 = evaluate basis_z(x,y,z) • 4 = evaluate basis_xx(x,y,z) • 5 = evaluate basis_yy(x,y,z) • 6 = evaluate basis_zz(x,y,z) • 7 = etc...
<i>xq</i>	Set to quad pt coordinate
<i>basis</i>	Set to all basis functions evaluated at all quadrature pts

Definition at line 2203 of file [vfetk.c](#).

7.3.5.39 Vfetk_PDE_simplexBasisInit()

```

VEXTERNC int Vfetk_PDE_simplexBasisInit (
    int key,
    int dim,
    int comp,
    int * ndof,
    int dof[] )

```

Initialize the bases for the trial or the test space, for a particular component of the system, at all quadrature points on the master simplex element.

Author

Mike Holst

Note

```

* The basis ordering is important. For a fixed quadrature
* point iq, you must follow the following ordering in p[iq][],
* based on how you specify the degrees of freedom in dof[]:
*
* <v_0 vDF_0>,      <v_1 vDF_0>,      ..., <v_{nv} vDF_0>
* <v_0 vDF_1>,      <v_1 vDF_1>,      ..., <v_{nv} vDF_1>

```

```

*
*      ...
*      <v_0 vDF_{nvDF}>, <v_0 vDF_{nvDF}>, ..., <v_{nv} vDF_{nvDF}>
*
*      <e_0 eDF_0>,      <e_1 eDF_0>,      ..., <e_{ne} eDF_0>
*      <e_0 eDF_1>,      <e_1 eDF_1>,      ..., <e_{ne} eDF_1>
*
*      ...
*      <e_0 eDF_{neDF}>, <e_1 eDF_{neDF}>, ..., <e_{ne} eDF_{neDF}>
*
*      <f_0 fDF_0>,      <f_1 fDF_0>,      ..., <f_{nf} fDF_0>
*      <f_0 fDF_1>,      <f_1 fDF_1>,      ..., <f_{nf} fDF_1>
*
*      ...
*      <f_0 fDF_{nfDF}>, <f_1 fDF_{nfDF}>, ..., <f_{nf} fDF_{nfDF}>
*
*      <s_0 sDF_0>,      <s_1 sDF_0>,      ..., <s_{ns} sDF_0>
*      <s_0 sDF_1>,      <s_1 sDF_1>,      ..., <s_{ns} sDF_1>
*
*      ...
*      <s_0 sDF_{nsDF}>, <s_1 sDF_{nsDF}>, ..., <s_{ns} sDF_{nsDF}>
*
*      For example, linear elements in R^3, with one degree of freedom at each *
*      vertex, would use the following ordering:
*
*      <v_0 vDF_0>, <v_1 vDF_0>, <v_2 vDF_0>, <v_3 vDF_0>
*
*      Quadratic elements in R^2, with one degree of freedom at each vertex and
*      edge, would use the following ordering:
*
*      <v_0 vDF_0>, <v_1 vDF_0>, <v_2 vDF_0>
*      <e_0 eDF_0>, <e_1 eDF_0>, <e_2 eDF_0>
*
*      You can use different trial and test spaces for each component of the
*      elliptic system, thereby allowing for the use of Petrov-Galerkin methods.
*      You MUST then tag the bilinear form symmetry entries as nonsymmetric in
*      your PDE constructor to reflect that  $DF(u)(w,v)$  will be different from
*       $DF(u)(v,w)$ , even if your form acts symmetrically when the same basis is
*      used for  $w$  and  $v$ .
*
*      You can also use different trial spaces for each component of the elliptic
*      system, and different test spaces for each component of the elliptic
*      system. This allows you to e.g. use a basis which is vertex-based for
*      one component, and a basis which is edge-based for another. This is
*      useful in fluid mechanics, eletromagnetics, or simply to play around with
*      different elements.
*
*      This function is called by MC to build new master elements whenever it
*      reads in a new mesh. Therefore, this function does not have to be all
*      that fast, and e.g. could involve symbolic computation.
*

```

Parameters

<i>key</i>	Basis type to evaluate (0 = trial, 1 = test, 2 = trialB, 3 = testB)
<i>dim</i>	Spatial dimension
<i>comp</i>	Which component of elliptic system to produce basis for?
<i>ndof</i>	Set to the number of degrees of freedom
<i>dof</i>	Set to degree of freedom per v/e/f/s

Definition at line 2140 of file [vfetk.c](#).

7.3.5.40 Vfetk_PDE_u_D()

```

VEXTERN void Vfetk_PDE_u_D (

```

```

PDE * thee,
int type,
int chart,
double txq[],
double F[] )

```

Evaluate the Dirichlet boundary condition at the given point.

Author

Nathan Baker

Bug This function is hard-coded to call only multiple-sphere Debye-Hü functions.
This function is not thread-safe.

Parameters

<i>thee</i>	PDE object
<i>type</i>	Vertex boundary type
<i>chart</i>	Chart for point coordinates
<i>txq</i>	Point coordinates
<i>F</i>	Set to boundary values

Definition at line [1867](#) of file [vfetk.c](#).

7.3.5.41 Vfetk_PDE_u_T()

```

VEXTERN void Vfetk_PDE_u_T (
    PDE * thee,
    int type,
    int chart,
    double txq[],
    double F[] )

```

Evaluate the "true solution" at the given point for comparison with the numerical solution.

Author

Nathan Baker

Note

This function only returns zero.

Bug This function is not thread-safe.

The signature here doesn't match what's in mc's src/pde/mc/pde.h, which g++ seems to dislike for GAMer integration. Trying a change of function signature to match to see if that makes g++ happy. Also see [vfetk.h](#) for similar signature change. - P. Ellis 11-8-2011

Parameters

<i>thee</i>	PDE object
<i>type</i>	Point type
<i>chart</i>	Chart for point coordinates
<i>txq</i>	Point coordinates
<i>F</i>	Set to value at point

Definition at line 1886 of file [vfetk.c](#).

7.3.5.42 Vfetk_qfEnergy()

```
VEXTERNC double Vfetk_qfEnergy (
    Vfetk * thee,
    int color )
```

Get the "fixed charge" contribution to the electrostatic energy.

Using the solution at the finest mesh level, get the electrostatic energy due to the interaction of the fixed charges with the potential: $G = \sum_i q_i u(r_i)$ and return the result in units of $k_B T$. Clearly, no self-interaction terms are removed. A factor a 1/2 has to be included to convert this to a real energy.

Author

Nathan Baker

Parameters

<i>thee</i>	Vfetk object
<i>color</i>	Partition restriction for energy evaluation, only used if non-negative

Returns

The fixed charge electrostatic energy in units of $k_B T$.

Parameters

<i>thee</i>	The Vfetk object
<i>color</i>	Partition restriction for energy evaluation, only used if non-negative

Definition at line 732 of file [vfetk.c](#).

7.3.5.43 Vfetk_readMesh()

```
VEXTERNC void Vfetk_readMesh (
    Vfetk * thee,
    int skey,
    Vio * sock )
```

Read in mesh and initialize associated internal structures.

Author

Nathan Baker

Note

See also

[Vfetc_genCube](#)

Parameters

<i>thee</i>	The Vfetc object
<i>skey</i>	The sock format key (0 = MCSF simplex format)
<i>sock</i>	Socket object ready for reading

7.3.5.44 Vfetc_setAtomColors()

```
VEEXTERNC void Vfetc_setAtomColors (
    Vfetc * thee )
```

Transfer color (partition ID) information from a partitioned mesh to the atoms.

Transfer color information from partitioned mesh to the atoms. In the case that a charge is shared between two partitions, the partition color of the first simplex is selected. Due to the arbitrary nature of this selection, THIS METHOD SHOULD ONLY BE USED IMMEDIATELY AFTER PARTITIONING!!!

Warning

This function should only be used immediately after mesh partitioning

Author

Nathan Baker

Note

This is a friend function of Vcsm

Parameters

<i>thee</i>	The Vfetc object
-------------	------------------

Definition at line 849 of file [vfetc.c](#).

7.3.5.45 Vfetc_setParameters()

```
VEEXTERNC void Vfetc_setParameters (
    Vfetc * thee,
    PBEparm * pbeparm,
    FEMparm * feparm )
```

Set the parameter objects.

Author

Nathan Baker

Parameters

<i>thee</i>	The Vfetc object
-------------	------------------

Parameters

<i>pbeparm</i>	Parameters for solution of the PBE
<i>feparm</i>	FEM-specific solution parameters

Definition at line 615 of file [vfetk.c](#).

7.3.5.46 Vfetk_write()

```

VEXTERNC int Vfetk_write (
    Vfetk * thee,
    const char * iodev,
    const char * iofmt,
    const char * thost,
    const char * fname,
    Bvec * vec,
    Vdata_Format format )

```

Write out data.

Author

Nathan Baker

Parameters

<i>thee</i>	Vfetk object
<i>vec</i>	FEtk Bvec vector to use
<i>format</i>	Format for data
<i>iodev</i>	Output device type (FILE/BUFF/UNIX/INET)
<i>iofmt</i>	Output device format (ASCII/XDR)
<i>thost</i>	Output hostname (for sockets)
<i>fname</i>	Output FILE/BUFF/UNIX/INET name

Note

This function is thread-safe

Bug Some values of format are not implemented

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	The Vfetk object
<i>iodev</i>	Output device type (FILE = file, BUFF = buffer, UNIX = unix pipe, INET = network socket)
<i>iofmt</i>	Output device format (ASCII = ascii/plaintext, XDR = xdr)
<i>thost</i>	Output hostname for sockets
<i>fname</i>	Output filename for other
<i>vec</i>	Data vector
<i>format</i>	Data format

Definition at line 2464 of file [vfetk.c](#).

7.4 Vpee class

This class provides some functionality for error esimation in parallel.

Files

- file [vpee.c](#)
Class Vpee methods.
- file [vpee.h](#)
Contains declarations for class Vpee.

Data Structures

- struct [sVpee](#)
Contains public data members for Vpee class/module.

Typedefs

- typedef struct [sVpee](#) [Vpee](#)
Declaration of the Vpee class as the Vpee structure.

Functions

- VEXTERNC [Vpee](#) * [Vpee_ctor](#) (Gem *gm, int localPartID, int killFlag, double killParam)
Construct the Vpee object.
- VEXTERNC int [Vpee_ctor2](#) ([Vpee](#) *thee, Gem *gm, int localPartID, int killFlag, double killParam)
FORTTRAN stub to construct the Vpee object.
- VEXTERNC void [Vpee_dtor](#) ([Vpee](#) **thee)
Object destructor.
- VEXTERNC void [Vpee_dtor2](#) ([Vpee](#) *thee)
FORTTRAN stub object destructor.
- VEXTERNC int [Vpee_markRefine](#) ([Vpee](#) *thee, AM *am, int level, int akey, int rcol, double etol, int bkey)
Mark simplices for refinement based on attenuated error estimates.
- VEXTERNC int [Vpee_numSS](#) ([Vpee](#) *thee)
Returns the number of simplices in the local partition.

7.4.1 Detailed Description

This class provides some functionality for error esimation in parallel.

This class provides some functionality for error esimation in parallel. The purpose is to modulate the error returned by some external error estimator according to the partitioning of the mesh. For example, the Bank/Holst parallel refinement routine essentially reduces the error outside the ``local" partition to zero. However, this leads to the need for a few final overlapping Schwarz solves to smooth out the errors near partition boundaries. Supposedly, if the region in which we allow error-based refinement includes the ``local" partition and an external buffer zone approximately equal in size to the local region, then the solution will asymptotically approach the solution obtained via more typical methods. This is essentially a more flexible parallel implementation of MC's AM_markRefine.

7.4.2 Typedef Documentation

7.4.2.1 Vpee

typedef struct [sVpee](#) [Vpee](#)

Declaration of the Vpee class as the Vpee structure.

Definition at line [112](#) of file [vpee.h](#).

7.4.3 Function Documentation

7.4.3.1 Vpee_ctor()

```
VEXTERNC Vpee * Vpee_ctor (
    Gem * gm,
    int localPartID,
    int killFlag,
    double killParam )
```

Construct the Vpee object.

Author

Nathan Baker

Returns

Newly constructed Vpee object

Parameters

<i>gm</i>	FEtk geometry manager object
<i>localPartID</i>	ID of the local partition (focus of refinement)
<i>killFlag</i>	A flag to indicate how error estimates are to be attenuated outside the local partition: <ul style="list-style-type: none"> • 0: no attenuation • 1: all error outside the local partition set to zero • 2: all error is set to zero outside a sphere of radius ($\text{killParam} * \text{partRadius}$), where partRadius is the radius of the sphere circumscribing the local partition • 3: all error is set to zero except for the local partition and its immediate neighbors
<i>killParam</i>	

See also

killFlag for usage

Definition at line 93 of file [vpee.c](#).

7.4.3.2 Vpee_ctor2()

```

VEXTERNC int Vpee_ctor2 (
    Vpee * thee,
    Gem * gm,
    int localPartID,
    int killFlag,
    double killParam )

```

FORTTRAN stub to construct the Vpee object.

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	The Vpee object
<i>gm</i>	FEtk geometry manager object
<i>localPartID</i>	ID of the local partition (focus of refinement)
<i>killFlag</i>	A flag to indicate how error estimates are to be attenuated outside the local partition: <ul style="list-style-type: none"> • 0: no attenuation • 1: all error outside the local partition set to zero • 2: all error is set to zero outside a sphere of radius (killParam*partRadius), where partRadius is the radius of the sphere circumscribing the local partition • 3: all error is set to zero except for the local partition and its immediate neighbors
<i>killParam</i>	

See also

killFlag for usage

Definition at line 114 of file [vpee.c](#).

7.4.3.3 Vpee_dtor()

```

VEXTERNC void Vpee_dtor (
    Vpee ** thee )

```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of the Vpee object
-------------	---

Definition at line 225 of file [vpee.c](#).

7.4.3.4 Vpee_dtor2()

```

VEXTERNC void Vpee_dtor2 (
    Vpee * thee )

```

FORTTRAN stub object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object to be destroyed
-------------	-----------------------------------

Definition at line 240 of file [vpee.c](#).

7.4.3.5 Vpee_markRefine()

```

VEXTERNC int Vpee_markRefine (
    Vpee * thee,
    AM * am,
    int level,
    int akey,
    int rcol,
    double etol,
    int bkey )

```

Mark simplices for refinement based on attenuated error estimates.

A wrapper/reimplementation of AM_markRefine that allows for more flexible attenuation of error-based markings outside the local partition. The error in each simplex is modified by the method (see killFlag) specified in the Vpee constructor. This allows the user to confine refinement to an arbitrary area around the local partition.

Author

Nathan Baker and Mike Holst

Note

This routine borrows very heavily from FEtk routines by Mike Holst.

Returns

The number of simplices marked for refinement.

Bug This function is no longer up-to-date with FEtk and may not function properly

Parameters

<i>thee</i>	The Vpee object
<i>am</i>	The FETk algebra manager currently used to solve the PB
<i>level</i>	The current level of the multigrid hierarchy
<i>akey</i>	The marking method: <ul style="list-style-type: none"> • -1: Reset markings --> killFlag has no effect. • 0: Uniform. • 1: User defined (geometry-based). • >1: A numerical estimate for the error has already been set in am and should be attenuated according to killFlag and used, in conjunction with etol, to mark simplices for refinement.
<i>rcol</i>	The ID of the main partition on which to mark (or -1 if all partitions should be marked). NOte that we shouldhave (rcol == thee->localPartID) for (thee->killFlag == 2 or 3)
<i>etol</i>	The error tolerance criterion for marking
<i>bkey</i>	How the error tolerance is interpreted: <ul style="list-style-type: none"> • 0: Simplex marked if error > etol. • 1: Simplex marked if error > sqrt(etol^2/L) where L\$ is the number of simplices

Definition at line 250 of file [vpee.c](#).

7.4.3.6 Vpee_numSS()

```

VEXTERNC int Vpee_numSS (
    Vpee * thee )

```

Returns the number of simplices in the local partition.

Author

Nathan Baker

Returns

Number of simplices in the local partition

Parameters

<i>thee</i>	The Vpee object
-------------	-----------------

Definition at line 479 of file [vpee.c](#).

7.5 APOLparm class

Parameter structure for APOL-specific variables from input files.

Files

- file [apolparm.c](#)
Class APOLparm methods.
- file [femparm.h](#)
Contains declarations for class APOLparm.

Data Structures

- struct [sAPOLparm](#)
Parameter structure for APOL-specific variables from input files.

Typedefs

- typedef enum [eAPOLparm_calcEnergy](#) [APOLparm_calcEnergy](#)
Define eAPOLparm_calcEnergy enumeration as APOLparm_calcEnergy.
- typedef enum [eAPOLparm_calcForce](#) [APOLparm_calcForce](#)
Define eAPOLparm_calcForce enumeration as APOLparm_calcForce.
- typedef enum [eAPOLparm_doCalc](#) [APOLparm_doCalc](#)
Define eAPOLparm_calcForce enumeration as APOLparm_calcForce.
- typedef struct [sAPOLparm](#) [APOLparm](#)
Declaration of the APOLparm class as the APOLparm structure.

Enumerations

- enum [eAPOLparm_calcEnergy](#) { [ACE_NO](#) =0 , [ACE_TOTAL](#) =1 , [ACE_COMPS](#) =2 }
Define energy calculation enumeration.
- enum [eAPOLparm_calcForce](#) { [ACF_NO](#) =0 , [ACF_TOTAL](#) =1 , [ACF_COMPS](#) =2 }
Define force calculation enumeration.
- enum [eAPOLparm_doCalc](#) { [ACD_NO](#) =0 , [ACD_YES](#) =1 , [ACD_ERROR](#) =2 }
Define force calculation enumeration.

Functions

- VEXTERNC [APOLparm](#) * [APOLparm_ctor](#) ()
Construct APOLparm.
- VEXTERNC Vrc_Codes [APOLparm_ctor2](#) ([APOLparm](#) *thee)
FORTTRAN stub to construct APOLparm.
- VEXTERNC void [APOLparm_dtor](#) ([APOLparm](#) **thee)
Object destructor.
- VEXTERNC void [APOLparm_dtor2](#) ([APOLparm](#) *thee)
FORTTRAN stub for object destructor.
- VEXTERNC Vrc_Codes [APOLparm_check](#) ([APOLparm](#) *thee)
Consistency check for parameter values stored in object.
- VEXTERNC void [APOLparm_copy](#) ([APOLparm](#) *thee, [APOLparm](#) *source)
Copy target object into thee.

7.5.1 Detailed Description

Parameter structure for APOL-specific variables from input files.

7.5.2 Typedef Documentation

7.5.2.1 APOLparm

[APOLparm](#)

Declaration of the APOLparm class as the APOLparm structure.

Definition at line 188 of file [apolparm.h](#).

7.5.2.2 APOLparm_calcEnergy

```
typedef enum eAPOLparm\_calcEnergy APOLparm\_calcEnergy
```

Define eAPOLparm_calcEnergy enumeration as APOLparm_calcEnergy.

Definition at line 89 of file [apolparm.h](#).

7.5.2.3 APOLparm_calcForce

```
typedef enum eAPOLparm\_calcForce APOLparm\_calcForce
```

Define eAPOLparm_calcForce enumeration as APOLparm_calcForce.

Definition at line 105 of file [apolparm.h](#).

7.5.2.4 APOLparm_doCalc

```
typedef enum eAPOLparm\_doCalc APOLparm\_doCalc
```

Define eAPOLparm_calcForce enumeration as APOLparm_calcForce.

Definition at line 121 of file [apolparm.h](#).

7.5.3 Enumeration Type Documentation

7.5.3.1 eAPOLparm_calcEnergy

[enum eAPOLparm_calcEnergy](#)

Define energy calculation enumeration.

Enumerator

ACE_NO	Do not perform energy calculation
ACE_TOTAL	Calculate total energy only
ACE_COMPS	Calculate per-atom energy components

Definition at line 79 of file [apolparm.h](#).

7.5.3.2 eAPOLparm_calcForce

[enum eAPOLparm_calcForce](#)

Define force calculation enumeration.

Enumerator

ACF_NO	Do not perform force calculation
ACF_TOTAL	Calculate total force only
ACF_COMPS	Calculate per-atom force components

Definition at line 95 of file [apolparm.h](#).

7.5.3.3 eAPOLparm_doCalc

```
enum eAPOLparm_doCalc
```

Define force calculation enumeration.

Enumerator

ACD_NO	Do not perform calculation
ACD_YES	Perform calculations
ACD_ERROR	Error setting up calculation

Definition at line 111 of file [apolparm.h](#).

7.5.4 Function Documentation

7.5.4.1 APOLparm_check()

```
VEXTERNC Vrc_Codes APOLparm_check (
    APOLparm * thee )
```

Consistency check for parameter values stored in object.

Author

David Gohara, Yong Huang

Parameters

<i>thee</i>	APOLparm object
-------------	-----------------

Returns

Success enumeration

Definition at line 179 of file [apolparm.c](#).

7.5.4.2 APOLparm_copy()

```
VEXTERNC void APOLparm_copy (
    APOLparm * thee,
    APOLparm * source )
```

Copy target object into thee.

Author

Nathan Baker

Parameters

<i>thee</i>	Destination object
<i>source</i>	Source object

Definition at line 108 of file [apolparm.c](#).

7.5.4.3 APOLparm_ctor()

VEXTERNC [APOLparm](#) * APOLparm_ctor ()
Construct APOLparm.

Author

David Gohara

Returns

Newly allocated and initialized Vpmgp object

Definition at line 65 of file [apolparm.c](#).

7.5.4.4 APOLparm_ctor2()

VEXTERNC Vrc_Codes APOLparm_ctor2 (
 [APOLparm](#) * *thee*)
FORTRAN stub to construct APOLparm.

Author

David Gohara, Yong Huang

Parameters

<i>thee</i>	Pointer to allocated APOLparm object
-------------	--------------------------------------

Returns

Success enumeration

Definition at line 76 of file [apolparm.c](#).

7.5.4.5 APOLparm_dtor()

VEXTERNC void APOLparm_dtor (
 [APOLparm](#) ** *thee*)

Object destructor.

Author

David Gohara

Parameters

<i>thee</i>	Pointer to memory location of APOLparm object
-------------	---

Definition at line 167 of file [apolparm.c](#).

7.5.4.6 APOLparm_dtor2()

```
VEXTERNC void APOLparm_dtor2 (
    APOLparm * thee )
```

FORTTRAN stub for object destructor.

Author

David Gohara

Parameters

<i>thee</i>	Pointer to APOLparm object
-------------	----------------------------

Definition at line 177 of file [apolparm.c](#).

7.6 BEMparm class

Parameter which holds useful parameters for generic multigrid calculations.

Files

- file [bemparm.c](#)
Class BEMparm methods.

Data Structures

- struct [sBEMparm](#)
Parameter structure for BEM-specific variables from input files.

Typedefs

- typedef enum [eBEMparm_CalcType](#) BEMparm_CalcType
Declare BEMparm_CalcType type.
- typedef struct [sBEMparm](#) BEMparm
Parameter structure for BEM-specific variables from input files.

Enumerations

- enum [eBEMparm_CalcType](#) { BCT_MANUAL =0 , BCT_NONE =1 }
Calculation type.

Functions

- VEXTERNC [BEMparm](#) * [BEMparm_ctor](#) ([BEMparm_CalcType](#) type)
Construct BEMparm object.
- VEXTERNC Vrc_Codes [BEMparm_ctor2](#) ([BEMparm](#) *thee, [BEMparm_CalcType](#) type)
FORTTRAN stub to construct BEMparm object.
- VEXTERNC void [BEMparm_dtor](#) ([BEMparm](#) **thee)
Object destructor.
- VEXTERNC void [BEMparm_dtor2](#) ([BEMparm](#) *thee)
FORTTRAN stub for object destructor.
- VEXTERNC Vrc_Codes [BEMparm_check](#) ([BEMparm](#) *thee)
Consistency check for parameter values stored in object.
- VEXTERNC Vrc_Codes [BEMparm_parseToken](#) ([BEMparm](#) *thee, char tok[VMAX_BUFSIZE], Vio *sock)
Parse an MG keyword from an input file.

7.6.1 Detailed Description

Parameter which holds useful parameters for generic multigrid calculations.

7.6.2 Typedef Documentation

7.6.2.1 BEMparm

```
typedef struct sBEMparm BEMparm
```

Parameter structure for BEM-specific variables from input files.

Author

Nathan Baker and Todd Dolinsky and Weihua Geng

Note

If you add/delete/change something in this class, the member functions – especially [BEMparm_copy](#) – must be modified accordingly

7.6.2.2 BEMparm_CalcType

```
typedef enum eBEMparm\_CalcType BEMparm\_CalcType
```

Declare [BEMparm_CalcType](#) type.

Definition at line [86](#) of file [bemparm.h](#).

7.6.3 Enumeration Type Documentation

7.6.3.1 eBEMparm_CalcType

```
enum eBEMparm\_CalcType
```

Calculation type.

Enumerator

BCT_MANUAL	bem-manual
BCT_NONE	not defined

Definition at line 77 of file [bemparm.h](#).

7.6.4 Function Documentation

7.6.4.1 BEMparm_check()

```
VEXTERNC Vrc_Codes BEMparm_check (
    BEMparm * thee )
```

Consistency check for parameter values stored in object.

Author

Nathan Baker

Parameters

<i>thee</i>	BEMparm object
-------------	----------------

Returns

Success enumeration

Definition at line 124 of file [bemparm.c](#).

7.6.4.2 BEMparm_ctor()

```
VEXTERNC BEMparm * BEMparm_ctor (
    BEMparm_CalcType type )
```

Construct BEMparm object.

Author

Nathan Baker

Parameters

<i>type</i>	Type of BEM calculation
-------------	-------------------------

Returns

Newly allocated and initialized BEMparm object

Definition at line 66 of file [bemparm.c](#).

7.6.4.3 BEMparm_ctor2()

```

VEXTERNC Vrc_Codes BEMparm_ctor2 (
    BEMparm * thee,
    BEMparm_CalcType type )

```

FORTTRAN stub to construct BEMparm object.

Author

Nathan Baker and Todd Dolinsky

Parameters

<i>thee</i>	Space for BEMparm object
<i>type</i>	Type of MG calculation

Returns

Success enumeration

Definition at line 77 of file [bemparm.c](#).

7.6.4.4 BEMparm_dtor()

```

VEXTERNC void BEMparm_dtor (
    BEMparm ** thee )

```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of BEMparm object
-------------	--

Definition at line 114 of file [bemparm.c](#).

7.6.4.5 BEMparm_dtor2()

```

VEXTERNC void BEMparm_dtor2 (
    BEMparm * thee )

```

FORTTRAN stub for object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to BEMparm object
-------------	---------------------------

Definition at line 122 of file [bemparm.c](#).

7.6.4.6 BEMparm_parseToken()

```
VEXTERNC Vrc_Codes BEMparm_parseToken (
    BEMparm * thee,
    char tok[VMAX_BUFSIZE],
    Vio * sock )
```

Parse an MG keyword from an input file.

Author

Nathan Baker and Todd Dolinsky

Parameters

<i>thee</i>	BEMparm object
<i>tok</i>	Token to parse
<i>sock</i>	Stream for more tokens

Returns

Success enumeration (1 if matched and assigned; -1 if matched, but there's some sort of error (i.e., too few args); 0 if not matched)

Definition at line 332 of file [bemparm.c](#).

7.7 FEMparm class

Parameter structure for FEM-specific variables from input files.

Files

- file [femparm.c](#)
Class FEMparm methods.
- file [femparm.h](#)
Contains declarations for class APOLparm.

Data Structures

- struct [sFEMparm](#)
Parameter structure for FEM-specific variables from input files.

Typedefs

- typedef enum [eFEMparm_EtolType](#) FEMparm_EtolType
Declare FEMparm_EtolType type.
- typedef enum [eFEMparm_EstType](#) FEMparm_EstType
Declare FEMparm_EstType type.
- typedef enum [eFEMparm_CalcType](#) FEMparm_CalcType
Declare FEMparm_CalcType type.
- typedef struct [sFEMparm](#) FEMparm
Declaration of the FEMparm class as the FEMparm structure.

Enumerations

- enum [eFEMparm_EtolType](#) { [FET_SIMP](#) =0 , [FET_GLOB](#) =1 , [FET_FRAC](#) =2 }
Adaptive refinement error estimate tolerance key.
- enum [eFEMparm_EstType](#) {
[FRT_UNIF](#) =0 , [FRT_GEOM](#) =1 , [FRT_RESI](#) =2 , [FRT_DUAL](#) =3 ,
[FRT_LOCA](#) =4 }
Adaptive refinement error estimator method.
- enum [eFEMparm_CalcType](#) { [FCT_MANUAL](#) , [FCT_NONE](#) }
Calculation type.

Functions

- VEXTERNC [FEMparm](#) * [FEMparm_ctor](#) ([FEMparm_CalcType](#) type)
Construct FEMparm.
- VEXTERNC int [FEMparm_ctor2](#) ([FEMparm](#) *thee, [FEMparm_CalcType](#) type)
FORTTRAN stub to construct FEMparm.
- VEXTERNC void [FEMparm_dtor](#) ([FEMparm](#) **thee)
Object destructor.
- VEXTERNC void [FEMparm_dtor2](#) ([FEMparm](#) *thee)
FORTTRAN stub for object destructor.
- VEXTERNC int [FEMparm_check](#) ([FEMparm](#) *thee)
Consistency check for parameter values stored in object.
- VEXTERNC void [FEMparm_copy](#) ([FEMparm](#) *thee, [FEMparm](#) *source)
Copy target object into thee.

7.7.1 Detailed Description

Parameter structure for FEM-specific variables from input files.

7.7.2 Typedef Documentation

7.7.2.1 FEMparm

[FEMparm](#)

Declaration of the FEMparm class as the FEMparm structure.

Definition at line [182](#) of file [femparm.h](#).

7.7.2.2 FEMparm_CalcType

`typedef enum eFEMparm_CalcType FEMparm_CalcType`
 Declare FEMparm_CalcType type.
 Definition at line 126 of file [femparm.h](#).

7.7.2.3 FEMparm_EstType

`typedef enum eFEMparm_EstType FEMparm_EstType`
 Declare FEMparm_EstType type.
 Definition at line 111 of file [femparm.h](#).

7.7.2.4 FEMparm_EtolType

`typedef enum eFEMparm_EtolType FEMparm_EtolType`
 Declare FEparm_EtolType type.

Author

Nathan Baker

Definition at line 90 of file [femparm.h](#).

7.7.3 Enumeration Type Documentation

7.7.3.1 eFEMparm_CalcType

`enum eFEMparm_CalcType`
 Calculation type.

Enumerator

FCT_MANUAL	fe-manual
FCT_NONE	unspecified

Definition at line 117 of file [femparm.h](#).

7.7.3.2 eFEMparm_EstType

`enum eFEMparm_EstType`
 Adaptive refinement error estimator method.

Note

Do not change these values; they correspond to settings in FEtk

Author

Nathan Baker

Enumerator

FRT_UNIF	Uniform refinement
FRT_GEOM	Geometry-based (i.e. surfaces and charges) refinement
FRT_RESI	Nonlinear residual estimate-based refinement
FRT_DUAL	Dual-solution weight nonlinear residual estimate-based refinement
FRT_LOCA	Local problem error estimate-based refinement

Definition at line 98 of file [femparm.h](#).

7.7.3.3 eFEMparm_EtolType

enum [eFEMparm_EtolType](#)

Adaptive refinement error estimate tolerance key.

Author

Nathan Baker

Enumerator

FET_SIMP	per-simplex error tolerance
FET_GLOB	global error tolerance
FET_FRAC	fraction of simplices we want to have refined

Definition at line 79 of file [femparm.h](#).

7.7.4 Function Documentation**7.7.4.1 FEMparm_check()**

```
VEXTERNC int FEMparm_check (
    FEMparm * thee )
```

Consistency check for parameter values stored in object.

Author

Nathan Baker

Parameters

<i>thee</i>	FEMparm object
-------------	----------------

Returns

1 if OK, 0 otherwise

Definition at line 143 of file [femparm.c](#).

7.7.4.2 FEMparm_copy()

```
VEXTERNC void FEMparm_copy (  
    FEMparm * thee,  
    FEMparm * source )
```

Copy target object into thee.

Author

Nathan Baker

Parameters

<i>thee</i>	Destination object
<i>source</i>	Source object

Definition at line 100 of file [femparm.c](#).

7.7.4.3 FEMparm_ctor()

```
VEXTERNC FEMparm * FEMparm_ctor (  
    FEMparm_CalcType type )
```

Construct FEMparm.

Author

Nathan Baker

Parameters

<i>type</i>	FEM calculation type
-------------	----------------------

Returns

Newly allocated and initialized Vpmgp object

Definition at line 65 of file [femparm.c](#).

7.7.4.4 FEMparm_ctor2()

```
VEXTERNC int FEMparm_ctor2 (  
    FEMparm * thee,  
    FEMparm_CalcType type )
```

FORTTRAN stub to construct FEMparm.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to allocated FEMparm object
<i>type</i>	FEM calculation type

Returns

1 if successful, 0 otherwise

Definition at line 76 of file [femparm.c](#).

7.7.4.5 FEMparm_dtor()

```
VEXTERNC void FEMparm_dtor (
    FEMparm ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of FEMparm object
-------------	--

Definition at line 133 of file [femparm.c](#).

7.7.4.6 FEMparm_dtor2()

```
VEXTERNC void FEMparm_dtor2 (
    FEMparm * thee )
```

FORTTRAN stub for object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to FEMparm object
-------------	---------------------------

Definition at line 141 of file [femparm.c](#).

7.8 GEOFLOWparm class

Parameter which holds useful parameters for GEOFLOWeric multigrid calculations.

Files

- file [geoflowparm.c](#)
Class GEOFLOWparm methods.
- file [geoflowparm.h](#)
Contains declarations for class GEOFLOWparm.

Data Structures

- struct [sGEOFLOWparm](#)

Parameter structure for GEOFLOW-specific variables from input files.

Typedefs

- typedef enum [eGEOFLOWparm_CalcType](#) [GEOFLOWparm_CalcType](#)
Declare GEOFLOWparm_CalcType type.
- typedef struct [sGEOFLOWparm](#) [GEOFLOWparm](#)
Parameter structure for GEOFLOW-specific variables from input files.

Enumerations

- enum [eGEOFLOWparm_CalcType](#) { GFCT_AUTO =1 }
Calculation type.

Functions

- VEXTERNC [GEOFLOWparm](#) * [GEOFLOWparm_ctor](#) ([GEOFLOWparm_CalcType](#) type)
Construct GEOFLOWparm object.
- VEXTERNC Vrc_Codes [GEOFLOWparm_ctor2](#) ([GEOFLOWparm](#) *thee, [GEOFLOWparm_CalcType](#) type)
FORTTRAN stub to construct GEOFLOWparm object ?????????!!!!!!!
- VEXTERNC void [GEOFLOWparm_dtor](#) ([GEOFLOWparm](#) **thee)
Object destructor.
- VEXTERNC void [GEOFLOWparm_dtor2](#) ([GEOFLOWparm](#) *thee)
FORTTRAN stub for object destructor ?????????!!!!!!!
- VEXTERNC Vrc_Codes [GEOFLOWparm_check](#) ([GEOFLOWparm](#) *thee)
Consistency check for parameter values stored in object.
- VEXTERNC Vrc_Codes [GEOFLOWparm_parseToken](#) ([GEOFLOWparm](#) *thee, char tok[VMAX_BUFSIZE], Vio *sock)
Parse an MG keyword from an input file.
- VEXTERNC void [GEOFLOWparm_copy](#) ([GEOFLOWparm](#) *thee, [GEOFLOWparm](#) *parm)
copy GEOFLOWparm object into thee.

7.8.1 Detailed Description

Parameter which holds useful parameters for GEOFLOWeric multigrid calculations.

7.8.2 Typedef Documentation

7.8.2.1 GEOFLOWparm

```
typedef struct sGEOFLOWparm GEOFLOWparm
```

Parameter structure for GEOFLOW-specific variables from input files.

Author

Andrew Stevens, Kyle Monson

Note

If you add/delete/change something in this class, the member functions – especially [GEOFLOWparm_copy](#) – must be modified accordingly

7.8.2.2 GEOFLOWparm_CalcType

typedef enum eGEOFLOWparm_CalcType GEOFLOWparm_CalcType
 Declare GEOFLOWparm_CalcType type.
 Definition at line 88 of file [geoflowparm.h](#).

7.8.3 Enumeration Type Documentation

7.8.3.1 eGEOFLOWparm_CalcType

enum eGEOFLOWparm_CalcType
 Calculation type.

Enumerator

GFCT_AUTO	GEOFLOW-auto
-----------	--------------

Definition at line 77 of file [geoflowparm.h](#).

7.8.4 Function Documentation

7.8.4.1 GEOFLOWparm_check()

```

VEXTERNC Vrc_Codes GEOFLOWparm_check (
    GEOFLOWparm * thee )

```

Consistency check for parameter values stored in object.

Author

Andrew Stevens, Kyle Monson

Parameters

<i>thee</i>	GEOFLOWparm object
-------------	--------------------

Returns

Success enumeration

Definition at line 101 of file [geoflowparm.c](#).

7.8.4.2 GEOFLOWparm_copy()

```

VEXTERNC void GEOFLOWparm_copy (
    GEOFLOWparm * thee,
    GEOFLOWparm * parm )

```

copy GEOFLOWparm object into thee.

Author

Parameters

<i>thee</i>	GEOFLOWparm object to be copied into
<i>parm</i>	GEOFLOWparm object.

Definition at line 127 of file [geoflowparm.c](#).

7.8.4.3 GEOFLOWparm_ctor()

```

VEXTERNC GEOFLOWparm * GEOFLOWparm_ctor (
    GEOFLOWparm_CalcType type )

```

Construct GEOFLOWparm object.

Author

Andrew Stevens, Kyle Monson

Parameters

<i>type</i>	Type of GEOFLOW calculation
-------------	-----------------------------

Returns

Newly allocated and initialized GEOFLOWparm object

Definition at line 66 of file [geoflowparm.c](#).

7.8.4.4 GEOFLOWparm_ctor2()

```

VEXTERNC Vrc_Codes GEOFLOWparm_ctor2 (
    GEOFLOWparm * thee,
    GEOFLOWparm_CalcType type )

```

FORTRAN stub to construct GEOFLOWparm object ?????????!!!!!!!

Author

Andrew Stevens, Kyle Monson

Parameters

<i>thee</i>	Space for GEOFLOWparm object
<i>type</i>	Type of MG calculation

Returns

Success enumeration

Definition at line 77 of file [geoflowparm.c](#).

7.8.4.5 GEOFLOWparm_dtor()

```

VEXTERNC void GEOFLOWparm_dtor (

```

```
GEOFLOWparm ** thee )
```

Object destructor.

Author

Andrew Stevens, Kyle Monson

Parameters

<i>thee</i>	Pointer to memory location of GEOFLOWparm object
-------------	--

Definition at line 91 of file [geoflowparm.c](#).

7.8.4.6 GEOFLOWparm_dtor2()

```
VEXTERNC void GEOFLOWparm_dtor2 (
    GEOFLOWparm * thee )
```

FORTRAN stub for object destructor ?????????!!!!!!!

Author

Andrew Stevens, Kyle Monson

Parameters

<i>thee</i>	Pointer to GEOFLOWparm object
-------------	-------------------------------

Definition at line 99 of file [geoflowparm.c](#).

7.8.4.7 GEOFLOWparm_parseToken()

```
VEXTERNC Vrc_Codes GEOFLOWparm_parseToken (
    GEOFLOWparm * thee,
    char tok[VMAX_BUFSIZE],
    Vio * sock )
```

Parse an MG keyword from an input file.

Author

Andrew Stevens, Kyle Monson

Parameters

<i>thee</i>	GEOFLOWparm object
<i>tok</i>	Token to parse
<i>sock</i>	Stream for more tokens

Returns

Success enumeration (1 if matched and assigned; -1 if matched, but there's some sort of error (i.e., too few args); 0 if not matched)

Definition at line 212 of file [geoflowparm.c](#).

7.9 MGparm class

Parameter which holds useful parameters for generic multigrid calculations.

Files

- file [mgparm.c](#)
Class MGparm methods.
- file [mgparm.h](#)
Contains declarations for class MGparm.

Data Structures

- struct [sMGparm](#)
Parameter structure for MG-specific variables from input files.

Typedefs

- typedef enum [eMGparm_CalcType](#) [MGparm_CalcType](#)
Declare MGparm_CalcType type.
- typedef enum [eMGparm_CentMeth](#) [MGparm_CentMeth](#)
Declare MGparm_CentMeth type.
- typedef struct [sMGparm](#) [MGparm](#)
Declaration of the MGparm class as the MGparm structure.

Enumerations

- enum [eMGparm_CalcType](#) {
[MCT_MANUAL](#) =0 , [MCT_AUTO](#) =1 , [MCT_PARALLEL](#) =2 , [MCT_DUMMY](#) =3 ,
[MCT_NONE](#) =4 }
 - enum [eMGparm_CentMeth](#) { [MCM_POINT](#) =0 , [MCM_MOLECULE](#) =1 , [MCM_FOCUS](#) =2 }
- Calculation type.*
- Centering method.*

Functions

- VEXTERNC Vrc_Codes [APOLparm_parseToken](#) ([APOLparm](#) *thee, char tok[VMAX_BUFSIZE], Vio *sock)
Parse an MG keyword from an input file.
- VEXTERNC Vrc_Codes [FEMparm_parseToken](#) ([FEMparm](#) *thee, char tok[VMAX_BUFSIZE], Vio *sock)
Parse an MG keyword from an input file.
- VEXTERNC int [MGparm_getNx](#) ([MGparm](#) *thee)
Get number of grid points in x direction.
- VEXTERNC int [MGparm_getNy](#) ([MGparm](#) *thee)
Get number of grid points in y direction.

- VEXTERNC int [MGparm_getNz](#) ([MGparm](#) *thee)
Get number of grid points in z direction.
- VEXTERNC double [MGparm_getHx](#) ([MGparm](#) *thee)
Get grid spacing in x direction (Å)
- VEXTERNC double [MGparm_getHy](#) ([MGparm](#) *thee)
Get grid spacing in y direction (Å)
- VEXTERNC double [MGparm_getHz](#) ([MGparm](#) *thee)
Get grid spacing in z direction (Å)
- VEXTERNC void [MGparm_setCenterX](#) ([MGparm](#) *thee, double x)
Set center x-coordinate.
- VEXTERNC void [MGparm_setCenterY](#) ([MGparm](#) *thee, double y)
Set center y-coordinate.
- VEXTERNC void [MGparm_setCenterZ](#) ([MGparm](#) *thee, double z)
Set center z-coordinate.
- VEXTERNC double [MGparm_getCenterX](#) ([MGparm](#) *thee)
Get center x-coordinate.
- VEXTERNC double [MGparm_getCenterY](#) ([MGparm](#) *thee)
Get center y-coordinate.
- VEXTERNC double [MGparm_getCenterZ](#) ([MGparm](#) *thee)
Get center z-coordinate.
- VEXTERNC [MGparm](#) * [MGparm_ctor](#) ([MGparm_CalcType](#) type)
Construct MGparm object.
- VEXTERNC Vrc_Codes [MGparm_ctor2](#) ([MGparm](#) *thee, [MGparm_CalcType](#) type)
FORTTRAN stub to construct MGparm object.
- VEXTERNC void [MGparm_dtor](#) ([MGparm](#) **thee)
Object destructor.
- VEXTERNC void [MGparm_dtor2](#) ([MGparm](#) *thee)
FORTTRAN stub for object destructor.
- VEXTERNC Vrc_Codes [MGparm_check](#) ([MGparm](#) *thee)
Consistency check for parameter values stored in object.
- VEXTERNC void [MGparm_copy](#) ([MGparm](#) *thee, [MGparm](#) *parm)
Copy MGparm object into thee.
- VEXTERNC Vrc_Codes [MGparm_parseToken](#) ([MGparm](#) *thee, char tok[VMAX_BUFSIZE], Vio *sock)
Parse an MG keyword from an input file.

7.9.1 Detailed Description

Parameter which holds useful parameters for generic multigrid calculations.

7.9.2 Typedef Documentation

7.9.2.1 MGparm

[MGparm](#)

Declaration of the MGparm class as the MGparm structure.

Definition at line 203 of file [mgparm.h](#).

7.9.2.2 MGparm_CalcType

`typedef enum eMGparm_CalcType MGparm_CalcType`
Declare MGparm_CalcType type.
Definition at line 89 of file [mgparm.h](#).

7.9.2.3 MGparm_CentMeth

`typedef enum eMGparm_CentMeth MGparm_CentMeth`
Declare MGparm_CentMeth type.
Definition at line 105 of file [mgparm.h](#).

7.9.3 Enumeration Type Documentation

7.9.3.1 eMGparm_CalcType

`enum eMGparm_CalcType`
Calculation type.

Enumerator

MCT_MANUAL	mg-manual
MCT_AUTO	mg-auto
MCT_PARALLEL	mg-para
MCT_DUMMY	mg-dummy
MCT_NONE	unspecified

Definition at line 77 of file [mgparm.h](#).

7.9.3.2 eMGparm_CentMeth

`enum eMGparm_CentMeth`
Centering method.

Enumerator

MCM_POINT	Center on a point
MCM_MOLECULE	Center on a molecule
MCM_FOCUS	Determined by focusing

Definition at line 95 of file [mgparm.h](#).

7.9.4 Function Documentation

7.9.4.1 APOLparm_parseToken()

```

VEXTERNC Vrc_Codes APOLparm_parseToken (
    APOLparm * thee,
    char tok[VMAX_BUFSIZE],
    Vio * sock )

```

Parse an MG keyword from an input file.

Author

David Gohara

Parameters

<i>thee</i>	MGparm object
<i>tok</i>	Token to parse
<i>sock</i>	Stream for more tokens

Returns

Success enumeration (1 if matched and assigned; -1 if matched, but there's some sort of error (i.e., too few args); 0 if not matched)

Definition at line 577 of file [apolparm.c](#).

7.9.4.2 FEMparm_parseToken()

```

VEXTERNC Vrc_Codes FEMparm_parseToken (
    FEMparm * thee,
    char tok[VMAX_BUFSIZE],
    Vio * sock )

```

Parse an MG keyword from an input file.

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
<i>tok</i>	Token to parse
<i>sock</i>	Stream for more tokens

Returns

VRC_SUCCESS if matched and assigned; VRC_FAILURE if matched, but there's some sort of error (i.e., too few args); VRC_WARNING if not matched

Definition at line 431 of file [femparm.c](#).

7.9.4.3 MGparm_check()

```

VEXTERNC Vrc_Codes MGparm_check (

```

```
MGparm * thee )
```

Consistency check for parameter values stored in object.

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
-------------	---------------

Returns

Success enumeration

Definition at line 185 of file [mgparm.c](#).

7.9.4.4 MGparm_copy()

```
VEXTERNC void MGparm_copy (  
    MGparm * thee,  
    MGparm * parm )
```

Copy MGparm object into thee.

Author

Nathan Baker and Todd Dolinsky

Parameters

<i>thee</i>	MGparm object (target for copy)
<i>parm</i>	MGparm object (source for copy)

Definition at line 341 of file [mgparm.c](#).

7.9.4.5 MGparm_ctor()

```
VEXTERNC MGparm * MGparm_ctor (  
    MGparm_CalcType type )
```

Construct MGparm object.

Author

Nathan Baker

Parameters

<i>type</i>	Type of MG calculation
-------------	------------------------

Returns

Newly allocated and initialized MGparm object

Definition at line 114 of file [mgparm.c](#).

7.9.4.6 MGparm_ctor2()

```
VEXTERNC Vrc_Codes MGparm_ctor2 (
    MGparm * thee,
    MGparm_CalcType type )
```

FORTTRAN stub to construct MGparm object.

Author

Nathan Baker and Todd Dolinsky

Parameters

<i>thee</i>	Space for MGparm object
<i>type</i>	Type of MG calculation

Returns

Success enumeration

Definition at line 125 of file [mgparm.c](#).

7.9.4.7 MGparm_dtor()

```
VEXTERNC void MGparm_dtor (
    MGparm ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of MGparm object
-------------	---

Definition at line 175 of file [mgparm.c](#).

7.9.4.8 MGparm_dtor2()

```
VEXTERNC void MGparm_dtor2 (
    MGparm * thee )
```

FORTTRAN stub for object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to MGparm object
-------------	--------------------------

Definition at line 183 of file [mgparm.c](#).

7.9.4.9 MGparm_getCenterX()

```
VEXTERNC double MGparm_getCenterX (  
    MGparm * thee )
```

Get center x-coordinate.

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
-------------	---------------

Returns

x-coordinate

Definition at line 77 of file [mgparm.c](#).

7.9.4.10 MGparm_getCenterY()

```
VEXTERNC double MGparm_getCenterY (  
    MGparm * thee )
```

Get center y-coordinate.

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
-------------	---------------

Returns

y-coordinate

Definition at line 81 of file [mgparm.c](#).

7.9.4.11 MGparm_getCenterZ()

```
VEXTERNC double MGparm_getCenterZ (  
    MGparm * thee )
```

```
MGparm * thee )
```

Get center z-coordinate.

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
-------------	---------------

Returns

z-coordinate

Definition at line 85 of file [mgparm.c](#).

7.9.4.12 MGparm_getHx()

```
VEXTERNC double MGparm_getHx (  
    MGparm * thee )
```

Get grid spacing in x direction (Å)

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
-------------	---------------

Returns

Grid spacing in the x direction

Definition at line 101 of file [mgparm.c](#).

7.9.4.13 MGparm_getHy()

```
VEXTERNC double MGparm_getHy (  
    MGparm * thee )
```

Get grid spacing in y direction (Å)

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
-------------	---------------

Returns

Grid spacing in the y direction

Definition at line 105 of file [mgparm.c](#).

7.9.4.14 MGparm_getHz()

```
VEXTERNC double MGparm_getHz (  
    MGparm * thee )
```

Get grid spacing in z direction (Å)

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
-------------	---------------

Returns

Grid spacing in the z direction

Definition at line 109 of file [mgparm.c](#).

7.9.4.15 MGparm_getNx()

```
VEXTERNC int MGparm_getNx (  
    MGparm * thee )
```

Get number of grid points in x direction.

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
-------------	---------------

Returns

Number of grid points in the x direction

Definition at line 89 of file [mgparm.c](#).

7.9.4.16 MGparm_getNy()

```
VEXTERNC int MGparm_getNy (  
    MGparm * thee )
```

Get number of grid points in y direction.

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
-------------	---------------

Returns

Number of grid points in the y direction

Definition at line 93 of file [mgparm.c](#).

7.9.4.17 MGparm_getNz()

```
VEXTERNC int MGparm_getNz (  
    MGparm * thee )
```

Get number of grid points in z direction.

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
-------------	---------------

Returns

Number of grid points in the z direction

Definition at line 97 of file [mgparm.c](#).

7.9.4.18 MGparm_parseToken()

```
VEXTERNC Vrc_Codes MGparm_parseToken (  
    MGparm * thee,  
    char tok[VMAX_BUFSIZE],  
    Vio * sock )
```

Parse an MG keyword from an input file.

Author

Nathan Baker and Todd Dolinsky

Parameters

<i>thee</i>	MGparm object
<i>tok</i>	Token to parse
<i>sock</i>	Stream for more tokens

Returns

Success enumeration (1 if matched and assigned; -1 if matched, but there's some sort of error (i.e., too few args); 0 if not matched)

Definition at line 919 of file [mgparm.c](#).

7.9.4.19 MGparm_setCenterX()

```
VEXTERNC void MGparm_setCenterX (  
    MGparm * thee,  
    double x )
```

Set center x-coordinate.

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
<i>x</i>	x-coordinate

Definition at line 65 of file [mgparm.c](#).

7.9.4.20 MGparm_setCenterY()

```
VEXTERNC void MGparm_setCenterY (  
    MGparm * thee,  
    double y )
```

Set center y-coordinate.

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
<i>y</i>	y-coordinate

Definition at line 69 of file [mgparm.c](#).

7.9.4.21 MGparm_setCenterZ()

```
VEXTERNC void MGparm_setCenterZ (  
    MGparm * thee,  
    double z )
```

Set center z-coordinate.

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
<i>z</i>	z-coordinate

Definition at line 73 of file [mgparm.c](#).

7.10 NOsh class

Class for parsing for fixed format input files.

Files

- file [nosh.c](#)
Class NOsh methods.
- file [nosh.h](#)
Contains declarations for class NOsh.

Data Structures

- struct [sNOsh_calc](#)
Calculation class for use when parsing fixed format input files.
- struct [sNOsh](#)
Class for parsing fixed format input files.

Macros

- `#define` [NOSH_MAXMOL](#) 20
Maximum number of molecules in a run.
- `#define` [NOSH_MAXCALC](#) 20
Maximum number of calculations in a run.
- `#define` [NOSH_MAXPRINT](#) 20
Maximum number of PRINT statements in a run.
- `#define` [NOSH_MAXPOP](#) 20
Maximum number of operations in a PRINT statement.

Typedefs

- typedef enum [eNOsh_MolFormat](#) [NOsh_MolFormat](#)
Declare NOsh_MolFormat type.
- typedef enum [eNOsh_CalcType](#) [NOsh_CalcType](#)
Declare NOsh_CalcType type.
- typedef enum [eNOsh_ParmFormat](#) [NOsh_ParmFormat](#)
Declare NOsh_ParmFormat type.
- typedef enum [eNOsh_PrintType](#) [NOsh_PrintType](#)
Declare NOsh_PrintType type.

- typedef struct `sNOsh` `NOsh`

Declaration of the NOsh class as the NOsh structure.

- typedef struct `sNOsh_calc` `NOsh_calc`

Declaration of the NOsh_calc class as the NOsh_calc structure.

Enumerations

- enum `eNOsh_MolFormat` { `NMF_PQR` =0 , `NMF_PDB` =1 , `NMF_XML` =2 }

Molecule file format types.

- enum `eNOsh_CalcType` {
`NCT_MG` =0 , `NCT_FEM` =1 , `NCT_APOL` =2 , `NCT_BEM` =3 ,
`NCT_GEOFLOW` =4 , `NCT_PBAM` =5 , `NCT_PBSAM` =6 }

NOsh calculation types.

- enum `eNOsh_ParmFormat` { `NPF_FLAT` =0 , `NPF_XML` =1 }

Parameter file format types.

- enum `eNOsh_PrintType` {
`NPT_ENERGY` =0 , `NPT_FORCE` =1 , `NPT_ELECENERGY` , `NPT_ELECFORCE` ,
`NPT_APOLENERGY` , `NPT_APOLFORCE` }

NOsh print types.

Functions

- VEXTERNC char * `NOsh_getMolpath` (`NOsh` *thee, int imol)
Returns path to specified molecule.
- VEXTERNC char * `NOsh_getDielXpath` (`NOsh` *thee, int imap)
Returns path to specified x-shifted dielectric map.
- VEXTERNC char * `NOsh_getDielYpath` (`NOsh` *thee, int imap)
Returns path to specified y-shifted dielectric map.
- VEXTERNC char * `NOsh_getDielZpath` (`NOsh` *thee, int imap)
Returns path to specified z-shifted dielectric map.
- VEXTERNC char * `NOsh_getKappapath` (`NOsh` *thee, int imap)
Returns path to specified kappa map.
- VEXTERNC char * `NOsh_getPotpath` (`NOsh` *thee, int imap)
Returns path to specified potential map.
- VEXTERNC char * `NOsh_getChargepath` (`NOsh` *thee, int imap)
Returns path to specified charge distribution map.
- VEXTERNC `NOsh_calc` * `NOsh_getCalc` (`NOsh` *thee, int icalc)
Returns specified calculation object.
- VEXTERNC int `NOsh_getDielfmt` (`NOsh` *thee, int imap)
Returns format of specified dielectric map.
- VEXTERNC int `NOsh_getKappafmt` (`NOsh` *thee, int imap)
Returns format of specified kappa map.
- VEXTERNC int `NOsh_getPotfmt` (`NOsh` *thee, int imap)
Returns format of specified potential map.
- VEXTERNC int `NOsh_getChargefmt` (`NOsh` *thee, int imap)
Returns format of specified charge map.
- VEXTERNC `NOsh_PrintType` `NOsh_printWhat` (`NOsh` *thee, int iprint)
Return an integer ID of the observable to print (.

- VEXTERNC char * [NOsh_elecname](#) (NOsh *thee, int ielec)
Return an integer mapping of an ELEC statement to a calculation ID (.).
- VEXTERNC int [NOsh_elec2calc](#) (NOsh *thee, int icalc)
Return the name of an elec statement.
- VEXTERNC int [NOsh_apol2calc](#) (NOsh *thee, int icalc)
Return the name of an apol statement.
- VEXTERNC int [NOsh_printNarg](#) (NOsh *thee, int iprint)
Return number of arguments to PRINT statement (.).
- VEXTERNC int [NOsh_printOp](#) (NOsh *thee, int iprint, int iarg)
Return integer ID for specified operation (.).
- VEXTERNC int [NOsh_printCalc](#) (NOsh *thee, int iprint, int iarg)
Return calculation ID for specified PRINT statement (.).
- VEXTERNC NOsh * [NOsh_ctor](#) (int rank, int size)
Construct NOsh.
- VEXTERNC NOsh_calc * [NOsh_calc_ctor](#) (NOsh_CalcType calcType)
Construct NOsh_calc.
- VEXTERNC int [NOsh_calc_copy](#) (NOsh_calc *thee, NOsh_calc *source)
Copy NOsh_calc object into thee.
- VEXTERNC void [NOsh_calc_dtor](#) (NOsh_calc **thee)
Object destructor.
- VEXTERNC int [NOsh_ctor2](#) (NOsh *thee, int rank, int size)
FORTTRAN stub to construct NOsh.
- VEXTERNC void [NOsh_dtor](#) (NOsh **thee)
Object destructor.
- VEXTERNC void [NOsh_dtor2](#) (NOsh *thee)
FORTTRAN stub for object destructor.
- VEXTERNC int [NOsh_parseInput](#) (NOsh *thee, Vio *sock)
Parse an input file from a socket.
- VEXTERNC int [NOsh_parseInputFile](#) (NOsh *thee, char *filename)
Parse an input file only from a file.
- VEXTERNC int [NOsh_setupElecCalc](#) (NOsh *thee, Valist *alist[NOSH_MAXMOL])
Setup the series of electrostatics calculations.
- VEXTERNC int [NOsh_setupApolCalc](#) (NOsh *thee, Valist *alist[NOSH_MAXMOL])
Setup the series of non-polar calculations.

7.10.1 Detailed Description

Class for parsing for fixed format input files.

7.10.2 Macro Definition Documentation

7.10.2.1 NOSH_MAXCALC

```
#define NOSH_MAXCALC 20
```

Maximum number of calculations in a run.

Definition at line 87 of file [nosh.h](#).

7.10.2.2 NOSH_MAXMOL

```
#define NOSH_MAXMOL 20
```

Maximum number of molecules in a run.

Definition at line 83 of file [nosh.h](#).

7.10.2.3 NOSH_MAXPOP

```
#define NOSH_MAXPOP 20
```

Maximum number of operations in a PRINT statement.

Definition at line 95 of file [nosh.h](#).

7.10.2.4 NOSH_MAXPRINT

```
#define NOSH_MAXPRINT 20
```

Maximum number of PRINT statements in a run.

Definition at line 91 of file [nosh.h](#).

7.10.3 Typedef Documentation

7.10.3.1 NOsh

```
typedef struct sNOsh NOsh
```

Declaration of the NOsh class as the NOsh structure.

Definition at line 277 of file [nosh.h](#).

7.10.3.2 NOsh_calc

```
NOsh_calc
```

Declaration of the NOsh_calc class as the NOsh_calc structure.

Definition at line 188 of file [nosh.h](#).

7.10.3.3 NOsh_CalcType

```
typedef enum eNOsh_CalcType NOsh_CalcType
```

Declare NOsh_CalcType type.

Definition at line 131 of file [nosh.h](#).

7.10.3.4 NOsh_MolFormat

```
typedef enum eNOsh_MolFormat NOsh_MolFormat
```

Declare NOsh_MolFormat type.

Definition at line 111 of file [nosh.h](#).

7.10.3.5 NOsh_ParmFormat

```
typedef enum eNOsh_ParmFormat NOsh_ParmFormat
```

Declare NOsh_ParmFormat type.
Definition at line 146 of file [nosh.h](#).

7.10.3.6 NOsh_PrintType

```
typedef enum eNOsh_PrintType NOsh_PrintType
```

Declare NOsh_PrintType type.
Definition at line 165 of file [nosh.h](#).

7.10.4 Enumeration Type Documentation

7.10.4.1 eNOsh_CalcType

```
enum eNOsh_CalcType
```

NOsh calculation types.

Enumerator

NCT_MG	Multigrid
NCT_FEM	Finite element
NCT_APOL	non-polar
NCT_BEM	Boundary element (TABI)
NCT_GEOFLOW	Geometric flow
NCT_PBAM	Analytical Poisson-Boltzmann Solver
NCT_PBSAM	Semi-Analytical Poisson-Boltzmann Solver

Definition at line 117 of file [nosh.h](#).

7.10.4.2 eNOsh_MolFormat

```
enum eNOsh_MolFormat
```

Molecule file format types.

Enumerator

NMF_PQR	PQR format
NMF_PDB	PDB format
NMF_XML	XML format

Definition at line 101 of file [nosh.h](#).

7.10.4.3 eNOsh_ParmFormat

```
enum eNOsh_ParmFormat
```

Parameter file format types.

Enumerator

NPF_FLAT	Flat-file format
NPF_XML	XML format

Definition at line 137 of file [nosh.h](#).

7.10.4.4 eNOsh_PrintType

enum [eNOsh_PrintType](#)

NOsh print types.

Enumerator

NPT_ENERGY	Energy (deprecated)
NPT_FORCE	Force (deprecated)
NPT_ELECENERGY	Elec Energy
NPT_ELECFORCE	Elec Force
NPT_APOLENERGY	Apol Energy
NPT_APOLFORCE	Apol Force

Definition at line 152 of file [nosh.h](#).

7.10.5 Function Documentation

7.10.5.1 NOsh_apol2calc()

```
VEXTERNC int NOsh_apol2calc (
    NOsh * thee,
    int icalc )
```

Return the name of an apol statement.

Author

David Gohara

Parameters

<i>thee</i>	NOsh object to use
<i>icalc</i>	ID of CALC statement

Returns

The name (if present) of an APOL statement

Definition at line 282 of file [nosh.c](#).

7.10.5.2 NOsh_calc_copy()

```
VEXTERNC int NOsh_calc_copy (
```

```
    NOsh_calc * thee,  
    NOsh_calc * source )
```

Copy NOsh_calc object into thee.

Author

Nathan Baker

Parameters

<i>thee</i>	Target object
<i>source</i>	Source object

Definition at line 467 of file [nosh.c](#).

7.10.5.3 NOsh_calc_ctor()

```
VEXTERNC NOsh_calc * NOsh_calc_ctor (  
    NOsh_CalcType calcType )
```

Construct NOsh_calc.

Author

Nathan Baker

Parameters

<i>calcType</i>	Calculation type
-----------------	------------------

Returns

Newly allocated and initialized NOsh object

Definition at line 374 of file [nosh.c](#).

7.10.5.4 NOsh_calc_dtor()

```
VEXTERNC void NOsh_calc_dtor (  
    NOsh_calc ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of NOsh_calc object
-------------	--

Definition at line 423 of file [nosh.c](#).

7.10.5.5 NOsh_ctor()

```
VECTERNC NOsh * NOsh_ctor (
    int rank,
    int size )
```

Construct NOsh.

Author

Nathan Baker

Parameters

<i>rank</i>	Rank of current processor in parallel calculation (0 if not parallel)
<i>size</i>	Number of processors in parallel calculation (1 if not parallel)

Returns

Newly allocated and initialized NOsh object

Definition at line 308 of file [nosh.c](#).

7.10.5.6 NOsh_ctor2()

```
VECTERNC int NOsh_ctor2 (
    NOsh * thee,
    int rank,
    int size )
```

FORTTRAN stub to construct NOsh.

Author

Nathan Baker

Parameters

<i>thee</i>	Space for NOsh objet
<i>rank</i>	Rank of current processor in parallel calculation (0 if not parallel)
<i>size</i>	Number of processors in parallel calculation (1 if not parallel)

Returns

1 if successful, 0 otherwise

Definition at line 319 of file [nosh.c](#).

7.10.5.7 NOsh_dtor()

```
VECTERNC void NOsh_dtor (
    NOsh ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of NOsh object
-------------	---

Definition at line 354 of file [nosh.c](#).

7.10.5.8 NOsh_dtor2()

```
VEXTERNC void NOsh_dtor2 (  
    NOsh * thee )  
FORTRAN stub for object destructor.
```

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
-------------	------------------------

Definition at line 362 of file [nosh.c](#).

7.10.5.9 NOsh_elec2calc()

```
VEXTERNC int NOsh_elec2calc (  
    NOsh * thee,  
    int icalc )  
Return the name of an elec statement.
```

Author

Todd Dolinsky

Parameters

<i>thee</i>	NOsh object to use
<i>icalc</i>	ID of CALC statement

Returns

The name (if present) of an ELEC statement

Definition at line 276 of file [nosh.c](#).

7.10.5.10 NOsh_elecname()

```
VEXTERNC char * NOsh_elecname (  

```

```
NOsh * thee,  
int ielec )
```

Return an integer mapping of an ELEC statement to a calculation ID (.

See also

elec2calc)

Author

Nathan Baker

Parameters

<i>thee</i>	NOsh object to use
<i>ielec</i>	ID of ELEC statement

Returns

An integer mapping of an ELEC statement to a calculation ID (

See also

elec2calc)

Definition at line 288 of file [nosh.c](#).

7.10.5.11 NOsh_getCalc()

```
VEXTERNC NOsh_calc * NOsh_getCalc (  
    NOsh * thee,  
    int icalc )
```

Returns specified calculation object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
<i>icalc</i>	Calculation ID of interest

Returns

Pointer to specified calculation object

Definition at line 235 of file [nosh.c](#).

7.10.5.12 NOsh_getChargefmt()

```
VEXTERNC int NOsh_getChargefmt (  
    NOsh * thee,
```

```
int imap )
```

Returns format of specified charge map.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
<i>imap</i>	Calculation ID of interest

Returns

Format of charge map

Definition at line 255 of file [nosh.c](#).

7.10.5.13 NOsh_getChargepath()

```
VEXTERNC char * NOsh_getChargepath (  
    NOsh * thee,  
    int imap )
```

Returns path to specified charge distribution map.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
<i>imap</i>	Map ID of interest

Returns

Path string

Definition at line 230 of file [nosh.c](#).

7.10.5.14 NOsh_getDielfmt()

```
VEXTERNC int NOsh_getDielfmt (  
    NOsh * thee,  
    int imap )
```

Returns format of specified dielectric map.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
<i>imap</i>	Calculation ID of interest

Returns

Format of dielectric map

Definition at line 240 of file [nosh.c](#).

7.10.5.15 NOsh_getDielXpath()

```
VEXTERNC char * NOsh_getDielXpath (
    NOsh * thee,
    int imap )
```

Returns path to specified x-shifted dielectric map.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
<i>imap</i>	Map ID of interest

Returns

Path string

Definition at line 205 of file [nosh.c](#).

7.10.5.16 NOsh_getDielYpath()

```
VEXTERNC char * NOsh_getDielYpath (
    NOsh * thee,
    int imap )
```

Returns path to specified y-shifted dielectric map.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
<i>imap</i>	Map ID of interest

Returns

Path string

Definition at line 210 of file [nosh.c](#).

7.10.5.17 NOsh_getDielZpath()

```
VEXTERNC char * NOsh_getDielZpath (
    NOsh * thee,
    int imap )
```

Returns path to specified z-shifted dielectric map.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
<i>imap</i>	Map ID of interest

Returns

Path string

Definition at line 215 of file [nosh.c](#).

7.10.5.18 NOsh_getKappafmt()

```
VEXTERNC int NOsh_getKappafmt (
    NOsh * thee,
    int imap )
```

Returns format of specified kappa map.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
<i>imap</i>	Calculation ID of interest

Returns

Format of kappa map

Definition at line 245 of file [nosh.c](#).

7.10.5.19 NOsh_getKappapath()

```
VEXTERNC char * NOsh_getKappapath (
```

```
NOsh * thee,  
int imap )
```

Returns path to specified kappa map.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
<i>imap</i>	Map ID of interest

Returns

Path string

Definition at line 220 of file [nosh.c](#).

7.10.5.20 NOsh_getMolpath()

```
EXTERNC char * NOsh_getMolpath (  
    NOsh * thee,  
    int imol )
```

Returns path to specified molecule.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
<i>imol</i>	Molecule ID of interest

Returns

Path string

Definition at line 200 of file [nosh.c](#).

7.10.5.21 NOsh_getPotfmt()

```
EXTERNC int NOsh_getPotfmt (  
    NOsh * thee,  
    int imap )
```

Returns format of specified potential map.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
<i>imap</i>	Calculation ID of interest

Returns

Format of potential map

Definition at line 250 of file [nosh.c](#).

7.10.5.22 NOsh_getPotpath()

```
VEXTERNC char * NOsh_getPotpath (
    NOsh * thee,
    int imap )
```

Returns path to specified potential map.

Author

David Gohara

Parameters

<i>thee</i>	Pointer to NOsh object
<i>imap</i>	Map ID of interest

Returns

Path string

Definition at line 225 of file [nosh.c](#).

7.10.5.23 NOsh_parseInput()

```
VEXTERNC int NOsh_parseInput (
    NOsh * thee,
    Vio * sock )
```

Parse an input file from a socket.

Note

Should be called before NOsh_setupCalc

Author

Nathan Baker and Todd Dolinsky

Parameters

<i>thee</i>	Pointer to NOsh object
<i>sock</i>	Stream of tokens to parse

Returns

1 if successful, 0 otherwise

Definition at line 513 of file [nosh.c](#).

7.10.5.24 NOsh_parseInputFile()

```
VEXTERNC int NOsh_parseInputFile (
    NOsh * thee,
    char * filename )
```

Parse an input file only from a file.

Note

Included for SWIG wrapper compatibility

Should be called before NOsh_setupCalc

Author

Nathan Baker and Todd Dolinsky

Parameters

<i>thee</i>	Pointer to NOsh object
<i>filename</i>	Name/path of readable file

Returns

1 if successful, 0 otherwise

Definition at line 498 of file [nosh.c](#).

7.10.5.25 NOsh_printCalc()

```
VEXTERNC int NOsh_printCalc (
    NOsh * thee,
    int iprint,
    int iarg )
```

Return calculation ID for specified PRINT statement (.

See also

printcalc)

Author

Nathan Baker

Parameters

<i>thee</i>	NOsh object to use
<i>iprint</i>	ID of PRINT statement
<i>iarg</i>	ID of operation in PRINT statement

Returns

Calculation ID for specified PRINT statement (

See also

printcalc)

Definition at line 301 of file [nosh.c](#).

7.10.5.26 NOsh_printNarg()

```
VEXTERNC int NOsh_printNarg (  
    NOsh * thee,  
    int iprint )
```

Return number of arguments to PRINT statement (.

See also

printrnarg)

Author

Nathan Baker

Parameters

<i>thee</i>	NOsh object to use
<i>iprint</i>	ID of PRINT statement

Returns

Number of arguments to PRINT statement (

See also

printrnarg)

Definition at line 270 of file [nosh.c](#).

7.10.5.27 NOsh_printOp()

```
VEXTERNC int NOsh_printOp (  
    NOsh * thee,  
    int iprint,  
    int iarg )
```

Return integer ID for specified operation (.

See also

printop)

Author

Nathan Baker

Parameters

<i>thee</i>	NOsh object to use
<i>iprint</i>	ID of PRINT statement
<i>iarg</i>	ID of operation in PRINT statement

Returns

Integer ID for specified operation (

See also

printop)

Definition at line 294 of file [nosh.c](#).

7.10.5.28 NOsh_printWhat()

```
VEXTERNC NOsh_PrintType NOsh_printWhat (
    NOsh * thee,
    int iprint )
```

Return an integer ID of the observable to print (.

See also

printwhat)

Author

Nathan Baker

Parameters

<i>thee</i>	NOsh object to use
<i>iprint</i>	ID of PRINT statement

Returns

An integer ID of the observable to print (

See also

printwhat)

Definition at line 264 of file [nosh.c](#).

7.10.5.29 NOsh_setupApolCalc()

```
VEXTERNC int NOsh_setupApolCalc (
    NOsh * thee,
    Valist * alist[NOSH_MAXMOL] )
```

Setup the series of non-polar calculations.

Note

Should be called after NOsh_parseInput*

Author

Nathan Baker and Todd Dolinsky

Parameters

<i>thee</i>	Pointer to NOsh object
<i>alist</i>	Array of pointers to Valist objects (molecules used to center mesh);

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	NOsh object
<i>alist</i>	Atom list for calculation

Definition at line 1469 of file [nosh.c](#).

7.10.5.30 NOsh_setupElecCalc()

```
VEEXTERNAL int NOsh_setupElecCalc (
    NOsh * thee,
    Valist * alist[NOSH_MAXMOL] )
```

Setup the series of electrostatics calculations.

Note

Should be called after NOsh_parseInput*

Author

Nathan Baker and Todd Dolinsky

Parameters

<i>thee</i>	Pointer to NOsh object
<i>alist</i>	Array of pointers to Valist objects (molecules used to center mesh);

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	NOsh object
<i>alist</i>	Atom list for calculation

Definition at line 1374 of file [nosh.c](#).

7.11 PBAMparm class

Parameter which holds useful parameters for Poisson-boltzmann analytical method calculations.

Files

- file [pbamparm.c](#)
Class PBAMparm methods.
- file [pbamparm.h](#)
Contains declarations for class PBAMparm.

Data Structures

- struct [sPBAMparm](#)
Parameter structure for PBAM-specific variables from input files.

Macros

- `#define CHR_MAXLEN 1000`
Number of things that can be written out in a single calculation.

Typedefs

- typedef enum [ePBAMparm_CalcType](#) [PBAMparm_CalcType](#)
Declare PBAMparm_CalcType type.
- typedef struct [sPBAMparm](#) [PBAMparm](#)
Parameter structure for PBAM-specific variables from input files.

Enumerations

- enum [ePBAMparm_CalcType](#) { [PBAMCT_AUTO](#) =1 }
Calculation type.

Functions

- VEXTERNC [PBAMparm](#) * [PBAMparm_ctor](#) ([PBAMparm_CalcType](#) type)
Construct PBAMparm object.
- VEXTERNC Vrc_Codes [PBAMparm_ctor2](#) ([PBAMparm](#) *thee, [PBAMparm_CalcType](#) type)
FORTTRAN stub to construct PBAMparm object ?????????!!!!!!
- VEXTERNC void [PBAMparm_dtor](#) ([PBAMparm](#) **thee)
Object destructor.
- VEXTERNC void [PBAMparm_dtor2](#) ([PBAMparm](#) *thee)
FORTTRAN stub for object destructor ?????????!!!!!!
- VEXTERNC Vrc_Codes [PBAMparm_check](#) ([PBAMparm](#) *thee)
Consistency check for parameter values stored in object.
- VEXTERNC Vrc_Codes [PBAMparm_parseToken](#) ([PBAMparm](#) *thee, char tok[VMAX_BUFSIZE], Vio *sock)
Parse an MG keyword from an input file.
- VEXTERNC void [PBAMparm_copy](#) ([PBAMparm](#) *thee, [PBAMparm](#) *parm)

copy PBAMparm object into thee.

- VPRIVATE Vrc_Codes [PBAMparm_parseSalt](#) (PBAMparm *thee, Vio *sock)
Find salt conc and save it as a structure variable.
- VPRIVATE Vrc_Codes [PBAMparm_parseRunType](#) (PBAMparm *thee, Vio *sock)
Find runType and save it as a structure variable.
- VPRIVATE Vrc_Codes [PBAMparm_parseRunName](#) (PBAMparm *thee, Vio *sock)
Find runName and save it as a structure variable.
- VPRIVATE Vrc_Codes [PBAMparm_parseRandorient](#) (PBAMparm *thee, Vio *sock)
Find randomorientation flag and save it as a boolean.
- VPRIVATE Vrc_Codes [PBAMparm_parsePBCS](#) (PBAMparm *thee, Vio *sock)
Find PBC flag and save the type and the boxlength.
- VPRIVATE Vrc_Codes [PBAMparm_parseUnits](#) (PBAMparm *thee, Vio *sock)
Find units flag and save units.
- VPRIVATE Vrc_Codes [PBAMparm_parse3Dmap](#) (PBAMparm *thee, Vio *sock)
Find 3D map filename and save it.
- VPRIVATE Vrc_Codes [PBAMparm_parseGrid2D](#) (PBAMparm *thee, Vio *sock)
Find 2D grid filename and save it.
- VPRIVATE Vrc_Codes [PBAMparm_parseDX](#) (PBAMparm *thee, Vio *sock)
Find DX filename and save it.
- VPRIVATE Vrc_Codes [PBAMparm_parseGridPts](#) (PBAMparm *thee, Vio *sock)
Find Grid points and save them.
- VPRIVATE Vrc_Codes [PBAMparm_parseTermcombine](#) (PBAMparm *thee, Vio *sock)
Find Termination logic and save it.
- VPRIVATE Vrc_Codes [PBAMparm_parseDiff](#) (PBAMparm *thee, Vio *sock)
Find diffusion coeffs for each molecule and save them.
- VPRIVATE Vrc_Codes [PBAMparm_parseXYZ](#) (PBAMparm *thee, Vio *sock)
Find xyz files for each molecule for each traj and save them.

7.11.1 Detailed Description

Parameter which holds useful parameters for Poisson-boltzmann analytical method calculations.

7.11.2 Macro Definition Documentation

7.11.2.1 CHR_MAXLEN

```
#define CHR_MAXLEN 1000
```

Number of things that can be written out in a single calculation.

Definition at line 76 of file [pbamparm.h](#).

7.11.3 Typedef Documentation

7.11.3.1 PBAMparm

```
typedef struct sPBAMparm PBAMparm
```

Parameter structure for PBAM-specific variables from input files.

Author

Andrew Stevens, Kyle Monson

Note

If you add/delete/change something in this class, the member functions – especially PBAMparm_copy – must be modified accordingly

7.11.3.2 PBAMparm_CalcType

```
typedef enum ePBAMparm_CalcType PBAMparm_CalcType
```

Declare PBAMparm_CalcType type.

Definition at line 95 of file [pbamparm.h](#).

7.11.4 Enumeration Type Documentation

7.11.4.1 ePBAMparm_CalcType

```
enum ePBAMparm_CalcType
```

Calculation type.

Enumerator

PBAMCT_AUTO	PBAM-auto
-------------	-----------

Definition at line 84 of file [pbamparm.h](#).

7.11.5 Function Documentation

7.11.5.1 PBAMparm_check()

```
VEXTERNC Vrc_Codes PBAMparm_check (
    PBAMparm * thee )
```

Consistency check for parameter values stored in object.

Author

Andrew Stevens, Kyle Monson

Parameters

<i>thee</i>	PBAMparm object
-------------	-----------------

Returns

Success enumeration

Definition at line 132 of file [pbamparm.c](#).

7.11.5.2 PBAMparm_copy()

```
VEXTERNC void PBAMparm_copy (
    PBAMparm * thee,
    PBAMparm * parm )
```

copy PBAMparm object into thee.

Author**Parameters**

<i>thee</i>	PBAMparm object to be copied into
<i>parm</i>	PBAMparm object.

Definition at line 157 of file [pbamparm.c](#).

7.11.5.3 PBAMparm_ctor()

```
VEXTERNC PBAMparm * PBAMparm_ctor (
    PBAMparm_CalcType type )
```

Construct PBAMparm object.

Author

Andrew Stevens, Kyle Monson

Parameters

<i>type</i>	Type of PBAM calculation
-------------	--------------------------

Returns

Newly allocated and initialized PBAMparm object

Definition at line 66 of file [pbamparm.c](#).

7.11.5.4 PBAMparm_ctor2()

```
VEXTERNC Vrc_Codes PBAMparm_ctor2 (
    PBAMparm * thee,
    PBAMparm_CalcType type )
```

FORTTRAN stub to construct PBAMparm object ?????????!!!!!!

Author

Andrew Stevens, Kyle Monson

Parameters

<i>thee</i>	Space for PBAMparm object
<i>type</i>	Type of MG calculation

Returns

Success enumeration

Definition at line 77 of file [pbamparm.c](#).

7.11.5.5 PBAMparm_dtor()

```
VEXTERNC void PBAMparm_dtor (  
    PBAMparm ** thee )
```

Object destructor.

Author

Andrew Stevens, Kyle Monson

Parameters

<i>thee</i>	Pointer to memory location of PBAMparm object
-------------	---

Definition at line 122 of file [pbamparm.c](#).

7.11.5.6 PBAMparm_dtor2()

```
VEXTERNC void PBAMparm_dtor2 (  
    PBAMparm * thee )
```

FORTRAN stub for object destructor ??????????!!!!!!!!!!!!

Author

Andrew Stevens, Kyle Monson

Parameters

<i>thee</i>	Pointer to PBAMparm object
-------------	----------------------------

Definition at line 130 of file [pbamparm.c](#).

7.11.5.7 PBAMparm_parse3Dmap()

```
VPRIVATE Vrc_Codes PBAMparm_parse3Dmap (  
    PBAMparm * thee,
```

```
Vio * sock )
```

Find 3D map filename and save it.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 371 of file [pbamparm.c](#).

7.11.5.8 PBAMparm_parseDiff()

```
VPRIVATE Vrc_Codes PBAMparm_parseDiff (  
    PBAMparm * thee,  
    Vio * sock )
```

Find diffusion coeffs for each molecule and save them.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 477 of file [pbamparm.c](#).

7.11.5.9 PBAMparm_parseDX()

```
VPRIVATE Vrc_Codes PBAMparm_parseDX (  
    PBAMparm * thee,  
    Vio * sock )
```

Find DX filename and save it.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 426 of file [pbamparm.c](#).

7.11.5.10 PBAMparm_parseGrid2D()

```
VPRIVATE Vrc_Codes PBAMparm_parseGrid2D (  
    PBAMparm * thee,  
    Vio * sock )
```

Find 2D grid filename and save it.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 391 of file [pbamparm.c](#).

7.11.5.11 PBAMparm_parseGridPts()

```
VPRIVATE Vrc_Codes PBAMparm_parseGridPts (  
    PBAMparm * thee,  
    Vio * sock )
```

Find Grid points and save them.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 351 of file [pbamparm.c](#).

7.11.5.12 PBAMparm_parsePBCS()

```
VPRIVATE Vrc_Codes PBAMparm_parsePBCS (  
    PBAMparm * thee,  
    Vio * sock )
```

Find PBC flag and save the type and the boxlength.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 310 of file [pbamparm.c](#).

7.11.5.13 PBAMparm_parseRandorient()

```
VPRIVATE Vrc_Codes PBAMparm_parseRandorient (
    PBAMparm * thee,
    Vio * sock )
```

Find randomorientation flag and save it as a boolean.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 304 of file [pbamparm.c](#).

7.11.5.14 PBAMparm_parseRunName()

```
VPRIVATE Vrc_Codes PBAMparm_parseRunName (
    PBAMparm * thee,
    Vio * sock )
```

Find runName and save it as a structure variable.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 289 of file [pbamparm.c](#).

7.11.5.15 PBAMparm_parseRunType()

```
VPRIVATE Vrc_Codes PBAMparm_parseRunType (
    PBAMparm * thee,
    Vio * sock )
```

Find runType and save it as a structure variable.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 271 of file [pbamparm.c](#).

7.11.5.16 PBAMparm_parseSalt()

```
VPRIVATE Vrc_Codes PBAMparm_parseSalt (  
    PBAMparm * thee,  
    Vio * sock )
```

Find salt conc and save it as a structure variable.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>parm</i>	The stream from which parameter is taken

Definition at line 252 of file [pbamparm.c](#).

7.11.5.17 PBAMparm_parseTermcombine()

```
VPRIVATE Vrc_Codes PBAMparm_parseTermcombine (  
    PBAMparm * thee,  
    Vio * sock )
```

Find Termination logic and save it.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 444 of file [pbamparm.c](#).

7.11.5.18 PBAMparm_parseToken()

```
VEXTERNC Vrc_Codes PBAMparm_parseToken (  
    PBAMparm * thee,  
    char tok[VMAX_BUFSIZE],  
    Vio * sock )
```

Parse an MG keyword from an input file.

Author

Andrew Stevens, Kyle Monson

Parameters

<i>thee</i>	PBAMparm object
<i>tok</i>	Token to parse
<i>sock</i>	Stream for more tokens

Returns

Success enumeration (1 if matched and assigned; -1 if matched, but there's some sort of error (i.e., too few args); 0 if not matched)

Definition at line 662 of file [pbamparm.c](#).

7.11.5.19 PBAMparm_parseUnits()

```
VPRIVATE Vrc_Codes PBAMparm_parseUnits (  
    PBAMparm * thee,  
    Vio * sock )
```

Find units flag and save units.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 336 of file [pbamparm.c](#).

7.11.5.20 PBAMparm_parseXYZ()

```
VPRIVATE Vrc_Codes PBAMparm_parseXYZ (  
    PBAMparm * thee,  
    Vio * sock )
```

Find xyz files for each molecule for each traj and save them.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 632 of file [pbamparm.c](#).

7.12 PBEparm class

Parameter structure for PBE variables independent of solver.

Files

- file [pbeparm.c](#)
Class PBEparm methods.
- file [pbeparm.h](#)
Contains declarations for class PBEparm.

Data Structures

- struct [sPBEparm](#)
Parameter structure for PBE variables from input files.

Macros

- `#define PBEPARAM_MAXWRITE 20`
Number of things that can be written out in a single calculation.

Typedefs

- typedef enum [ePBEparm_calcEnergy](#) [PBEparm_calcEnergy](#)
Define ePBEparm_calcEnergy enumeration as PBEparm_calcEnergy.
- typedef enum [ePBEparm_calcForce](#) [PBEparm_calcForce](#)
Define ePBEparm_calcForce enumeration as PBEparm_calcForce.
- typedef struct [sPBEparm](#) [PBEparm](#)
Declaration of the PBEparm class as the PBEparm structure.

Enumerations

- enum [ePBEparm_calcEnergy](#) { [PCE_NO](#) =0 , [PCE_TOTAL](#) =1 , [PCE_COMPS](#) =2 }
Define energy calculation enumeration.
- enum [ePBEparm_calcForce](#) { [PCF_NO](#) =0 , [PCF_TOTAL](#) =1 , [PCF_COMPS](#) =2 }
Define force calculation enumeration.

Functions

- VEXTERNC double [PBEparm_getIonCharge](#) ([PBEparm](#) *thee, int iion)
Get charge (e) of specified ion species.
- VEXTERNC double [PBEparm_getIonConc](#) ([PBEparm](#) *thee, int iion)
Get concentration (M) of specified ion species.
- VEXTERNC double [PBEparm_getIonRadius](#) ([PBEparm](#) *thee, int iion)
Get radius (A) of specified ion species.
- VEXTERNC [PBEparm](#) * [PBEparm_ctor](#) ()
Construct PBEparm object.
- VEXTERNC int [PBEparm_ctor2](#) ([PBEparm](#) *thee)
FORTTRAN stub to construct PBEparm object.
- VEXTERNC void [PBEparm_dtor](#) ([PBEparm](#) **thee)

Object destructor.

- VEXTERNC void [PBEparm_dtor2](#) ([PBEparm](#) *thee)

FORTTRAN stub for object destructor.

- VEXTERNC int [PBEparm_check](#) ([PBEparm](#) *thee)

Consistency check for parameter values stored in object.

- VEXTERNC void [PBEparm_copy](#) ([PBEparm](#) *thee, [PBEparm](#) *parm)

Copy PBEparm object into thee.

- VEXTERNC int [PBEparm_parseToken](#) ([PBEparm](#) *thee, char tok[VMAX_BUFSIZE], Vio *sock)

Parse a keyword from an input file.

7.12.1 Detailed Description

Parameter structure for PBE variables independent of solver.

7.12.2 Macro Definition Documentation

7.12.2.1 PBEPARM_MAXWRITE

```
#define PBEPARM_MAXWRITE 20
```

Number of things that can be written out in a single calculation.

Definition at line 75 of file [pbeparm.h](#).

7.12.3 Typedef Documentation

7.12.3.1 PBEparm

```
typedef struct sPBEparm PBEparm
```

Declaration of the PBEparm class as the PBEparm structure.

Definition at line 213 of file [pbeparm.h](#).

7.12.3.2 PBEparm_calcEnergy

```
typedef enum ePBEparm_calcEnergy PBEparm_calcEnergy
```

Define ePBEparm_calcEnergy enumeration as PBEparm_calcEnergy.

Definition at line 91 of file [pbeparm.h](#).

7.12.3.3 PBEparm_calcForce

```
typedef enum ePBEparm_calcForce PBEparm_calcForce
```

Define ePBEparm_calcForce enumeration as PBEparm_calcForce.

Definition at line 107 of file [pbeparm.h](#).

7.12.4 Enumeration Type Documentation

7.12.4.1 ePBEparm_calcEnergy

enum [ePBEparm_calcEnergy](#)

Define energy calculation enumeration.

Enumerator

PCE_NO	Do not perform energy calculation
PCE_TOTAL	Calculate total energy only
PCE_COMPS	Calculate per-atom energy components

Definition at line 81 of file [pbeparm.h](#).

7.12.4.2 ePBEparm_calcForce

enum [ePBEparm_calcForce](#)

Define force calculation enumeration.

Enumerator

PCF_NO	Do not perform force calculation
PCF_TOTAL	Calculate total force only
PCF_COMPS	Calculate per-atom force components

Definition at line 97 of file [pbeparm.h](#).

7.12.5 Function Documentation

7.12.5.1 PBEparm_check()

```
VEXTERNC int PBEparm_check (  
    PBEparm * thee )
```

Consistency check for parameter values stored in object.

Author

Nathan Baker

Returns

1 if OK, 0 otherwise

Parameters

<i>thee</i>	Object to be checked
-------------	----------------------

Definition at line 183 of file [pbeparm.c](#).

7.12.5.2 PBEparm_copy()

```
VEXTERNC void PBEparm_copy (
    PBEparm * thee,
    PBEparm * parm )
```

Copy PBEparm object into thee.

Author

Nathan Baker

Parameters

<i>thee</i>	Target for copy
<i>parm</i>	Source for copy

Definition at line 283 of file [pbeparm.c](#).

7.12.5.3 PBEparm_ctor()

```
VEXTERNC PBEparm * PBEparm_ctor ( )
```

Construct PBEparm object.

Author

Nathan Baker

Returns

Newly allocated and initialized PBEparm object

Definition at line 104 of file [pbeparm.c](#).

7.12.5.4 PBEparm_ctor2()

```
VEXTERNC int PBEparm_ctor2 (
    PBEparm * thee )
```

FORTTRAN stub to construct PBEparm object.

Author

Nathan Baker

Returns

1 if succesful, 0 otherwise

Parameters

<i>thee</i>	Memory location for object
-------------	----------------------------

Definition at line 115 of file [pbeparm.c](#).

7.12.5.5 PBEparm_dtor()

```
VEXTERNC void PBEparm_dtor (  
    PBEparm ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object
-------------	--------------------------------------

Definition at line 173 of file [pbeparm.c](#).

7.12.5.6 PBEparm_dtor2()

```
VEXTERNC void PBEparm_dtor2 (  
    PBEparm * thee )
```

FORTTRAN stub for object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object to be destroyed
-------------	-----------------------------------

Definition at line 181 of file [pbeparm.c](#).

7.12.5.7 PBEparm_getIonCharge()

```
VEXTERNC double PBEparm_getIonCharge (  
    PBEparm * thee,  
    int iion )
```

Get charge (e) of specified ion species.

Author

Nathan Baker

Returns

Charge of ion species (e)

Parameters

<i>thee</i>	PBEparm object
<i>iion</i>	Ion species ID/index

Definition at line 65 of file [pbeparm.c](#).

7.12.5.8 PBEparm_getIonConc()

```
VEXTERNC double PBEparm_getIonConc (
    PBEparm * thee,
    int iion )
```

Get concentration (M) of specified ion species.

Author

Nathan Baker

Returns

Concentration of ion species (M)

Parameters

<i>thee</i>	PBEparm object
<i>iion</i>	Ion species ID/index

Definition at line 71 of file [pbeparm.c](#).

7.12.5.9 PBEparm_getIonRadius()

```
VEXTERNC double PBEparm_getIonRadius (
    PBEparm * thee,
    int iion )
```

Get radius (A) of specified ion species.

Author

Nathan Baker

Returns

Radius of ion species (A)

Parameters

<i>thee</i>	PBEparm object
<i>iion</i>	Ion species ID/index

Definition at line 77 of file [pbeparm.c](#).

7.12.5.10 PBEparm_parseToken()

```
VEXTERNC int PBEparm_parseToken (
    PBEparm * thee,
    char tok[VMAX_BUFSIZE],
```



```
Vio * sock )
```

Parse a keyword from an input file.

Author

Nathan Baker

Returns

1 if matched and assigned; -1 if matched, but there's some sort of error (i.e., too few args); 0 if not matched

Parameters

<i>thee</i>	Parsing object
<i>tok</i>	Token to parse
<i>sock</i>	Socket for additional tokens

Definition at line 1215 of file [pbeparm.c](#).

7.13 PBSAMparm class

Parameter which holds useful parameters for Poisson-boltzmann analytical method calculations.

Files

- file [pbsamparm.c](#)
Class PBSAMparm methods.
- file [pbsamparm.h](#)
Contains declarations for class PBSAMparm.

Data Structures

- struct [sPBSAMparm](#)
Parameter structure for PBSAM-specific variables from input files.

Macros

- #define [CHR_MAXLEN](#) 1000
Number of things that can be written out in a single calculation.

Typedefs

- typedef enum [ePBSAMparm_CalcType](#) [PBSAMparm_CalcType](#)
Declare PBSAMparm_CalcType type.
- typedef struct [sPBSAMparm](#) [PBSAMparm](#)
Parameter structure for PBSAM-specific variables from input files.

Enumerations

- enum [ePBSAMparm_CalcType](#) { [PBSAMCT_AUTO](#) =1 }
Calculation type.

Functions

- VEXTERNC [PBSAMparm](#) * [PBSAMparm_ctor](#) ([PBSAMparm_CalcType](#) type)
Construct PBSAMparm object.
- VEXTERNC Vrc_Codes [PBSAMparm_ctor2](#) ([PBSAMparm](#) *thee, [PBSAMparm_CalcType](#) type)
FORTTRAN stub to construct PBSAMparm object ?????????!!!!!!!
- VEXTERNC void [PBSAMparm_dtor](#) ([PBSAMparm](#) **thee)
Object destructor.
- VEXTERNC void [PBSAMparm_dtor2](#) ([PBSAMparm](#) *thee)
FORTTRAN stub for object destructor ?????????!!!!!!!
- VEXTERNC Vrc_Codes [PBSAMparm_check](#) ([PBSAMparm](#) *thee)
Consistency check for parameter values stored in object.
- VEXTERNC Vrc_Codes [PBSAMparm_parseToken](#) ([PBSAMparm](#) *thee, char tok[VMAX_BUFSIZE], Vio *sock)
Parse an MG keyword from an input file.
- VEXTERNC void [PBSAMparm_copy](#) ([PBSAMparm](#) *thee, [PBSAMparm](#) *parm)
copy PBSAMparm object into thee.
- VPRIVATE Vrc_Codes [PBSAMparm_parseTolsp](#) ([PBSAMparm](#) *thee, Vio *sock)
Find sphere tolerance for coarse-graining.
- VPRIVATE Vrc_Codes [PBSAMparm_parseSurf](#) ([PBSAMparm](#) *thee, Vio *sock)
Find vertex files for each molecule and save them.
- VPRIVATE Vrc_Codes [PBSAMparm_parselmat](#) ([PBSAMparm](#) *thee, Vio *sock)
Find IMAT files for each molecule and save them.
- VPRIVATE Vrc_Codes [PBSAMparm_parseExp](#) ([PBSAMparm](#) *thee, Vio *sock)
Find expansion files for each molecule and save them.
- VPRIVATE Vrc_Codes [PBSAMparm_parseMSMS](#) ([PBSAMparm](#) *thee, Vio *sock)
Find msms flag for if MSMS is to be run.

7.13.1 Detailed Description

Parameter which holds useful parameters for Poisson-boltzmann analytical method calculations.

7.13.2 Macro Definition Documentation

7.13.2.1 CHR_MAXLEN

```
#define CHR_MAXLEN 1000
```

Number of things that can be written out in a single calculation.

Definition at line 76 of file [pbsamparm.h](#).

7.13.3 Typedef Documentation

7.13.3.1 PBSAMparm

```
typedef struct sPBSAMparm PBSAMparm
```

Parameter structure for PBSAM-specific variables from input files.

Author

Lisa Felberg

Note

If you add/delete/change something in this class, the member functions – especially PBSAMparm_copy – must be modified accordingly

7.13.3.2 PBSAMparm_CalcType

```
typedef enum ePBSAMparm_CalcType PBSAMparm_CalcType
```

Declare PBSAMparm_CalcType type.

Definition at line 95 of file [pbsamparm.h](#).

7.13.4 Enumeration Type Documentation

7.13.4.1 ePBSAMparm_CalcType

```
enum ePBSAMparm_CalcType
```

Calculation type.

Enumerator

PBSAMCT_AUTO	PBSAM-auto
--------------	------------

Definition at line 84 of file [pbsamparm.h](#).

7.13.5 Function Documentation

7.13.5.1 PBSAMparm_check()

```
VEXTERNC Vrc_Codes PBSAMparm_check (
    PBSAMparm * thee )
```

Consistency check for parameter values stored in object.

Author

Lisa Felberg

Parameters

<i>thee</i>	PBSAMparm object
-------------	------------------

Returns

Success enumeration

Definition at line 110 of file [pbsamparm.c](#).

7.13.5.2 PBSAMparm_copy()

```
VEXTERNC void PBSAMparm_copy (
    PBSAMparm * thee,
    PBSAMparm * parm )
```

copy PBSAMparm object into thee.

Author**Parameters**

<i>thee</i>	PBSAMparm object to be copied into
<i>parm</i>	PBSAMparm object.

Definition at line 135 of file [pbsamparm.c](#).

7.13.5.3 PBSAMparm_ctor()

```
VEXTERNC PBSAMparm * PBSAMparm_ctor (
    PBSAMparm_CalcType type )
```

Construct PBSAMparm object.

Author

Lisa Felberg

Parameters

<i>type</i>	Type of PBSAM calculation
-------------	---------------------------

Returns

Newly allocated and initialized PBSAMparm object

Definition at line 66 of file [pbsamparm.c](#).

7.13.5.4 PBSAMparm_ctor2()

```
VEXTERNC Vrc_Codes PBSAMparm_ctor2 (
    PBSAMparm * thee,
    PBSAMparm_CalcType type )
```

FORTTRAN stub to construct PBSAMparm object ?????????!!!!!!

Author

Lisa Felberg

Parameters

<i>thee</i>	Space for PBSAMparm object
<i>type</i>	Type of MG calculation

Returns

Success enumeration

Definition at line 77 of file [pbsamparm.c](#).

7.13.5.5 PBSAMparm_dtor()

```
VEXTERNC void PBSAMparm_dtor (  
    PBSAMparm ** thee )
```

Object destructor.

Author

Lisa Felberg

Parameters

<i>thee</i>	Pointer to memory location of PBSAMparm object
-------------	--

Definition at line 100 of file [pbsamparm.c](#).

7.13.5.6 PBSAMparm_dtor2()

```
VEXTERNC void PBSAMparm_dtor2 (  
    PBSAMparm * thee )
```

FORTTRAN stub for object destructor ??????????!!!!!!!!!!!!

Author

Lisa Felberg

Parameters

<i>thee</i>	Pointer to PBSAMparm object
-------------	-----------------------------

Definition at line 108 of file [pbsamparm.c](#).

7.13.5.7 PBSAMparm_parseExp()

```
VPRIVATE Vrc_Codes PBSAMparm_parseExp (  
    PBSAMparm * thee,
```

```
Vio * sock )
```

Find expansion files for each molecule and save them.

Author

Parameters

<i>thee</i>	PBSAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 218 of file [pbsamparm.c](#).

7.13.5.8 PBSAMparm_parselmat()

```
VPRIVATE Vrc_Codes PBSAMparm_parseImat (  
    PBSAMparm * thee,  
    Vio * sock )
```

Find IMAT files for each molecule and save them.

Author

Parameters

<i>thee</i>	PBSAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 203 of file [pbsamparm.c](#).

7.13.5.9 PBSAMparm_parseMSMS()

```
VPRIVATE Vrc_Codes PBSAMparm_parseMSMS (  
    PBSAMparm * thee,  
    Vio * sock )
```

Find msms flag for if MSMS is to be run.

Author

Parameters

<i>thee</i>	PBSAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 182 of file [pbsamparm.c](#).

7.13.5.10 PBSAMparm_parseSurf()

```
VPRIVATE Vrc_Codes PBSAMparm_parseSurf (
    PBSAMparm * thee,
    Vio * sock )
```

Find vertex files for each molecule and save them.

Author

Parameters

<i>thee</i>	PBSAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 166 of file [pbsamparm.c](#).

7.13.5.11 PBSAMparm_parseToken()

```
VEXTERNC Vrc_Codes PBSAMparm_parseToken (
    PBSAMparm * thee,
    char tok[VMAX_BUFSIZE],
    Vio * sock )
```

Parse an MG keyword from an input file.

Author

Lisa Felberg

Parameters

<i>thee</i>	PBSAMparm object
<i>tok</i>	Token to parse
<i>sock</i>	Stream for more tokens

Returns

Success enumeration (1 if matched and assigned; -1 if matched, but there's some sort of error (i.e., too few args); 0 if not matched)

Definition at line 252 of file [pbsamparm.c](#).

7.13.5.12 PBSAMparm_parseTolsp()

```
VPRIVATE Vrc_Codes PBSAMparm_parseTolsp (
    PBSAMparm * thee,
    Vio * sock )
```

Find sphere tolerance for coarse-graining.

Author

Parameters

<i>thee</i>	PBSAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 232 of file [pbsamparm.c](#).

7.14 Vacc class

Solvent- and ion-accessibility oracle.

Files

- file [vacc.c](#)
Class Vacc methods.
- file [vacc.h](#)
Contains declarations for class Vacc.

Data Structures

- struct [sVaccSurf](#)
Surface object list of per-atom surface points.
- struct [sVacc](#)
Oracle for solvent- and ion-accessibility around a biomolecule.

Typedefs

- typedef struct [sVaccSurf](#) [VaccSurf](#)
Declaration of the VaccSurf class as the VaccSurf structure.
- typedef struct [sVacc](#) [Vacc](#)
Declaration of the Vacc class as the Vacc structure.

Functions

- VEXTERNC unsigned long int [Vacc_memChk](#) ([Vacc](#) *thee)
Get number of bytes in this object and its members.
- VEXTERNC [VaccSurf](#) * [VaccSurf_ctor](#) (Vmem *mem, double probe_radius, int nsphere)
Allocate and construct the surface object; do not assign surface points to positions.
- VEXTERNC int [VaccSurf_ctor2](#) ([VaccSurf](#) *thee, Vmem *mem, double probe_radius, int nsphere)
Construct the surface object using previously allocated memory; do not assign surface points to positions.
- VEXTERNC void [VaccSurf_dtor](#) ([VaccSurf](#) **thee)
Destroy the surface object and free its memory.
- VEXTERNC void [VaccSurf_dtor2](#) ([VaccSurf](#) *thee)
Destroy the surface object.
- VEXTERNC [VaccSurf](#) * [VaccSurf_refSphere](#) (Vmem *mem, int npts)
Set up an array of points for a reference sphere of unit radius.
- VEXTERNC [VaccSurf](#) * [Vacc_atomSurf](#) ([Vacc](#) *thee, [Vatom](#) *atom, [VaccSurf](#) *ref, double probe_radius)
Set up an array of points corresponding to the SAS due to a particular atom.
- VEXTERNC [Vacc](#) * [Vacc_ctor](#) ([Valist](#) *alist, [Vclist](#) *clist, double surf_density)

- Construct the accessibility object.*

 - VEXTERNC int `Vacc_ctor2` (`Vacc *thee`, `Valist *alist`, `Vclist *clist`, double `surf_density`)

FORTTRAN stub to construct the accessibility object.
- VEXTERNC void `Vacc_dtor` (`Vacc **thee`)

Destroy object.

 - VEXTERNC void `Vacc_dtor2` (`Vacc *thee`)

FORTTRAN stub to destroy object.
- VEXTERNC double `Vacc_vdwAcc` (`Vacc *thee`, double `center[VAPBS_DIM]`)

Report van der Waals accessibility.
- VEXTERNC double `Vacc_ivdwAcc` (`Vacc *thee`, double `center[VAPBS_DIM]`, double `radius`)

Report inflated van der Waals accessibility.
- VEXTERNC double `Vacc_molAcc` (`Vacc *thee`, double `center[VAPBS_DIM]`, double `radius`)

Report molecular accessibility.
- VEXTERNC double `Vacc_fastMolAcc` (`Vacc *thee`, double `center[VAPBS_DIM]`, double `radius`)

Report molecular accessibility quickly.
- VEXTERNC double `Vacc_splineAcc` (`Vacc *thee`, double `center[VAPBS_DIM]`, double `win`, double `infrad`)

Report spline-based accessibility.
- VEXTERNC void `Vacc_splineAccGrad` (`Vacc *thee`, double `center[VAPBS_DIM]`, double `win`, double `infrad`, double `*grad`)

Report gradient of spline-based accessibility.
- VEXTERNC double `Vacc_splineAccAtom` (`Vacc *thee`, double `center[VAPBS_DIM]`, double `win`, double `infrad`, `Vatom *atom`)

Report spline-based accessibility for a given atom.
- VEXTERNC void `Vacc_splineAccGradAtomUnnorm` (`Vacc *thee`, double `center[VAPBS_DIM]`, double `win`, double `infrad`, `Vatom *atom`, double `*force`)

Report gradient of spline-based accessibility with respect to a particular atom (see `Vpmg_splineAccAtom`)
- VEXTERNC void `Vacc_splineAccGradAtomNorm` (`Vacc *thee`, double `center[VAPBS_DIM]`, double `win`, double `infrad`, `Vatom *atom`, double `*force`)

Report gradient of spline-based accessibility with respect to a particular atom normalized by the accessibility value due to that atom at that point (see `Vpmg_splineAccAtom`)
- VEXTERNC void `Vacc_splineAccGradAtomNorm4` (`Vacc *thee`, double `center[VAPBS_DIM]`, double `win`, double `infrad`, `Vatom *atom`, double `*force`)

Report gradient of spline-based accessibility with respect to a particular atom normalized by a 4th order accessibility value due to that atom at that point (see `Vpmg_splineAccAtom`)
- VEXTERNC void `Vacc_splineAccGradAtomNorm3` (`Vacc *thee`, double `center[VAPBS_DIM]`, double `win`, double `infrad`, `Vatom *atom`, double `*force`)

Report gradient of spline-based accessibility with respect to a particular atom normalized by a 3rd order accessibility value due to that atom at that point (see `Vpmg_splineAccAtom`)
- VEXTERNC double `Vacc_SASA` (`Vacc *thee`, double `radius`)

Build the solvent accessible surface (SAS) and calculate the solvent accessible surface area.
- VEXTERNC double `Vacc_totalSASA` (`Vacc *thee`, double `radius`)

Return the total solvent accessible surface area (SASA)
- VEXTERNC double `Vacc_atomSASA` (`Vacc *thee`, double `radius`, `Vatom *atom`)

Return the atomic solvent accessible surface area (SASA)
- VEXTERNC `VaccSurf *` `Vacc_atomSASPoints` (`Vacc *thee`, double `radius`, `Vatom *atom`)

Get the set of points for this atom's solvent-accessible surface.
- VEXTERNC void `Vacc_atomdSAV` (`Vacc *thee`, double `radius`, `Vatom *atom`, double `*dSA`)

Get the derivative of solvent accessible volume.

- VEXTERN void `Vacc_atomdSASA` (`Vacc` *thee, double dpos, double radius, `Vatom` *atom, double *dSA)
Get the derivatve of solvent accessible area.
- VEXTERN void `Vacc_totalAtomdSASA` (`Vacc` *thee, double dpos, double radius, `Vatom` *atom, double *dSA)
Testing purposes only.
- VEXTERN void `Vacc_totalAtomdSAV` (`Vacc` *thee, double dpos, double radius, `Vatom` *atom, double *dSA, `Vclist` *clist)
Total solvent accessible volume.
- VEXTERN double `Vacc_totalSAV` (`Vacc` *thee, `Vclist` *clist, `APOLparm` *apolparm, double radius)
Return the total solvent accessible volume (SAV)
- VEXTERN int `Vacc_wcaEnergy` (`Vacc` *thee, `APOLparm` *apolparm, `Valist` *alist, `Vclist` *clist)
Return the WCA integral energy.
- VEXTERN int `Vacc_wcaForceAtom` (`Vacc` *thee, `APOLparm` *apolparm, `Vclist` *clist, `Vatom` *atom, double *force)
Return the WCA integral force.
- VEXTERN int `Vacc_wcaEnergyAtom` (`Vacc` *thee, `APOLparm` *apolparm, `Valist` *alist, `Vclist` *clist, int iatom, double *value)
Calculate the WCA energy for an atom.

7.14.1 Detailed Description

Solvent- and ion-accessibility oracle.

7.14.2 Typedef Documentation

7.14.2.1 Vacc

```
typedef struct sVacc Vacc
```

Declaration of the Vacc class as the Vacc structure.

Definition at line 131 of file `vacc.h`.

7.14.2.2 VaccSurf

```
typedef struct sVaccSurf VaccSurf
```

Declaration of the VaccSurf class as the VaccSurf structure.

Definition at line 101 of file `vacc.h`.

7.14.3 Function Documentation

7.14.3.1 Vacc_atomdSASA()

```
VEXTERN void Vacc_atomdSASA (
    Vacc * thee,
    double dpos,
    double radius,
    Vatom * atom,
    double * dSA )
```

Get the derivatve of solvent accessible area.

Author

Jason Wagoner, David Gohara, Nathan Baker

Parameters

<i>thee</i>	Acessibility object
<i>dpos</i>	Atom position offset
<i>radius</i>	Probe radius (Å)
<i>atom</i>	Atom of interest
<i>dSA</i>	Array holding answers of calc

Definition at line 1320 of file [vacc.c](#).

7.14.3.2 Vacc_atomdSAV()

```
VEXTERNC void Vacc_atomdSAV (  
    Vacc * thee,  
    double radius,  
    Vatom * atom,  
    double * dSA )
```

Get the derivative of solvent accessible volume.

Author

Jason Wagoner, Nathan Baker

Parameters

<i>thee</i>	Acessibility object
<i>radius</i>	Probe radius (Å)
<i>atom</i>	Atom of interest
<i>dSA</i>	Array holding answers of calc

Definition at line 1200 of file [vacc.c](#).

7.14.3.3 Vacc_atomSASA()

```
VEXTERNC double Vacc_atomSASA (  
    Vacc * thee,  
    double radius,  
    Vatom * atom )
```

Return the atomic solvent accessible surface area (SASA)

Note

Alias for Vacc_SASA

Author

Nathan Baker

Returns

Atomic solvent accessible area (\AA^2)

Parameters

<i>thee</i>	Accessibility object
<i>radius</i>	Probe molecule radius (\AA)
<i>atom</i>	Atom of interest

Definition at line 780 of file [vacc.c](#).

7.14.3.4 Vacc_atomSASPoints()

```
VEXTERNC VaccSurf * Vacc_atomSASPoints (
    Vacc * thee,
    double radius,
    Vatom * atom )
```

Get the set of points for this atom's solvent-accessible surface.

Author

Nathan Baker

Returns

Pointer to VaccSurf object for this atom

Parameters

<i>thee</i>	Accessibility object
<i>radius</i>	Probe molecule radius (\AA)
<i>atom</i>	Atom of interest

Definition at line 982 of file [vacc.c](#).

7.14.3.5 Vacc_atomSurf()

```
VEXTERNC VaccSurf * Vacc_atomSurf (
    Vacc * thee,
    Vatom * atom,
    VaccSurf * ref,
    double probe_radius )
```

Set up an array of points corresponding to the SAS due to a particular atom.

Author

Nathan Baker

Returns

Atom sphere surface object

Parameters

<i>thee</i>	Accessibility object for molecule
<i>atom</i>	Atom for which the surface should be constructed
<i>ref</i>	Reference sphere which sets the resolution for the surface.

See also

[VaccSurf_refSphere](#)

Parameters

<i>probe_radius</i>	Probe radius (in Å)
---------------------	---------------------

Definition at line 868 of file [vacc.c](#).

7.14.3.6 Vacc_ctor()

```
VEXTERNC Vacc * Vacc_ctor (
    Valist * alist,
    Vclist * clist,
    double surf_density )
```

Construct the accessibility object.

Author

Nathan Baker

Returns

Newly allocated Vacc object

Parameters

<i>alist</i>	Molecule for accessibility queries
<i>clist</i>	Pre-constructed cell list for looking up atoms near specific positions
<i>surf_density</i>	Minimum per-atom solvent accessible surface point density (in pts/Å ²)

Definition at line 132 of file [vacc.c](#).

7.14.3.7 Vacc_ctor2()

```
VEXTERNC int Vacc_ctor2 (
    Vacc * thee,
    Valist * alist,
    Vclist * clist,
    double surf_density )
```

FORTTRAN stub to construct the accessibility object.

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	Memory for Vacc objet
<i>alist</i>	Molecule for accessibility queries
<i>clist</i>	Pre-constructed cell list for looking up atoms near specific positions
<i>surf_density</i>	Minimum per-atom solvent accessible surface point density (in pts/A ²)

Definition at line 213 of file [vacc.c](#).**7.14.3.8 Vacc_dtor()**

```
VEXTERNC void Vacc_dtor (
    Vacc ** thee )
```

Destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object
-------------	--------------------------------------

Definition at line 245 of file [vacc.c](#).**7.14.3.9 Vacc_dtor2()**

```
VEXTERNC void Vacc_dtor2 (
    Vacc * thee )
```

FORTRAN stub to destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object
-------------	-------------------

Definition at line 255 of file [vacc.c](#).

7.14.3.10 Vacc_fastMolAcc()

```
VEXTERNC double Vacc_fastMolAcc (  
    Vacc * thee,  
    double center[VAPBS_DIM],  
    double radius )
```

Report molecular accessibility quickly.

Given a point which is INSIDE the collection of inflated van der Waals spheres, but OUTSIDE the collection of non-inflated van der Waals spheres, determine accessibility of a probe (of radius radius) at a given point, given a collection of atomic spheres. Uses molecular (Connolly) surface definition.

Note

THIS ASSUMES YOU HAVE TESTED THAT THIS POINT IS DEFINITELY INSIDE THE INFLATED AND NON-
INFLATED VAN DER WAALS SURFACES!

Author

Nathan Baker

Returns

Characteristic function value between 1.0 (accessible) and 0.0 (inaccessible)

Bug This routine has a slight bug which can generate very small internal regions of high dielectric (thanks to John Mongan and Jess Swanson for finding this)

Parameters

<i>thee</i>	Accessibility object
<i>center</i>	Probe center coordinates
<i>radius</i>	Probe radius (in Å)

Definition at line 637 of file [vacc.c](#).

7.14.3.11 Vacc_ivdwAcc()

```
VEXTERNC double Vacc_ivdwAcc (  
    Vacc * thee,  
    double center[VAPBS_DIM],  
    double radius )
```

Report inflated van der Waals accessibility.

Determines if a point is within the union of the spheres centered at the atomic centers with radii equal to the sum of the atomic van der Waals radius and the probe radius.

Author

Nathan Baker

Returns

Characteristic function value between 1.0 (accessible) and 0.0 (inaccessible)

Parameters

<i>thee</i>	Accessibility object
<i>center</i>	Probe center coordinates
<i>radius</i>	Probe radius (Å)

7.14.3.12 Vacc_memChk()

```
VEXTERNC unsigned long int Vacc_memChk (  
    Vacc * thee )
```

Get number of bytes in this object and its members.

Author

Nathan Baker

Returns

Number of bytes allocated for object

Parameters

<i>thee</i>	Object for memory check
-------------	-------------------------

Definition at line 63 of file [vacc.c](#).

7.14.3.13 Vacc_molAcc()

```
VEXTERNC double Vacc_molAcc (  
    Vacc * thee,  
    double center[VAPBS_DIM],  
    double radius )
```

Report molecular accessibility.

Determine accessibility of a probe (of radius radius) at a given point, given a collection of atomic spheres. Uses molecular (Connolly) surface definition.

Author

Nathan Baker

Returns

Characteristic function value between 1.0 (accessible) and 0.0 (inaccessible)

Bug This routine has a slight bug which can generate very small internal regions of high dielectric (thanks to John Mongan and Jess Swanson for finding this)

Parameters

<i>thee</i>	Accessibility object
<i>center</i>	Probe center coordinates
<i>radius</i>	Probe radius (in Å)

Definition at line 608 of file [vacc.c](#).

7.14.3.14 Vacc_SASA()

```
VEXTERNC double Vacc_SASA (
    Vacc * thee,
    double radius )
```

Build the solvent accessible surface (SAS) and calculate the solvent accessible surface area.

Note

Similar to UHBD FORTRAN routine by Brock Luty (returns UHBD's asas2)

Author

Nathan Baker (original FORTRAN routine by Brock Luty)

Returns

Total solvent accessible area (\AA^2)

Parameters

<i>thee</i>	Accessibility object
<i>radius</i>	Probe molecule radius (\AA)

Definition at line 713 of file [vacc.c](#).

7.14.3.15 Vacc_splineAcc()

```
VEXTERNC double Vacc_splineAcc (
    Vacc * thee,
    double center[VAPBS_DIM],
    double win,
    double infrad )
```

Report spline-based accessibility.

Determine accessibility at a given point, given a collection of atomic spheres. Uses Benoit Roux (Im et al, Comp Phys Comm, 111, 59–75, 1998) definition suitable for force evalation; basically a cubic spline.

Author

Nathan Baker

Returns

Characteristic function value between 1.0 (accessible) and 0.0 (inaccessible)

Parameters

<i>thee</i>	Accessibility object
<i>center</i>	Probe center coordinates
<i>win</i>	Spline window (\AA)
<i>infrad</i>	Inflation radius (\AA) for ion access.

Definition at line 528 of file [vacc.c](#).

7.14.3.16 Vacc_splineAccAtom()

```
VEXTERNC double Vacc_splineAccAtom (
    Vacc * thee,
    double center[VAPBS_DIM],
    double win,
    double infrad,
    Vatom * atom )
```

Report spline-based accessibility for a given atom.

Determine accessibility at a given point for a given atomic spheres. Uses Benoit Roux (Im et al, Comp Phys Comm, 111, 59–75, 1998) definition suitable for force evalation; basically a cubic spline.

Author

Nathan Baker

Returns

Characteristic function value between 1.0 (accessible) and 0.0 (inaccessible)

Parameters

<i>thee</i>	Accessibility object
<i>center</i>	Probe center coordinates
<i>win</i>	Spline window (Å)
<i>infrad</i>	Inflation radius (Å) for ion access.
<i>atom</i>	Atom

Definition at line 438 of file [vacc.c](#).

7.14.3.17 Vacc_splineAccGrad()

```
VEXTERNC void Vacc_splineAccGrad (
    Vacc * thee,
    double center[VAPBS_DIM],
    double win,
    double infrad,
    double * grad )
```

Report gradient of spline-based accessibility.

Author

Nathan Baker

Parameters

<i>thee</i>	Accessibility object
<i>center</i>	Probe center coordinates
<i>win</i>	Spline window (Å)

Parameters

<i>infrad</i>	Inflation radius (Å) for ion access.
<i>grad</i>	3-vector set to gradient of accessibility

Definition at line 561 of file [vacc.c](#).

7.14.3.18 Vacc_splineAccGradAtomNorm()

```
VEXTERNC void Vacc_splineAccGradAtomNorm (
    Vacc * thee,
    double center[VAPBS_DIM],
    double win,
    double infrad,
    Vatom * atom,
    double * force )
```

Report gradient of spline-based accessibility with respect to a particular atom normalized by the accessibility value due to that atom at that point (see [Vpmg_splineAccAtom](#))

Determine accessibility at a given point, given a collection of atomic spheres. Uses Benoit Roux (Im et al, Comp Phys Comm, 111, 59–75, 1998) definition suitable for force evaluation; basically a cubic spline.

Author

Nathan Baker

Parameters

<i>thee</i>	Accessibility object
<i>center</i>	Probe center coordinates
<i>win</i>	Spline window (Å)
<i>infrad</i>	Inflation radius (Å) for ion access.
<i>atom</i>	Atom
<i>force</i>	VAPBS_DIM-vector set to gradient of accessibility

Definition at line 316 of file [vacc.c](#).

7.14.3.19 Vacc_splineAccGradAtomNorm3()

```
VEXTERNC void Vacc_splineAccGradAtomNorm3 (
    Vacc * thee,
    double center[VAPBS_DIM],
    double win,
    double infrad,
    Vatom * atom,
    double * force )
```

Report gradient of spline-based accessibility with respect to a particular atom normalized by a 3rd order accessibility value due to that atom at that point (see [Vpmg_splineAccAtom](#))

Author

Michael Schnieders

Parameters

<i>thee</i>	Accessibility object
<i>center</i>	Probe center coordinates
<i>win</i>	Spline window (Å)
<i>infrad</i>	Inflation radius (Å) for ion access.
<i>atom</i>	Atom
<i>force</i>	VAPBS_DIM-vector set to gradient of accessibility

Definition at line 1099 of file [vacc.c](#).

7.14.3.20 Vacc_splineAccGradAtomNorm4()

```

VEXTERNC void Vacc_splineAccGradAtomNorm4 (
    Vacc * thee,
    double center[VAPBS_DIM],
    double win,
    double infrad,
    Vatom * atom,
    double * force )

```

Report gradient of spline-based accessibility with respect to a particular atom normalized by a 4th order accessibility value due to that atom at that point (see [Vpmg_splineAccAtom](#))

Author

Michael Schnieders

Parameters

<i>thee</i>	Accessibility object
<i>center</i>	Probe center coordinates
<i>win</i>	Spline window (Å)
<i>infrad</i>	Inflation radius (Å) for ion access.
<i>atom</i>	Atom
<i>force</i>	VAPBS_DIM-vector set to gradient of accessibility

Definition at line 1006 of file [vacc.c](#).

7.14.3.21 Vacc_splineAccGradAtomUnnorm()

```

VEXTERNC void Vacc_splineAccGradAtomUnnorm (
    Vacc * thee,
    double center[VAPBS_DIM],
    double win,
    double infrad,
    Vatom * atom,
    double * force )

```

Report gradient of spline-based accessibility with respect to a particular atom (see [Vpmg_splineAccAtom](#))

Determine accessibility at a given point, given a collection of atomic spheres. Uses Benoit Roux (Im et al, Comp Phys Comm, 111, 59–75, 1998) definition suitable for force evaluation; basically a cubic spline.

Author

Nathan Baker

Parameters

<i>thee</i>	Accessibility object
<i>center</i>	Probe center coordinates
<i>win</i>	Spline window (Å)
<i>infrad</i>	Inflation radius (Å) for ion access.
<i>atom</i>	Atom
<i>force</i>	VAPBS_DIM-vector set to gradient of accessibility

Definition at line 377 of file [vacc.c](#).**7.14.3.22 Vacc_totalAtomdSASA()**

```
VEEXTERNC void Vacc_totalAtomdSASA (
    Vacc * thee,
    double dpos,
    double radius,
    Vatom * atom,
    double * dSA )
```

Testing purposes only.

Author

David Gohara, Nathan Baker

Parameters

<i>thee</i>	Accessibility object
<i>dpos</i>	Atom position offset
<i>radius</i>	Probe radius (Å)
<i>atom</i>	Atom of interest
<i>dSA</i>	Array holding answers of calc

Definition at line 1389 of file [vacc.c](#).**7.14.3.23 Vacc_totalAtomdSAV()**

```
VEEXTERNC void Vacc_totalAtomdSAV (
    Vacc * thee,
    double dpos,
    double radius,
    Vatom * atom,
    double * dSA,
    Vclist * clist )
```

Total solvent accessible volume.

Author

David Gohara, Nathan Baker

Parameters

<i>thee</i>	Acessibility object
<i>dpos</i>	Atom position offset
<i>radius</i>	Probe radius (Å)
<i>atom</i>	Atom of interest
<i>dSA</i>	Array holding answers of calc
<i>clist</i>	clist for this calculation

Definition at line 1448 of file [vacc.c](#).

7.14.3.24 Vacc_totalSASA()

```
VEXTERNC double Vacc_totalSASA (  
    Vacc * thee,  
    double radius )
```

Return the total solvent accessible surface area (SASA)

Note

Alias for Vacc_SASA

Author

Nathan Baker

Returns

Total solvent accessible area (Å²)

Parameters

<i>thee</i>	Accessibility object
<i>radius</i>	Probe molecule radius (Å)

Definition at line 774 of file [vacc.c](#).

7.14.3.25 Vacc_totalSAV()

```
VEXTERNC double Vacc_totalSAV (  
    Vacc * thee,  
    Vclist * clist,  
    APOLparm * apolparm,  
    double radius )
```

Return the total solvent accessible volume (SAV)

Note

Alias for Vacc_SAV

Author

David Gohara

Returns

Total solvent accessible volume (\AA^3)

Parameters

<i>thee</i>	Accessibility object
<i>clist</i>	Clist for acc object
<i>apolparm</i>	Apolar parameters – could be VNULL if none required for this calculation. If VNULL, then default settings are used
<i>radius</i>	Probe molecule radius (\AA)

Definition at line 1503 of file [vacc.c](#).

7.14.3.26 Vacc_vdwAcc()

```
VEXTERNC double Vacc_vdwAcc (
    Vacc * thee,
    double center[VAPBS_DIM] )
```

Report van der Waals accessibility.

Determines if a point is within the union of the atomic spheres (with radii equal to their van der Waals radii).

Author

Nathan Baker

Returns

Characteristic function value between 1.0 (accessible) and 0.0 (inaccessible)

Parameters

<i>thee</i>	Accessibility object
<i>center</i>	Probe center coordinates

7.14.3.27 Vacc_wcaEnergy()

```
VEXTERNC int Vacc_wcaEnergy (
    Vacc * thee,
    APOLparm * apolparm,
    Valist * alist,
    Vclist * clist )
```

Return the WCA integral energy.

Author

David Gohara

Returns

Success flag

Parameters

<i>thee</i>	Accessibility object
<i>apolparm</i>	Apolar calculation parameters
<i>alist</i>	Alist for acc object
<i>clist</i>	Clist for acc object

Definition at line 1721 of file [vacc.c](#).**7.14.3.28 Vacc_wcaEnergyAtom()**

```
VEXTERNC int Vacc_wcaEnergyAtom (  
    Vacc * thee,  
    APOLparm * apolparm,  
    Valist * alist,  
    Vclist * clist,  
    int iatom,  
    double * value )
```

Calculate the WCA energy for an atom.

Author

Dave Gohara and Nathan Baker

Returns

Success flag

Parameters

<i>thee</i>	Accessibility object
<i>apolparm</i>	Apolar calculation parameters
<i>alist</i>	Atom list
<i>clist</i>	Cell list associated with Vacc object
<i>iatom</i>	Index for atom of interest
<i>value</i>	Set to energy value

Definition at line 1580 of file [vacc.c](#).**7.14.3.29 Vacc_wcaForceAtom()**

```
VEXTERNC int Vacc_wcaForceAtom (  
    Vacc * thee,
```



```
    APOLparm * apolparm,  
    Vclist * clist,  
    Vatom * atom,  
    double * force )
```

Return the WCA integral force.

Author

David Gohara

Returns

WCA energy (kJ/mol/A)

Parameters

<i>thee</i>	Accessibility object
<i>apolparm</i>	Apolar calculation parameters
<i>clist</i>	Clist for acc object
<i>atom</i>	Current atom
<i>force</i>	Force for atom

Definition at line 1756 of file [vacc.c](#).

7.14.3.30 VaccSurf_ctor()

```
VEXTERNC VaccSurf * VaccSurf_ctor (  
    Vmem * mem,  
    double probe_radius,  
    int nsphere )
```

Allocate and construct the surface object; do not assign surface points to positions.

Author

Nathan Baker

Returns

Newly allocated and constructed surface object

Parameters

<i>mem</i>	Memory manager (can be VNULL)
<i>probe_radius</i>	Probe radius (in A) for this surface
<i>nsphere</i>	Number of points in sphere

Definition at line 803 of file [vacc.c](#).

7.14.3.31 VaccSurf_ctor2()

```
VEXTERNC int VaccSurf_ctor2 (
```

```

    VaccSurf * thee,
    Vmem * mem,
    double probe_radius,
    int nsphere )

```

Construct the surface object using previously allocated memory; do not assign surface points to positions.

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	Allocated memory
<i>mem</i>	Memory manager (can be VNULL)
<i>probe_radius</i>	Probe radius (in A) for this surface
<i>nsphere</i>	Number of points in sphere

Definition at line 813 of file [vacc.c](#).

7.14.3.32 VaccSurf_dtor()

```

VEXTERNC void VaccSurf_dtor (
    VaccSurf ** thee )

```

Destroy the surface object and free its memory.

Author

Nathan Baker

Parameters

<i>thee</i>	Object to be destroyed
-------------	------------------------

Definition at line 839 of file [vacc.c](#).

7.14.3.33 VaccSurf_dtor2()

```

VEXTERNC void VaccSurf_dtor2 (
    VaccSurf * thee )

```

Destroy the surface object.

Author

Nathan Baker

Parameters

<i>thee</i>	Object to be destroyed
-------------	------------------------

Definition at line 853 of file [vacc.c](#).

7.14.3.34 VaccSurf_refSphere()

```

VEXTERNC VaccSurf * VaccSurf_refSphere (
    Vmem * mem,
    int npts )

```

Set up an array of points for a reference sphere of unit radius.

Generates approximately npts # of points (actual number stored in thee->npts) somewhat uniformly distributed across a sphere of unit radius centered at the origin.

Note

This routine was shamelessly ripped off from sphere.f from UHBD as developed by Michael K. Gilson.

Author

Nathan Baker (original FORTRAN code by Mike Gilson)

Returns

Reference sphere surface object

Parameters

<i>mem</i>	Memory object
<i>npts</i>	Requested number of points on sphere

Definition at line 926 of file [vacc.c](#).

7.15 Valist class

Container class for list of atom objects.

Files

- file [valist.h](#)

Contains declarations for class Valist.

Data Structures

- struct [sValist](#)

Container class for list of atom objects.

Typedefs

- typedef struct [sValist](#) Valist

Declaration of the Valist class as the Valist structure.

Functions

- VEXTERNC `Vatom * Valist_getAtomList (Valist *thee)`
Get actual array of atom objects from the list.
- VEXTERNC double `Valist_getCenterX (Valist *thee)`
Get x-coordinate of molecule center.
- VEXTERNC double `Valist_getCenterY (Valist *thee)`
Get y-coordinate of molecule center.
- VEXTERNC double `Valist_getCenterZ (Valist *thee)`
Get z-coordinate of molecule center.
- VEXTERNC int `Valist_getNumberAtoms (Valist *thee)`
Get number of atoms in the list.
- VEXTERNC `Vatom * Valist_getAtom (Valist *thee, int i)`
Get pointer to particular atom in list.
- VEXTERNC unsigned long int `Valist_memChk (Valist *thee)`
Get total memory allocated for this object and its members.
- VEXTERNC `Valist * Valist_ctor ()`
Construct the atom list object.
- VEXTERNC `Vrc_Codes Valist_ctor2 (Valist *thee)`
FORTTRAN stub to construct the atom list object.
- VEXTERNC void `Valist_dtor (Valist **thee)`
Destroys atom list object.
- VEXTERNC void `Valist_dtor2 (Valist *thee)`
FORTTRAN stub to destroy atom list object.
- VEXTERNC `Vrc_Codes Valist_readPQR (Valist *thee, Vparam *param, Vio *sock)`
Fill atom list with information from a PQR file.
- VEXTERNC `Vrc_Codes Valist_readPDB (Valist *thee, Vparam *param, Vio *sock)`
Fill atom list with information from a PDB file.
- VEXTERNC `Vrc_Codes Valist_readXML (Valist *thee, Vparam *param, Vio *sock)`
Fill atom list with information from an XML file.
- VEXTERNC `Vrc_Codes Valist_getStatistics (Valist *thee)`
Load up Valist with various statistics.

7.15.1 Detailed Description

Container class for list of atom objects.

7.15.2 Typedef Documentation

7.15.2.1 Valist

```
typedef struct sValist Valist
```

Declaration of the Valist class as the Valist structure.

Definition at line 95 of file `valist.h`.

7.15.3 Function Documentation

7.15.3.1 Valist_ctor()

```
VEXTERNC Valist * Valist_ctor ( )
```

Construct the atom list object.

Author

Nathan Baker

Returns

Pointer to newly allocated (empty) atom list

Definition at line 138 of file [valist.c](#).

7.15.3.2 Valist_ctor2()

```
VEXTERNC Vrc_Codes Valist_ctor2 (
    Valist * thee )
```

FORTTRAN stub to construct the atom list object.

Author

Nathan Baker, Yong Huang

Returns

Success enumeration

Parameters

<i>thee</i>	Storage for new atom list
-------------	---------------------------

Definition at line 155 of file [valist.c](#).

7.15.3.3 Valist_dtor()

```
VEXTERNC void Valist_dtor (
    Valist ** thee )
```

Destroys atom list object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to storage for atom list
-------------	----------------------------------

Definition at line 167 of file [valist.c](#).

7.15.3.4 Valist_dtor2()

```
EXTERNC void Valist_dtor2 (  
    Valist * thee )
```

FORTTRAN stub to destroy atom list object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to atom list object
-------------	-----------------------------

Definition at line 176 of file [valist.c](#).

7.15.3.5 Valist_getAtom()

```
EXTERNC Vatom * Valist_getAtom (  
    Valist * thee,  
    int i )
```

Get pointer to particular atom in list.

Author

Nathan Baker

Returns

Pointer to atom object i

Parameters

<i>thee</i>	Atom list object
<i>i</i>	Index of atom in list

Definition at line 115 of file [valist.c](#).

7.15.3.6 Valist_getAtomList()

```
EXTERNC Vatom * Valist_getAtomList (  
    Valist * thee )
```

Get actual array of atom objects from the list.

Author

Nathan Baker

Returns

Array of atom objects

Parameters

<i>thee</i>	Atom list object
-------------	------------------

Definition at line 95 of file [valist.c](#).

7.15.3.7 Valist_getCenterX()

```
VEXTERNC double Valist_getCenterX (  
    Valist * thee )
```

Get x-coordinate of molecule center.

Author

Nathan Baker

Returns

X-coordinate of molecule center

Parameters

<i>thee</i>	Atom list object
-------------	------------------

Definition at line 66 of file [valist.c](#).

7.15.3.8 Valist_getCenterY()

```
VEXTERNC double Valist_getCenterY (  
    Valist * thee )
```

Get y-coordinate of molecule center.

Author

Nathan Baker

Returns

Y-coordinate of molecule center

Parameters

<i>thee</i>	Atom list object
-------------	------------------

Definition at line 76 of file [valist.c](#).

7.15.3.9 Valist_getCenterZ()

```
VEXTERNC double Valist_getCenterZ (  
    Valist * thee )
```

Get z-coordinate of molecule center.

Author

Nathan Baker

Returns

Z-coordinate of molecule center

Parameters

<i>thee</i>	Atom list object
-------------	------------------

Definition at line 85 of file [valist.c](#).

7.15.3.10 Valist_getNumberAtoms()

```
VEXTERNC int Valist_getNumberAtoms (  
    Valist * thee )
```

Get number of atoms in the list.

Author

Nathan Baker

Returns

Number of atoms in list

Parameters

<i>thee</i>	Atom list object
-------------	------------------

Definition at line 105 of file [valist.c](#).

7.15.3.11 Valist_getStatistics()

```
VEXTERNC Vrc_Codes Valist_getStatistics (  
    Valist * thee )
```

Load up Valist with various statistics.

Author

Nathan Baker, Yong Huang

Returns

Success enumeration

Definition at line 869 of file [valist.c](#).

7.15.3.12 Valist_memChk()

```
VEXTERNC unsigned long int Valist_memChk (  
    Valist * thee )
```

Get total memory allocated for this object and its members.

Author

Nathan Baker

Returns

Total memory in bytes

Parameters

<i>thee</i>	Atom list object
-------------	------------------

Definition at line 129 of file [valist.c](#).

7.15.3.13 Valist_readPDB()

```
VEXTERNC Vrc_Codes Valist_readPDB (  
    Valist * thee,  
    Vparam * param,  
    Vio * sock )
```

Fill atom list with information from a PDB file.

Author

Nathan Baker, Todd Dolinsky, Yong Huang

Returns

Success enumeration

Note

We don't actually respect PDB format; instead recognize whitespace- or tab-delimited fields which allows us to deal with structures with coordinates > 999 or < -999.

Parameters

<i>thee</i>	Atom list object
<i>param</i>	A pre-initialized parameter object
<i>sock</i>	Socket read for reading PDB file

Definition at line 515 of file [valist.c](#).

7.15.3.14 Valist_readPQR()

```
VEXTERNC Vrc_Codes Valist_readPQR (  
    Valist * thee,  
    Vparam * param,  
    Vio * sock )
```

Fill atom list with information from a PQR file.

Author

Nathan Baker, Yong Huang

Returns

Success enumeration

Note

- A PQR file has PDB structure with charge and radius in the last two columns instead of weight and occupancy
- We don't actually respect PDB format; instead recognize whitespace- or tab-delimited fields which allows us to deal with structures with coordinates > 999 or < -999.

Parameters

<i>thee</i>	Atom list object
<i>param</i>	A pre-initialized parameter object
<i>sock</i>	Socket reading for reading PQR file

Definition at line 606 of file [valist.c](#).

7.15.3.15 Valist_readXML()

```
VEEXTERNC Vrc_Codes Valist_readXML (
    Valist * thee,
    Vparam * param,
    Vio * sock )
```

Fill atom list with information from an XML file.

Author

Todd Dolinsky, Yong Huang

Returns

Success enumeration

Note

- The XML file must adhere to some guidelines, notably the presence of an <atom> tag with all other useful information (x, y, z, charge, and radius) as nested elements.

Parameters

<i>thee</i>	Atom list object
<i>param</i>	A pre-initialized parameter object
<i>sock</i>	Socket reading for reading PQR file

Definition at line 725 of file [valist.c](#).

7.16 Vatom class

Atom class for interfacing APBS with PDB files.

Files

- file [vatom.c](#)
Class Vatom methods.
- file [vatom.h](#)
Contains declarations for class Vatom.

Data Structures

- struct [sVatom](#)
Contains public data members for Vatom class/module.

Macros

- #define [VMAX_RECLEN](#) 64
Residue name length.

Typedefs

- typedef struct [sVatom](#) [Vatom](#)
Declaration of the Vatom class as the Vatom structure.

Functions

- VEXTERNC double * [Vatom_getPosition](#) ([Vatom](#) *thee)
Get atomic position.
- VEXTERNC void [Vatom_setRadius](#) ([Vatom](#) *thee, double radius)
Set atomic radius.
- VEXTERNC double [Vatom_getRadius](#) ([Vatom](#) *thee)
Get atomic position.
- VEXTERNC void [Vatom_setPartID](#) ([Vatom](#) *thee, int partID)
Set partition ID.
- VEXTERNC double [Vatom_getPartID](#) ([Vatom](#) *thee)
Get partition ID.
- VEXTERNC void [Vatom_setAtomID](#) ([Vatom](#) *thee, int id)
Set atom ID.
- VEXTERNC double [Vatom_getAtomID](#) ([Vatom](#) *thee)
Get atom ID.
- VEXTERNC void [Vatom_setCharge](#) ([Vatom](#) *thee, double charge)
Set atomic charge.
- VEXTERNC double [Vatom_getCharge](#) ([Vatom](#) *thee)
Get atomic charge.
- VEXTERNC void [Vatom_setEpsilon](#) ([Vatom](#) *thee, double epsilon)
Set atomic epsilon.
- VEXTERNC double [Vatom_getEpsilon](#) ([Vatom](#) *thee)
Get atomic epsilon.

- VEXTERNC unsigned long int [Vatom_memChk](#) ([Vatom](#) *thee)
Return the memory used by this structure (and its contents) in bytes.
- VEXTERNC void [Vatom_setResName](#) ([Vatom](#) *thee, char resName[VMAX_RECLEN])
Set residue name.
- VEXTERNC void [Vatom_setAtomName](#) ([Vatom](#) *thee, char atomName[VMAX_RECLEN])
Set atom name.
- VEXTERNC void [Vatom_getResName](#) ([Vatom](#) *thee, char resName[VMAX_RECLEN])
Retrieve residue name.
- VEXTERNC void [Vatom_getAtomName](#) ([Vatom](#) *thee, char atomName[VMAX_RECLEN])
Retrieve atom name.
- VEXTERNC [Vatom](#) * [Vatom_ctor](#) ()
Constructor for the Vatom class.
- VEXTERNC int [Vatom_ctor2](#) ([Vatom](#) *thee)
FORTTRAN stub constructor for the Vatom class.
- VEXTERNC void [Vatom_dtor](#) ([Vatom](#) **thee)
Object destructor.
- VEXTERNC void [Vatom_dtor2](#) ([Vatom](#) *thee)
FORTTRAN stub object destructor.
- VEXTERNC void [Vatom_setPosition](#) ([Vatom](#) *thee, double position[3])
Set the atomic position.
- VEXTERNC void [Vatom_copyTo](#) ([Vatom](#) *thee, [Vatom](#) *dest)
Copy information to another atom.
- VEXTERNC void [Vatom_copyFrom](#) ([Vatom](#) *thee, [Vatom](#) *src)
Copy information to another atom.

7.16.1 Detailed Description

Atom class for interfacing APBS with PDB files.

7.16.2 Macro Definition Documentation

7.16.2.1 VMAX_RECLEN

```
#define VMAX_RECLEN 64
```

Residue name length.

Author

Nathan Baker, David Gohara, Mike Schneiders

Definition at line 77 of file [vatom.h](#).

7.16.3 Typedef Documentation

7.16.3.1 Vatom

```
typedef struct sVatom Vatom
```

Declaration of the Vatom class as the Vatom structure.

Definition at line 114 of file [vatom.h](#).

7.16.4 Function Documentation

7.16.4.1 Vatom_copyFrom()

```
VEXTERNC void Vatom_copyFrom (
    Vatom * thee,
    Vatom * src )
```

Copy information to another atom.

Author

Nathan Baker

Parameters

<i>thee</i>	Destination for atom information
<i>src</i>	Source for atom information

Definition at line 186 of file [vatom.c](#).

7.16.4.2 Vatom_copyTo()

```
VEXTERNC void Vatom_copyTo (
    Vatom * thee,
    Vatom * dest )
```

Copy information to another atom.

Author

Nathan Baker

Parameters

<i>thee</i>	Source for atom information
<i>dest</i>	Destination for atom information

Definition at line 177 of file [vatom.c](#).

7.16.4.3 Vatom_ctor()

```
VEXTERNC Vatom * Vatom_ctor ( )
```

Constructor for the Vatom class.

Author

Nathan Baker

Returns

Pointer to newly allocated Vatom object

Definition at line 142 of file [vatom.c](#).

7.16.4.4 Vatom_ctor2()

```
VEXTERNC int Vatom_ctor2 (  
    Vatom * thee )
```

FORTTRAN stub constructor for the Vatom class.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to Vatom allocated memory location
-------------	--

Returns

1 if succesful, 0 otherwise

Definition at line 153 of file [vatom.c](#).

7.16.4.5 Vatom_dtor()

```
VEXTERNC void Vatom_dtor (  
    Vatom ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object to be destroyed
-------------	--

Definition at line 158 of file [vatom.c](#).

7.16.4.6 Vatom_dtor2()

```
VEXTERNC void Vatom_dtor2 (  
    Vatom * thee )
```

FORTTRAN stub object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object to be destroyed
-------------	-----------------------------------

Definition at line 166 of file [vatom.c](#).

7.16.4.7 Vatom_getAtomID()

```
VEXTERNC double Vatom_getAtomID (
    Vatom * thee )
```

Get atom ID.

Author

Nathan Baker

Parameters

<i>thee</i>	Vatom object
-------------	--------------

Returns

Unique non-negative number

Definition at line 84 of file [vatom.c](#).

7.16.4.8 Vatom_getAtomName()

```
VEXTERNC void Vatom_getAtomName (
    Vatom * thee,
    char atomName[VMAX_RECLEN] )
```

Retrieve atom name.

Author

Jason Wagoner

Parameters

<i>thee</i>	Vatom object
<i>atomName</i>	Atom name

Definition at line 214 of file [vatom.c](#).

7.16.4.9 Vatom_getCharge()

```
VEXTERNC double Vatom_getCharge (
    Vatom * thee )
```

Get atomic charge.

Author

Nathan Baker

Parameters

<i>thee</i>	Vatom object
-------------	--------------

Returns

Atom partial charge (in e)

Definition at line 119 of file [vatom.c](#).

7.16.4.10 Vatom_getEpsilon()

```
VEXTERNC double Vatom_getEpsilon (
    Vatom * thee )
```

Get atomic epsilon.

Author

David Gohara

Parameters

<i>thee</i>	Vatom object
-------------	--------------

Returns

Atomic epsilon (in Å)

Definition at line 132 of file [vatom.c](#).

7.16.4.11 Vatom_getPartID()

```
VEXTERNC double Vatom_getPartID (
    Vatom * thee )
```

Get partition ID.

Author

Nathan Baker

Parameters

<i>thee</i>	Vatom object
-------------	--------------

Returns

Partition ID; a negative value means this atom is not assigned to any partition

Definition at line 70 of file [vatom.c](#).

7.16.4.12 Vatom_getPosition()

```
VEXTERNC double * Vatom_getPosition (
    Vatom * thee )
```

Get atomic position.

Author

Nathan Baker

Parameters

<i>thee</i>	Vatom object
-------------	--------------

Returns

Pointer to 3*double array of atomic coordinates (in Å)

Definition at line 63 of file [vatom.c](#).**7.16.4.13 Vatom_getRadius()**

```
VEXTERNC double Vatom_getRadius (  
    Vatom * thee )
```

Get atomic position.

Author

Nathan Baker

Parameters

<i>thee</i>	Vatom object
-------------	--------------

Returns

Atomic radius (in Å)

Definition at line 105 of file [vatom.c](#).**7.16.4.14 Vatom_getResName()**

```
VEXTERNC void Vatom_getResName (  
    Vatom * thee,  
    char resName[VMAX_RECLEN] )
```

Retrieve residue name.

Author

Jason Wagoner

Parameters

<i>thee</i>	Vatom object
<i>resName</i>	Residue Name

Definition at line 199 of file [vatom.c](#).

7.16.4.15 Vatom_memChk()

```
VEXTERNC unsigned long int Vatom_memChk (  
    Vatom * thee )
```

Return the memory used by this structure (and its contents) in bytes.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpmg object
-------------	-------------

Returns

The memory used by this structure and its contents in bytes

Definition at line 138 of file [vatom.c](#).

7.16.4.16 Vatom_setAtomID()

```
VEXTERNC void Vatom_setAtomID (  
    Vatom * thee,  
    int id )
```

Set atom ID.

Author

Nathan Baker

Parameters

<i>thee</i>	Vatom object
<i>id</i>	Unique non-negative number

Definition at line 91 of file [vatom.c](#).

7.16.4.17 Vatom_setAtomName()

```
VEXTERNC void Vatom_setAtomName (  
    Vatom * thee,  
    char atomName[VMAX_RECLEN] )
```

Set atom name.

Author

Jason Wagoner

Parameters

<i>thee</i>	Vatom object
<i>atomName</i>	Atom name

Definition at line 207 of file [vatom.c](#).

7.16.4.18 Vatom_setCharge()

```
VEXTERNC void Vatom_setCharge (
    Vatom * thee,
    double charge )
```

Set atomic charge.

Author

Nathan Baker

Parameters

<i>thee</i>	Vatom object
<i>charge</i>	Atom partial charge (in e)

Definition at line 112 of file [vatom.c](#).

7.16.4.19 Vatom_setEpsilon()

```
VEXTERNC void Vatom_setEpsilon (
    Vatom * thee,
    double epsilon )
```

Set atomic epsilon.

Author

David Gohara

Parameters

<i>thee</i>	Vatom object
<i>epsilon</i>	Atomic epsilon (in Å)

Definition at line 126 of file [vatom.c](#).

7.16.4.20 Vatom_setPartID()

```
VEXTERNC void Vatom_setPartID (
    Vatom * thee,
    int partID )
```

Set partition ID.

Author

Nathan Baker

Parameters

<i>thee</i>	Vatom object
-------------	--------------

Parameters

<i>partID</i>	Partition ID; a negative value means this atom is not assigned to any partition
---------------	---

Definition at line 77 of file [vatom.c](#).

7.16.4.21 Vatom_setPosition()

```
VEXTERNC void Vatom_setPosition (
    Vatom * thee,
    double position[3] )
```

Set the atomic position.

Author

Nathan Baker

Parameters

<i>thee</i>	Vatom object to be modified
<i>position</i>	Coordinates (in Å)

Definition at line 168 of file [vatom.c](#).

7.16.4.22 Vatom_setRadius()

```
VEXTERNC void Vatom_setRadius (
    Vatom * thee,
    double radius )
```

Set atomic radius.

Author

Nathan Baker

Parameters

<i>thee</i>	Vatom object
<i>radius</i>	Atomic radius (in Å)

Definition at line 98 of file [vatom.c](#).

7.16.4.23 Vatom_setResName()

```
VEXTERNC void Vatom_setResName (
    Vatom * thee,
    char resName[VMAX_RECLEN] )
```

Set residue name.

Author

Jason Wagoner

Parameters

<i>thee</i>	Vatom object
<i>resName</i>	Residue Name

Definition at line 192 of file [vatom.c](#).

7.17 Vcap class

Collection of routines which cap certain exponential and hyperbolic functions.

Files

- file [vcap.c](#)
Class Vcap methods.
- file [vcap.h](#)
Contains declarations for class Vcap.

Macros

- #define [EXPMAX](#) 85.00
Maximum argument for exp(), sinh(), or cosh()
- #define [EXPMIN](#) -85.00
Minimum argument for exp(), sinh(), or cosh()

Functions

- VEXTERNC double [Vcap_exp](#) (double x, int *ichop)
Provide a capped exp() function.
- VEXTERNC double [Vcap_sinh](#) (double x, int *ichop)
Provide a capped sinh() function.
- VEXTERNC double [Vcap_cosh](#) (double x, int *ichop)
Provide a capped cosh() function.

7.17.1 Detailed Description

Collection of routines which cap certain exponential and hyperbolic functions.

Note

These routines are based on FORTRAN code by Mike Holst

7.17.2 Macro Definition Documentation

7.17.2.1 EXPMAX

```
#define EXPMAX 85.00
```

Maximum argument for `exp()`, `sinh()`, or `cosh()`

Definition at line 72 of file [vcap.h](#).

7.17.2.2 EXPMIN

```
#define EXPMIN -85.00
```

Minimum argument for `exp()`, `sinh()`, or `cosh()`

Definition at line 77 of file [vcap.h](#).

7.17.3 Function Documentation

7.17.3.1 Vcap_cosh()

```
VEXTERNC double Vcap_cosh (
    double x,
    int * ichop )
```

Provide a capped `cosh()` function.

If the argument `x` of `Vcap_cosh()` exceeds `EXPMAX` or `EXPMIN`, then we return `cosh(EXPMAX)` or `cosh(EXPMIN)` rather than `cosh(x)`.

Note

Original FORTRAN routine from PMG library by Mike Holst Original notes: to control overflow in the hyperbolic and exp functions, note that the following are the argument limits of the various functions on various machines after which overflow occurs: Convex C240, Sun 3/60, Sun SPARC, IBM RS/6000: `sinh`, `cosh`, `exp`: maximal argument (abs value) = 88.0d0 `dsinh`, `dcosh`, `dexp`: maximal argument (abs value) = 709.0d0

Author

Nathan Baker (based on FORTRAN code by Mike Holst)

Returns

`cosh(x)` or capped equivalent

Parameters

<code>x</code>	Argument to <code>cosh()</code>
<code>ichop</code>	Set to 1 if function capped, 0 otherwise

Definition at line 91 of file [vcap.c](#).

7.17.3.2 Vcap_exp()

```
VEXTERNC double Vcap_exp (
    double x,
    int * ichop )
```

Provide a capped exp() function.

```
If the argument x of Vcap_exp() exceeds EXPMAX or EXPMIN, then we
return exp(EXPMAX) or exp(EXPMIN) rather than exp(x).
```

Note

Original FORTRAN routine from PMG library by Mike Holst Original notes: to control overflow in the hyperbolic and exp functions, note that the following are the argument limits of the various functions on various machines after which overflow occurs: Convex C240, Sun 3/60, Sun SPARC, IBM RS/6000: sinh, cosh, exp: maximal argument (abs value) = 88.0d0 dsinh, dcosh, dexp: maximal argument (abs value) = 709.0d0

Author

Nathan Baker (based on FORTRAN code by Mike Holst)

Returns

exp(x) or capped equivalent

Parameters

<i>x</i>	Argument to exp()
<i>ichop</i>	Set to 1 if function capped, 0 otherwise

Definition at line 59 of file [vcap.c](#).

7.17.3.3 Vcap_sinh()

```
VEXTERNC double Vcap_sinh (
    double x,
    int * ichop )
```

Provide a capped sinh() function.

```
If the argument x of Vcap_sinh() exceeds EXPMAX or EXPMIN, then we
return sinh(EXPMAX) or sinh(EXPMIN) rather than sinh(x).
```

Note

Original FORTRAN routine from PMG library by Mike Holst Original notes: to control overflow in the hyperbolic and exp functions, note that the following are the argument limits of the various functions on various machines after which overflow occurs: Convex C240, Sun 3/60, Sun SPARC, IBM RS/6000: sinh, cosh, exp: maximal argument (abs value) = 88.0d0 dsinh, dcosh, dexp: maximal argument (abs value) = 709.0d0

Author

Nathan Baker (based on FORTRAN code by Mike Holst)

Returns

sinh(x) or capped equivalent

Parameters

<i>x</i>	Argument to sinh()
<i>ichop</i>	Set to 1 if function capped, 0 otherwise

Definition at line 75 of file [vcap.c](#).

7.18 Vclist class

Atom cell list.

Files

- file [vclist.c](#)
Class Vclist methods.
- file [vclist.h](#)
Contains declarations for class Vclist.

Data Structures

- struct [sVclistCell](#)
Atom cell list cell.
- struct [sVclist](#)
Atom cell list.

Typedefs

- typedef struct [sVclistCell](#) [VclistCell](#)
Declaration of the VclistCell class as the VclistCell structure.
- typedef struct [sVclist](#) [Vclist](#)
Declaration of the Vclist class as the Vclist structure.
- typedef enum [eVclist_DomainMode](#) [Vclist_DomainMode](#)
Declaration of Vclist_DomainMode enumeration type.

Enumerations

- enum [eVclist_DomainMode](#) { [CLIST_AUTO_DOMAIN](#) , [CLIST_MANUAL_DOMAIN](#) }
Atom cell list domain setup mode.

Functions

- VEXTERNC unsigned long int [Vclist_memChk](#) ([Vclist](#) *thee)
Get number of bytes in this object and its members.
- VEXTERNC double [Vclist_maxRadius](#) ([Vclist](#) *thee)
Get the max probe radius value (in Å) the cell list was constructed with.
- VEXTERNC [Vclist](#) * [Vclist_ctor](#) ([Valist](#) *alist, double max_radius, int npts[[VAPBS_DIM](#)], [Vclist_DomainMode](#) mode, double lower_corner[[VAPBS_DIM](#)], double upper_corner[[VAPBS_DIM](#)])
Construct the cell list object.
- VEXTERNC [Vrc_Codes](#) [Vclist_ctor2](#) ([Vclist](#) *thee, [Valist](#) *alist, double max_radius, int npts[[VAPBS_DIM](#)], [Vclist_DomainMode](#) mode, double lower_corner[[VAPBS_DIM](#)], double upper_corner[[VAPBS_DIM](#)])

FORTTRAN stub to construct the cell list object.

- VEXTERNC void [Vclist_dtor](#) ([Vclist](#) **thee)

Destroy object.

- VEXTERNC void [Vclist_dtor2](#) ([Vclist](#) *thee)

FORTTRAN stub to destroy object.

- VEXTERNC [VclistCell](#) * [Vclist_getCell](#) ([Vclist](#) *thee, double position[[VAPBS_DIM](#)])

Return cell corresponding to specified position or return VNULL.

- VEXTERNC [VclistCell](#) * [VclistCell_ctor](#) (int natoms)

Allocate and construct a cell list cell object.

- VEXTERNC [Vrc_Codes](#) [VclistCell_ctor2](#) ([VclistCell](#) *thee, int natoms)

Construct a cell list object.

- VEXTERNC void [VclistCell_dtor](#) ([VclistCell](#) **thee)

Destroy object.

- VEXTERNC void [VclistCell_dtor2](#) ([VclistCell](#) *thee)

FORTTRAN stub to destroy object.

7.18.1 Detailed Description

Atom cell list.

7.18.2 Typedef Documentation

7.18.2.1 Vclist

```
typedef struct sVclist Vclist
```

Declaration of the Vclist class as the Vclist structure.

Definition at line 136 of file [vclist.h](#).

7.18.2.2 Vclist_DomainMode

```
Vclist_DomainMode
```

Declaration of Vclist_DomainMode enumeration type.

Definition at line 94 of file [vclist.h](#).

7.18.2.3 VclistCell

```
typedef struct sVclistCell VclistCell
```

Declaration of the VclistCell class as the VclistCell structure.

Definition at line 110 of file [vclist.h](#).

7.18.3 Enumeration Type Documentation

7.18.3.1 eVclist_DomainMode

enum `eVclist_DomainMode`

Atom cell list domain setup mode.

Author

Nathan Baker

Enumerator

<code>CLIST_AUTO_DOMAIN</code>	Setup the cell list domain automatically to encompass the entire molecule
<code>CLIST_MANUAL_DOMAIN</code>	Specify the cell list domain manually through the constructor

Definition at line 82 of file `vclist.h`.

7.18.4 Function Documentation

7.18.4.1 Vclist_ctor()

```
VEXTERNC Vclist * Vclist_ctor (
    Valist * alist,
    double max_radius,
    int npts[VAPBS_DIM],
    Vclist_DomainMode mode,
    double lower_corner[VAPBS_DIM],
    double upper_corner[VAPBS_DIM] )
```

Construct the cell list object.

Author

Nathan Baker

Returns

Newly allocated `Vclist` object

Parameters

<i>alist</i>	Molecule for cell list queries
<i>max_radius</i>	Max probe radius (Å) to be queried
<i>npts</i>	Number of in hash table points in each direction
<i>mode</i>	Mode to construct table
<i>lower_corner</i>	Hash table lower corner for manual construction (see mode variable); ignored otherwise
<i>upper_corner</i>	Hash table upper corner for manual construction (see mode variable); ignored otherwise

Definition at line 75 of file `vclist.c`.

7.18.4.2 Vclist_ctor2()

```
VEXTERNC Vrc_Codes Vclist_ctor2 (
    Vclist * thee,
    Valist * alist,
    double max_radius,
    int npts[VAPBS_DIM],
    Vclist_DomainMode mode,
    double lower_corner[VAPBS_DIM],
    double upper_corner[VAPBS_DIM] )
```

FORTTRAN stub to construct the cell list object.

Author

Nathan Baker, Yong Huang

Returns

Success enumeration

Parameters

<i>thee</i>	Memory for Vclist objet
<i>alist</i>	Molecule for cell list queries
<i>max_radius</i>	Max probe radius (Å) to be queried
<i>npts</i>	Number of in hash table points in each direction
<i>mode</i>	Mode to construct table
<i>lower_corner</i>	Hash table lower corner for manual construction (see mode variable); ignored otherwise
<i>upper_corner</i>	Hash table upper corner for manual construction (see mode variable); ignored otherwise

Definition at line 343 of file [vclist.c](#).

7.18.4.3 Vclist_dtor()

```
VEXTERNC void Vclist_dtor (
    Vclist ** thee )
```

Destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object
-------------	--------------------------------------

Definition at line 397 of file [vclist.c](#).

7.18.4.4 Vclist_dtor2()

```
VEXTERNC void Vclist_dtor2 (
```

```
Vclist * thee )
```

FORTTRAN stub to destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object
-------------	-------------------

Definition at line 408 of file [vclist.c](#).

7.18.4.5 Vclist_getCell()

```
VEXTERNC VclistCell * Vclist_getCell (
    Vclist * thee,
    double position[VAPBS_DIM] )
```

Return cell corresponding to specified position or return VNULL.

Author

Nathan Baker

Returns

Pointer to VclistCell object or VNULL if no cell available (away from molecule).

Parameters

<i>thee</i>	Pointer to Vclist cell list
<i>position</i>	Position to evaluate

Definition at line 423 of file [vclist.c](#).

7.18.4.6 Vclist_maxRadius()

```
VEXTERNC double Vclist_maxRadius (
    Vclist * thee )
```

Get the max probe radius value (in A) the cell list was constructed with.

Author

Nathan Baker

Returns

Max probe radius (in A)

Parameters

<i>thee</i>	Cell list object
-------------	------------------

Definition at line 68 of file [vclist.c](#).

7.18.4.7 Vclist_memChk()

```
VEXTERNC unsigned long int Vclist_memChk (
    Vclist * thee )
```

Get number of bytes in this object and its members.

Author

Nathan Baker

Returns

Number of bytes allocated for object

Parameters

<i>thee</i>	Object for memory check
-------------	-------------------------

Definition at line 63 of file [vclist.c](#).

7.18.4.8 VclistCell_ctor()

```
VEXTERNC VclistCell * VclistCell_ctor (
    int natoms )
```

Allocate and construct a cell list cell object.

Author

Nathan Baker

Returns

Pointer to newly-allocated and constructed object.

Parameters

<i>natoms</i>	Number of atoms associated with this cell
---------------	---

Definition at line 452 of file [vclist.c](#).

7.18.4.9 VclistCell_ctor2()

```
VEXTERNC Vrc_Codes VclistCell_ctor2 (
    VclistCell * thee,
    int natoms )
```

Construct a cell list object.

Author

Nathan Baker, Yong Huang

Returns

Success enumeration

Parameters

<i>thee</i>	Memory location for object
<i>natoms</i>	Number of atoms associated with this cell

Definition at line [464](#) of file [vclist.c](#).

7.18.4.10 VclistCell_dtor()

```
VEXTERNC void VclistCell_dtor (
    VclistCell ** thee )
```

Destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object
-------------	--------------------------------------

Definition at line [486](#) of file [vclist.c](#).

7.18.4.11 VclistCell_dtor2()

```
VEXTERNC void VclistCell_dtor2 (
    VclistCell * thee )
```

FORTTRAN stub to destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object
-------------	-------------------

Definition at line [497](#) of file [vclist.c](#).

7.19 Vgreen class

Provides capabilities for pointwise evaluation of free space Green's function for point charges in a uniform dielectric.

Files

- file [vgreen.c](#)

Class Vgreen methods.

- file [vgreen.h](#)

Contains declarations for class Vgreen.

Data Structures

- struct [sVgreen](#)

Contains public data members for Vgreen class/module.

Typedefs

- typedef struct [sVgreen](#) [Vgreen](#)

Declaration of the Vgreen class as the Vgreen structure.

Functions

- VEXTERNC [Valist](#) * [Vgreen_getValist](#) ([Vgreen](#) *thee)
Get the atom list associated with this Green's function object.
- VEXTERNC unsigned long int [Vgreen_memChk](#) ([Vgreen](#) *thee)
Return the memory used by this structure (and its contents) in bytes.
- VEXTERNC [Vgreen](#) * [Vgreen_ctor](#) ([Valist](#) *alist)
Construct the Green's function oracle.
- VEXTERNC int [Vgreen_ctor2](#) ([Vgreen](#) *thee, [Valist](#) *alist)
FORTTRAN stub to construct the Green's function oracle.
- VEXTERNC void [Vgreen_dtor](#) ([Vgreen](#) **thee)
Destruct the Green's function oracle.
- VEXTERNC void [Vgreen_dtor2](#) ([Vgreen](#) *thee)
FORTTRAN stub to destruct the Green's function oracle.
- VEXTERNC int [Vgreen_helmholtz](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *val, double kappa)
Get the Green's function for Helmholtz's equation integrated over the atomic point charges.
- VEXTERNC int [Vgreen_helmholtzD](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *gradx, double *grady, double *gradz, double kappa)
Get the gradient of Green's function for Helmholtz's equation integrated over the atomic point charges.
- VEXTERNC int [Vgreen_coulomb_direct](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *val)
Get the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation.
- VEXTERNC int [Vgreen_coulomb](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *val)
Get the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation or H. E. Johnston, R. Krasny FMM library (if available)
- VEXTERNC int [Vgreen_coulombD_direct](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *pot, double *gradx, double *grady, double *gradz)
Get gradient of the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation.
- VEXTERNC int [Vgreen_coulombD](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *pot, double *gradx, double *grady, double *gradz)
Get gradient of the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using either direct summation or H. E. Johnston/R. Krasny FMM library (if available)

7.19.1 Detailed Description

Provides capabilities for pointwise evaluation of free space Green's function for point charges in a uniform dielectric.

Note

Right now, these are very slow methods without any fast multipole acceleration.

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
*
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* CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE)
* ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF
* THE POSSIBILITY OF SUCH DAMAGE.
*
*
```

7.19.2 Typedef Documentation

7.19.2.1 Vgreen

```
typedef struct sVgreen Vgreen
```

Declaration of the Vgreen class as the Vgreen structure.

Definition at line 101 of file [vgreen.h](#).

7.19.3 Function Documentation

7.19.3.1 Vgreen_coulomb()

```

VEXTERNC int Vgreen_coulomb (
    Vgreen * thee,
    int npos,
    double * x,
    double * y,
    double * z,
    double * val )

```

Get the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation or H. E. Johnston, R. Krasny FMM library (if available)

Returns the potential ϕ defined by

$$\phi(r) = \sum_i \frac{q_i}{r_i}$$

where q_i is the atomic charge (in e) and r_i is the distance to the observation point r . The potential is scaled to units of V.

Author

Nathan Baker

Parameters

<i>thee</i>	Vgreen object
<i>npos</i>	The number of positions to evaluate
<i>x</i>	The npos x-coordinates
<i>y</i>	The npos y-coordinates
<i>z</i>	The npos z-coordinates
<i>val</i>	The npos values

Returns

1 if successful, 0 otherwise

Definition at line 258 of file [vgreen.c](#).

7.19.3.2 Vgreen_coulomb_direct()

```

VEXTERNC int Vgreen_coulomb_direct (
    Vgreen * thee,
    int npos,
    double * x,
    double * y,
    double * z,
    double * val )

```

Get the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation.

Returns the potential ϕ defined by

$$\phi(r) = \sum_i \frac{q_i}{r_i}$$

where q_i is the atomic charge (in e) and r_i is the distance to the observation point r . The potential is scaled to units of V.

Author

Nathan Baker

Parameters

<i>thee</i>	Vgreen object
<i>npos</i>	The number of positions to evaluate
<i>x</i>	The npos x-coordinates
<i>y</i>	The npos y-coordinates
<i>z</i>	The npos z-coordinates
<i>val</i>	The npos values

Returns

1 if successful, 0 otherwise

Definition at line 224 of file [vgreen.c](#).

7.19.3.3 Vgreen_coulombD()

```

VEXTERNC int Vgreen_coulombD (
    Vgreen * thee,
    int npos,
    double * x,
    double * y,
    double * z,
    double * pot,
    double * gradx,
    double * grady,
    double * gradz )

```

Get gradient of the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using either direct summation or H. E. Johnston/R. Krasny FMM library (if available)

Returns the field $\nabla\phi$ defined by

$$\nabla\phi(r) = \sum_i \frac{q_i}{r_i}$$

where q_i is the atomic charge (in e) and r_i is the distance to the observation point r . The field is scaled to units of V/Å.

Author

Nathan Baker

Parameters

<i>thee</i>	Vgreen object
<i>npos</i>	The number of positions to evaluate
<i>x</i>	The npos x-coordinates
<i>y</i>	The npos y-coordinates
<i>z</i>	The npos z-coordinates

Parameters

<i>pot</i>	The npos potential values
<i>gradx</i>	The npos gradient x-components
<i>grady</i>	The npos gradient y-components
<i>gradz</i>	The npos gradient z-components

Returns

1 if successful, 0 otherwise

Definition at line 362 of file [vgreen.c](#).

7.19.3.4 Vgreen_coulombD_direct()

```

VEXTERNC int Vgreen_coulombD_direct (
    Vgreen * thee,
    int npos,
    double * x,
    double * y,
    double * z,
    double * pot,
    double * gradx,
    double * grady,
    double * gradz )

```

Get gradient of the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation.

Returns the field $\nabla\phi$ defined by

$$\nabla\phi(r) = \sum_i \frac{q_i}{r_i}$$

where q_i is the atomic charge (in e) and r_i is the distance to the observation point r . The field is scaled to units of V/Å.

Author

Nathan Baker

Parameters

<i>thee</i>	Vgreen object
<i>npos</i>	The number of positions to evaluate
<i>x</i>	The npos x-coordinates
<i>y</i>	The npos y-coordinates
<i>z</i>	The npos z-coordinates
<i>pot</i>	The npos potential values
<i>gradx</i>	The npos gradient x-components
<i>grady</i>	The npos gradient y-components
<i>gradz</i>	The npos gradient z-components

Returns

1 if successful, 0 otherwise

Definition at line 310 of file [vgreen.c](#).

7.19.3.5 Vgreen_ctor()

```
VEXTERNC Vgreen * Vgreen_ctor (
    Valist * alist )
```

Construct the Green's function oracle.

Author

Nathan Baker

Parameters

<i>alist</i>	Atom (charge) list associated with object
--------------	---

Returns

Pointer to newly allocated Green's function oracle

Definition at line 156 of file [vgreen.c](#).

7.19.3.6 Vgreen_ctor2()

```
VEXTERNC int Vgreen_ctor2 (
    Vgreen * thee,
    Valist * alist )
```

FORTTRAN stub to construct the Green's function oracle.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory allocated for object
<i>alist</i>	Atom (charge) list associated with object

Returns

1 if successful, 0 otherwise

Definition at line 167 of file [vgreen.c](#).

7.19.3.7 Vgreen_dtor()

```
VEXTERNC void Vgreen_dtor (
    Vgreen ** thee )
```

Destruct the Green's function oracle.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location for object
-------------	---------------------------------------

Definition at line 192 of file [vgreen.c](#).**7.19.3.8 Vgreen_dtor2()**

```
VEEXTERNAL void Vgreen_dtor2 (  
    Vgreen * thee )
```

FORTRAN stub to destruct the Green's function oracle.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object
-------------	-------------------

Definition at line 200 of file [vgreen.c](#).**7.19.3.9 Vgreen_getValist()**

```
VEEXTERNAL Valist * Vgreen_getValist (  
    Vgreen * thee )
```

Get the atom list associated with this Green's function object.

Author

Nathan Baker

Parameters

<i>thee</i>	Vgreen object
-------------	---------------

Returns

Pointer to Valist object associated with this Green's function object

Definition at line 142 of file [vgreen.c](#).**7.19.3.10 Vgreen_helmholtz()**

```
VEEXTERNAL int Vgreen_helmholtz (  
    Vgreen * thee,  
    int npos,  
    double * x,
```

```
double * y,
double * z,
double * val,
double kappa )
```

Get the Green's function for Helmholtz's equation integrated over the atomic point charges.
Returns the potential ϕ defined by

$$\phi(r) = \sum_i \frac{q_i e^{-\kappa r_i}}{r_i}$$

where κ is the inverse screening length (in Å) q_i is the atomic charge (in e), and r_i is the distance from atom i to the observation point r . The potential is scaled to units of V.

Author

Nathan Baker

Bug Not implemented yet

Note

Not implemented yet

Parameters

<i>thee</i>	Vgreen object
<i>npos</i>	Number of positions to evaluate
<i>x</i>	The npos x-coordinates
<i>y</i>	The npos y-coordinates
<i>z</i>	The npos z-coordinates
<i>val</i>	The npos values
<i>kappa</i>	The value of κ (see above)

Returns

1 if successful, 0 otherwise

Definition at line 209 of file [vgreen.c](#).

7.19.3.11 Vgreen_helmholtzD()

```
VEXTERNC int Vgreen_helmholtzD (
    Vgreen * thee,
    int npos,
    double * x,
    double * y,
    double * z,
    double * gradx,
    double * grady,
    double * gradz,
    double kappa )
```

Get the gradient of Green's function for Helmholtz's equation integrated over the atomic point charges.

Returns the field $\nabla\phi$ defined by

$$\nabla\phi(r) = \nabla \sum_i \frac{q_i e^{-\kappa r_i}}{r_i}$$

where κ is the inverse screening length (in Å). q_i is the atomic charge (in e), and r_i is the distance from atom i to the observation point r . The potential is scaled to units of V/Å.

Author

Nathan Baker

Bug Not implemented yet

Note

Not implemented yet

Parameters

<i>thee</i>	Vgreen object
<i>npos</i>	The number of positions to evaluate
<i>x</i>	The npos x-coordinates
<i>y</i>	The npos y-coordinates
<i>z</i>	The npos z-coordinates
<i>gradx</i>	The npos gradient x-components
<i>grady</i>	The npos gradient y-components
<i>gradz</i>	The npos gradient z-components
<i>kappa</i>	The value of κ (see above)

Returns

int 1 if successful, 0 otherwise

Definition at line 216 of file [vgreen.c](#).

7.19.3.12 Vgreen_memChk()

```
VEXTERNC unsigned long int Vgreen_memChk (
    Vgreen * thee )
```

Return the memory used by this structure (and its contents) in bytes.

Author

Nathan Baker

Parameters

<i>thee</i>	Vgreen object
-------------	---------------

Returns

The memory used by this structure and its contents in bytes

Definition at line 149 of file [vgreen.c](#).

7.20 Vhal class

A "class" which consists solely of macro definitions which are used by several other classes.

Files

- file [vhal.h](#)
Contains generic macro definitions for APBS.

Macros

- `#define APBS_TIMER_WALL_CLOCK` 26
APBS total execution timer ID.
- `#define APBS_TIMER_SETUP` 27
APBS setup timer ID.
- `#define APBS_TIMER_SOLVER` 28
APBS solver timer ID.
- `#define APBS_TIMER_ENERGY` 29
APBS energy timer ID.
- `#define APBS_TIMER_FORCE` 30
APBS force timer ID.
- `#define APBS_TIMER_TEMP1` 31
APBS temp timer #1 ID.
- `#define APBS_TIMER_TEMP2` 32
APBS temp timer #2 ID.
- `#define MAXMOL` 5
The maximum number of molecules that can be involved in a single PBE calculation.
- `#define MAXION` 10
The maximum number of ion species that can be involved in a single PBE calculation.
- `#define MAXFOCUS` 5
The maximum number of times an MG calculation can be focused.
- `#define VMGNLEV` 4
Minimum number of levels in a multigrid calculations.
- `#define VREDFRAC` 0.25
Maximum reduction of grid spacing during a focusing calculation.
- `#define VAPBS_NVS` 4
Number of vertices per simplex (hard-coded to 3D)
- `#define VAPBS_DIM` 3
Our dimension.
- `#define VAPBS_RIGHT` 0
Face definition for a volume.
- `#define VAPBS_FRONT` 1
Face definition for a volume.

- `#define VAPBS_UP 2`
Face definition for a volume.
- `#define VAPBS_LEFT 3`
Face definition for a volume.
- `#define VAPBS_BACK 4`
Face definition for a volume.
- `#define VAPBS_DOWN 5`
Face definition for a volume.
- `#define VPMGSMALL 1e-12`
A small number used in Vpmg to decide if points are on/off grid-lines or non-zero (etc.)
- `#define SINH_MIN -85.0`
Used to set the min values acceptable for sinh chopping.
- `#define SINH_MAX 85.0`
Used to set the max values acceptable for sinh chopping.
- `#define VF77_MANGLE(name, NAME) name`
Name-mangling macro for using FORTRAN functions in C code.
- `#define VFLOOR(value) floor(value)`
Wrapped floor to fix floating point issues in the Intel compiler.
- `#define VEMBED(rctag)`
Allows embedding of RCS ID tags in object files.

Typedefs

- `typedef enum eVhal_PBEType Vhal_PBEType`
Declaration of the Vhal_PBEType type as the Vhal_PBEType enum.
- `typedef enum eVhal_IPKEYType Vhal_IPKEYType`
Declaration of the Vhal_IPKEYType type as the Vhal_IPKEYType enum.
- `typedef enum eVhal_NONLINType Vhal_NONLINType`
Declaration of the Vhal_NONLINType type as the Vhal_NONLINType enum.
- `typedef enum eVoutput_Format Voutput_Format`
Declaration of the Voutput_Format type as the VOutput_Format enum.
- `typedef enum eVbcfl Vbcfl`
Declare Vbcfl type.
- `typedef enum eVsurf_Meth Vsurf_Meth`
Declaration of the Vsurf_Meth type as the Vsurf_Meth enum.
- `typedef enum eVchrg_Meth Vchrg_Meth`
Declaration of the Vchrg_Meth type as the Vchrg_Meth enum.
- `typedef enum eVchrg_Src Vchrg_Src`
Declaration of the Vchrg_Src type as the Vchrg_Meth enum.
- `typedef enum eVdata_Type Vdata_Type`
Declaration of the Vdata_Type type as the Vdata_Type enum.
- `typedef enum eVdata_Format Vdata_Format`
Declaration of the Vdata_Format type as the Vdata_Format enum.

Enumerations

- enum `eVrc_Codes` { `VRC_WARNING` = -1 , `VRC_FAILURE` = 0 , `VRC_SUCCESS` = 1 }
Return code enumerations.
- enum `eVsol_Meth` {
`VSOL_CGMG` , `VSOL_Newton` , `VSOL_MG` , `VSOL_CG` ,
`VSOL_SOR` , `VSOL_RBGS` , `VSOL_WJ` , `VSOL_Richardson` ,
`VSOL_CGMGAqua` , `VSOL_NewtonAqua` }
Solution Method enumerations.
- enum `eVsurf_Meth` {
`VSM_MOL` = 0 , `VSM_MOLSMOOTH` = 1 , `VSM_SPLINE` = 2 , `VSM_SPLINE3` = 3 ,
`VSM_SPLINE4` = 4 }
Types of molecular surface definitions.
- enum `eVhal_PBEType` {
`PBE_LPBE` , `PBE_NPBE` , `PBE_LRPBE` , `PBE_NRPBE` ,
`PBE_SMPBE` }
Version of PBE to solve.
- enum `eVhal_IPKEYType` { `IPKEY_SMPBE` = -2 , `IPKEY_LPBE` , `IPKEY_NPBE` }
Type of ipkey to use for MG methods.
- enum `eVhal_NONLINType` {
`NONLIN_LPBE` = 0 , `NONLIN_NPBE` , `NONLIN_SMPBE` , `NONLIN_LPBEAQUA` ,
`NONLIN_NPBEAQUA` }
Type of nonlinear to use for MG methods.
- enum `eVoutput_Format` { `OUTPUT_NULL` , `OUTPUT_FLAT` }
Output file format.
- enum `eVbcfl` {
`BCFL_ZERO` = 0 , `BCFL_SDH` = 1 , `BCFL_MDH` = 2 , `BCFL_UNUSED` = 3 ,
`BCFL_FOCUS` = 4 , `BCFL_MEM` = 5 , `BCFL_MAP` = 6 }
Types of boundary conditions.
- enum `eVchrg_Meth` { `VCM_TRIL` = 0 , `VCM_BSPL2` = 1 , `VCM_BSPL4` = 2 }
Types of charge discretization methods.
- enum `eVchrg_Src` { `VCM_CHARGE` = 0 , `VCM_PERMANENT` = 1 , `VCM_INDUCED` = 2 , `VCM_NLINDUCED` = 3 }
Charge source.
- enum `eVdata_Type` {
`VDT_CHARGE` , `VDT_POT` , `VDT_ATOMPOT` , `VDT_SMOL` ,
`VDT_SSPL` , `VDT_VDW` , `VDT_IVDW` , `VDT_LAP` ,
`VDT_EDENS` , `VDT_NDENS` , `VDT_QDENS` , `VDT_DIELX` ,
`VDT_DIELY` , `VDT_DIELZ` , `VDT_KAPPA` }
Types of (scalar) data that can be written out of APBS.
- enum `eVdata_Format` {
`VDF_DX` = 0 , `VDF_UHBD` = 1 , `VDF_AVS` = 2 , `VDF_MCSF` = 3 ,
`VDF_GZ` = 4 , `VDF_FLAT` = 5 , `VDF_DXBIN` = 6 }
Format of data for APBS I/O.

7.20.1 Detailed Description

A "class" which consists solely of macro definitions which are used by several other classes.

7.20.2 Macro Definition Documentation

7.20.2.1 APBS_TIMER_ENERGY

```
#define APBS_TIMER_ENERGY 29
```

APBS energy timer ID.
Definition at line 347 of file [vhal.h](#).

7.20.2.2 APBS_TIMER_FORCE

```
#define APBS_TIMER_FORCE 30
```

APBS force timer ID.
Definition at line 353 of file [vhal.h](#).

7.20.2.3 APBS_TIMER_SETUP

```
#define APBS_TIMER_SETUP 27
```

APBS setup timer ID.
Definition at line 335 of file [vhal.h](#).

7.20.2.4 APBS_TIMER_SOLVER

```
#define APBS_TIMER_SOLVER 28
```

APBS solver timer ID.
Definition at line 341 of file [vhal.h](#).

7.20.2.5 APBS_TIMER_TEMP1

```
#define APBS_TIMER_TEMP1 31
```

APBS temp timer #1 ID.
Definition at line 359 of file [vhal.h](#).

7.20.2.6 APBS_TIMER_TEMP2

```
#define APBS_TIMER_TEMP2 32
```

APBS temp timer #2 ID.
Definition at line 365 of file [vhal.h](#).

7.20.2.7 APBS_TIMER_WALL_CLOCK

```
#define APBS_TIMER_WALL_CLOCK 26
```

APBS total execution timer ID.
Definition at line 329 of file [vhal.h](#).

7.20.2.8 MAXFOCUS

```
#define MAXFOCUS 5
```

The maximum number of times an MG calculation can be focused.
Definition at line 382 of file [vhal.h](#).

7.20.2.9 MAXION

```
#define MAXION 10
```

The maximum number of ion species that can be involved in a single PBE calculation.

Definition at line 377 of file [vhal.h](#).

7.20.2.10 MAXMOL

```
#define MAXMOL 5
```

The maximum number of molecules that can be involved in a single PBE calculation.

Definition at line 371 of file [vhal.h](#).

7.20.2.11 SINH_MAX

```
#define SINH_MAX 85.0
```

Used to set the max values acceptable for sinh chopping.

Definition at line 456 of file [vhal.h](#).

7.20.2.12 SINH_MIN

```
#define SINH_MIN -85.0
```

Used to set the min values acceptable for sinh chopping.

Definition at line 450 of file [vhal.h](#).

7.20.2.13 VAPBS_BACK

```
#define VAPBS_BACK 4
```

Face definition for a volume.

Note

Consistent with PMG if RIGHT = EAST, BACK = SOUTH

Definition at line 432 of file [vhal.h](#).

7.20.2.14 VAPBS_DIM

```
#define VAPBS_DIM 3
```

Our dimension.

Definition at line 402 of file [vhal.h](#).

7.20.2.15 VAPBS_DOWN

```
#define VAPBS_DOWN 5
```

Face definition for a volume.

Note

Consistent with PMG if RIGHT = EAST, BACK = SOUTH

Definition at line 438 of file [vhal.h](#).

7.20.2.16 VAPBS_FRONT

```
#define VAPBS_FRONT 1
```

Face definition for a volume.

Note

Consistent with PMG if RIGHT = EAST, BACK = SOUTH

Definition at line 414 of file [vhal.h](#).

7.20.2.17 VAPBS_LEFT

```
#define VAPBS_LEFT 3
```

Face definition for a volume.

Note

Consistent with PMG if RIGHT = EAST, BACK = SOUTH

Definition at line 426 of file [vhal.h](#).

7.20.2.18 VAPBS_NVS

```
#define VAPBS_NVS 4
```

Number of vertices per simplex (hard-coded to 3D)

Definition at line 397 of file [vhal.h](#).

7.20.2.19 VAPBS_RIGHT

```
#define VAPBS_RIGHT 0
```

Face definition for a volume.

Note

Consistent with PMG if RIGHT = EAST, BACK = SOUTH

Definition at line 408 of file [vhal.h](#).

7.20.2.20 VAPBS_UP

```
#define VAPBS_UP 2
```

Face definition for a volume.

Note

Consistent with PMG if RIGHT = EAST, BACK = SOUTH

Definition at line 420 of file [vhal.h](#).

7.20.2.21 VEMBED

```
#define VEMBED(  
    rctag )
```

Value:

```
VPRIVATE const char* rctag; \  
static void* use_rcsid=(0 ? &use_rcsid : (void*)&rcsid);
```

Allows embedding of RCS ID tags in object files.

Author

Mike Holst

Definition at line 556 of file [vhal.h](#).

7.20.2.22 VF77_MANGLE

```
#define VF77_MANGLE(  
    name,  
    NAME ) name
```

Name-mangling macro for using FORTRAN functions in C code.

Definition at line 532 of file [vhal.h](#).

7.20.2.23 VFLOOR

```
#define VFLOOR(  
    value ) floor(value)
```

Wrapped floor to fix floating point issues in the Intel compiler.

Author

Todd Dolinsky

Definition at line 547 of file [vhal.h](#).

7.20.2.24 VMGNLEV

```
#define VMGNLEV 4
```

Minimum number of levels in a multigrid calculations.

Definition at line 387 of file [vhal.h](#).

7.20.2.25 VPMGSMALL

```
#define VPMGSMALL 1e-12
```

A small number used in Vpmg to decide if points are on/off grid-lines or non-zero (etc.)

Definition at line 444 of file [vhal.h](#).

7.20.2.26 VREDFRAC

```
#define VREDFRAC 0.25
```

Maximum reduction of grid spacing during a focusing calculation.

Definition at line 392 of file [vhal.h](#).

7.20.3 Typedef Documentation**7.20.3.1 Vbcfl**

```
typedef enum eVbcfl Vbcfl
```

Declare Vbcfl type.

Definition at line 223 of file [vhal.h](#).

7.20.3.2 Vchrg_Meth

[Vchrg_Meth](#)

Declaration of the Vchrg_Meth type as the Vchrg_Meth enum.

Definition at line 244 of file [vhal.h](#).

7.20.3.3 Vchrg_Src

[Vchrg_Src](#)

Declaration of the Vchrg_Src type as the Vchrg_Meth enum.

Definition at line 262 of file [vhal.h](#).

7.20.3.4 Vdata_Format

[Vdata_Format](#)

Declaration of the Vdata_Format type as the Vdata_Format enum.

Definition at line 323 of file [vhal.h](#).

7.20.3.5 Vdata_Type

[Vdata_Type](#)

Declaration of the Vdata_Type type as the Vdata_Type enum.

Definition at line 302 of file [vhal.h](#).

7.20.3.6 Vhal_IPKEYType

```
typedef enum eVhal_IPKEYType Vhal_IPKEYType
```

Declaration of the Vhal_IPKEYType type as the Vhal_IPKEYType enum.

Definition at line 167 of file [vhal.h](#).

7.20.3.7 Vhal_NONLINType

```
typedef enum eVhal_NONLINType Vhal_NONLINType
```

Declaration of the Vhal_NONLINType type as the Vhal_NONLINType enum.

Definition at line 185 of file [vhal.h](#).

7.20.3.8 Vhal_PBEType

```
typedef enum eVhal_PBEType Vhal_PBEType
```

Declaration of the Vhal_PBEType type as the Vhal_PBEType enum.

Definition at line 151 of file [vhal.h](#).

7.20.3.9 Voutput_Format

```
typedef enum eVoutput_Format Voutput_Format
```

Declaration of the Voutput_Format type as the VOutput_Format enum.

Definition at line 200 of file [vhal.h](#).

7.20.3.10 Vsurf_Meth

`Vsurf_Meth`

Declaration of the `Vsurf_Meth` type as the `Vsurf_Meth` enum.

Definition at line 133 of file `vhal.h`.

7.20.4 Enumeration Type Documentation

7.20.4.1 eVbcfl

enum `eVbcfl`

Types of boundary conditions.

Author

Nathan Baker

Enumerator

BCFL_ZERO	Zero Dirichlet boundary conditions
BCFL_SDH	Single-sphere Debye-Huckel Dirichlet boundary condition
BCFL_MDH	Multiple-sphere Debye-Huckel Dirichlet boundary condition
BCFL_UNUSED	Unused boundary condition method (placeholder)
BCFL_FOCUS	Focusing Dirichlet boundary condition
BCFL_MEM	Focusing membrane boundary condition
BCFL_MAP	Skip first level of focusing use an external map

Definition at line 207 of file `vhal.h`.

7.20.4.2 eVchrg_Meth

enum `eVchrg_Meth`

Types of charge discretization methods.

Author

Nathan Baker

Enumerator

VCM_TRIL	Trilinear interpolation of charge to 8 nearest grid points. The traditional method; not particularly good to use with PBE forces.
VCM_BSPL2	Cubic B-spline across nearest- and next-nearest-neighbors. Mainly for use in grid-sensitive applications (such as force calculations).
VCM_BSPL4	5th order B-spline for AMOEBA permanent multipoles.

Definition at line 230 of file `vhal.h`.

7.20.4.3 eVchrg_Src

enum [eVchrg_Src](#)

Charge source.

Author

Michael Schnieders

Enumerator

VCM_CHARGE	Partial Charge source distribution
VCM_PERMANENT	Permanent Multipole source distribution
VCM_INDUCED	Induced Dipole source distribution
VCM_NLINDUCED	NL Induced Dipole source distribution

Definition at line [251](#) of file [vhal.h](#).

7.20.4.4 eVdata_Format

enum [eVdata_Format](#)

Format of data for APBS I/O.

Author

Nathan Baker

Enumerator

VDF_DX	OpenDX (Data Explorer) format
VDF_UHBD	UHBD format
VDF_AVS	AVS UCD format
VDF_MCSF	FEtk MC Simplex Format (MCSF)
VDF_GZ	Binary file (GZip)
VDF_FLAT	Write flat file
VDF_DXBIN	OpendDX (Data Explorer) binary format

Definition at line [309](#) of file [vhal.h](#).

7.20.4.5 eVdata_Type

enum [eVdata_Type](#)

Types of (scalar) data that can be written out of APBS.

Author

Nathan Baker

Enumerator

VDT_CHARGE	Charge distribution (e)
------------	-------------------------

Enumerator

VDT_POT	Potential (kT/e)
VDT_ATOMPOT	Atom potential (kT/e)
VDT_SMOL	Solvent accessibility defined by molecular/Connolly surface definition (1 = accessible, 0 = inaccessible)
VDT_SSPL	Spline-based solvent accessibility (1 = accessible, 0 = inaccessible)
VDT_VDW	van der Waals-based accessibility (1 = accessible, 0 = inaccessible)
VDT_IVDW	Ion accessibility/inflated van der Waals (1 = accessible, 0 = inaccessible)
VDT_LAP	Laplacian of potential (kT/e/A ²)
VDT_EDENS	Energy density $\epsilon(\nabla u)^2$, where u is potential (kT/e/A) ²
VDT_NDENS	Ion number density $\sum c_i \exp(-q_i u)^2$, where u is potential (output in M)
VDT_QDENS	Ion charge density $\sum q_i c_i \exp(-q_i u)^2$, where u is potential (output in $e_c M$)
VDT_DIELX	Dielectric x-shifted map as calculated with the currently specified scheme (dimensionless)
VDT_DIELY	Dielectric y-shifted map as calculated with the currently specified scheme (dimensionless)
VDT_DIELZ	Dielectric y-shifted map as calculated with the currently specified scheme (dimensionless)
VDT_KAPPA	Kappa map as calculated with the currently specified scheme (⁻³)

Definition at line 269 of file [vhal.h](#).

7.20.4.6 eVhal_IPKEYType

enum [eVhal_IPKEYType](#)

Type of ipkey to use for MG methods.

Enumerator

IPKEY_SMPBE	SMPBE ipkey
IPKEY_LPBE	LPBE ipkey
IPKEY_NPBE	NPBE ipkey

Definition at line 157 of file [vhal.h](#).

7.20.4.7 eVhal_NONLINType

enum [eVhal_NONLINType](#)

Type of nonlinear to use for MG methods.

Definition at line 173 of file [vhal.h](#).

7.20.4.8 eVhal_PBEType

enum [eVhal_PBEType](#)

Version of PBE to solve.

Enumerator

PBE_LPBE	Traditional Poisson-Boltzmann equation, linearized
----------	--

Enumerator

PBE_NPBE	Traditional Poisson-Boltzmann equation, full
PBE_LRPBE	Regularized Poisson-Boltzmann equation, linearized
PBE_SMPBE	< Regularized Poisson-Boltzmann equation, full SM PBE

Definition at line 139 of file [vhal.h](#).

7.20.4.9 eVoutput_Format

enum [eVoutput_Format](#)

Output file format.

Enumerator

OUTPUT_NULL	No output
OUTPUT_FLAT	Output in flat-file format

Definition at line 191 of file [vhal.h](#).

7.20.4.10 eVrc_Codes

enum [eVrc_Codes](#)

Return code enumerations.

Author

David Gohara

Note

Note that the enumerated values are opposite the standard for FAILURE and SUCCESS

Enumerator

VRC_FAILURE	A non-fatal error
VRC_SUCCESS	A fatal error

Definition at line 66 of file [vhal.h](#).

7.20.4.11 eVsol_Meth

enum [eVsol_Meth](#)

Solution Method enumerations.

Author

David Gohara

Note

Note that the enumerated values are opposite the standard for FAILURE and SUCCESS

Definition at line 81 of file [vhal.h](#).

7.20.4.12 eVsurf_Meth

enum [eVsurf_Meth](#)

Types of molecular surface definitions.

Author

Nathan Baker

Enumerator

VSM_MOL	Ion accessibility is defined using inflated van der Waals radii, the dielectric coefficient () is defined using the molecular (Conolly) surface definition without smoothing
VSM_MOLSMOOTH	As VSM_MOL but with a simple harmonic average smoothing
VSM_SPLINE	Spline-based surface definitions. This is primarily for use with force calculations, since it requires substantial reparameterization of radii. This is based on the work of Im et al, Comp. Phys. Comm. 111 , (1998) and uses a cubic spline to define a smoothly varying characteristic function for the surface-based parameters. Ion accessibility is defined using inflated van der Waals radii with the spline function and the dielectric coefficient is defined using the standard van der Waals radii with the spline function.
VSM_SPLINE3	A 5th order polynomial spline is used to create a smoothly varying characteristic function (continuity through 2nd derivatives) for surface based paramters.
VSM_SPLINE4	A 7th order polynomial spline is used to create a smoothly varying characteristic function (continuity through 3rd derivatives) for surface based paramters.

Definition at line 102 of file [vhal.h](#).

7.21 Matrix wrapper class

A header for including data wrapping matrices.

Files

- file [vmatrix.h](#)

Contains inclusions for matrix data wrappers.

7.21.1 Detailed Description

A header for including data wrapping matrices.

7.22 Vparam class

Reads and assigns charge/radii parameters.

Files

- file [vparam.c](#)
Class [Vparam](#) methods.
- file [vparam.h](#)
Contains declarations for class [Vparam](#).

Data Structures

- struct [sVparam_AtomData](#)
AtomData sub-class; stores atom data.
- struct [Vparam_ResData](#)
ResData sub-class; stores residue data.
- struct [Vparam](#)
Reads and assigns charge/radii parameters.

Typedefs

- typedef struct [sVparam_AtomData](#) [Vparam_AtomData](#)
Declaration of the [Vparam_AtomData](#) class as the [sVparam_AtomData](#) structure.
- typedef struct [Vparam_ResData](#) [Vparam_ResData](#)
Declaration of the [Vparam_ResData](#) class as the [Vparam_ResData](#) structure.
- typedef struct [Vparam](#) [Vparam](#)
Declaration of the [Vparam](#) class as the [Vparam](#) structure.

Functions

- VPRIVATE int [readFlatFileLine](#) (Vio *sock, [Vparam_AtomData](#) *atom)
Read a single line of the flat file database.
- VPRIVATE int [readXMLFileAtom](#) (Vio *sock, [Vparam_AtomData](#) *atom)
Read atom information from an XML file.
- VEXTERNC unsigned long int [Vparam_memChk](#) ([Vparam](#) *thee)
Get number of bytes in this object and its members.
- VEXTERNC [Vparam_AtomData](#) * [Vparam_AtomData_ctor](#) ()
Construct the object.
- VEXTERNC int [Vparam_AtomData_ctor2](#) ([Vparam_AtomData](#) *thee)
FORTTRAN stub to construct the object.
- VEXTERNC void [Vparam_AtomData_dtor](#) ([Vparam_AtomData](#) **thee)
Destroy object.
- VEXTERNC void [Vparam_AtomData_dtor2](#) ([Vparam_AtomData](#) *thee)
FORTTRAN stub to destroy object.
- VEXTERNC void [Vparam_AtomData_copyTo](#) ([Vparam_AtomData](#) *thee, [Vparam_AtomData](#) *dest)
Copy current atom object to destination.
- VEXTERNC void [Vparam_ResData_copyTo](#) ([Vparam_ResData](#) *thee, [Vparam_ResData](#) *dest)
Copy current residue object to destination.
- VEXTERNC void [Vparam_AtomData_copyFrom](#) ([Vparam_AtomData](#) *thee, [Vparam_AtomData](#) *src)
Copy current atom object from another.
- VEXTERNC [Vparam_ResData](#) * [Vparam_ResData_ctor](#) (Vmem *mem)
Construct the object.

- VEXTERNC int [Vparam_ResData_ctor2](#) ([Vparam_ResData](#) *thee, Vmem *mem)
FORTTRAN stub to construct the object.
- VEXTERNC void [Vparam_ResData_dtor](#) ([Vparam_ResData](#) **thee)
Destroy object.
- VEXTERNC void [Vparam_ResData_dtor2](#) ([Vparam_ResData](#) *thee)
FORTTRAN stub to destroy object.
- VEXTERNC [Vparam](#) * [Vparam_ctor](#) ()
Construct the object.
- VEXTERNC int [Vparam_ctor2](#) ([Vparam](#) *thee)
FORTTRAN stub to construct the object.
- VEXTERNC void [Vparam_dtor](#) ([Vparam](#) **thee)
Destroy object.
- VEXTERNC void [Vparam_dtor2](#) ([Vparam](#) *thee)
FORTTRAN stub to destroy object.
- VEXTERNC [Vparam_ResData](#) * [Vparam_getResData](#) ([Vparam](#) *thee, char resName[VMAX_ARGLEN])
Get residue data.
- VEXTERNC [Vparam_AtomData](#) * [Vparam_getAtomData](#) ([Vparam](#) *thee, char resName[VMAX_ARGLEN], char atomName[VMAX_ARGLEN])
Get atom data.
- VEXTERNC int [Vparam_readFlatFile](#) ([Vparam](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname)
Read a flat-file format parameter database.
- VEXTERNC int [Vparam_readXMLFile](#) ([Vparam](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname)
Read an XML format parameter database.

Variables

- VPRIVATE char * [MCwhiteChars](#) = " =,;\t\n\r"
Whitespace characters for socket reads.
- VPRIVATE char * [MCcommChars](#) = "#%"
Comment characters for socket reads.
- VPRIVATE char * [MCxmlwhiteChars](#) = " =,;\t\n\r<>"
Whitespace characters for XML socket reads.

7.22.1 Detailed Description

Reads and assigns charge/radii parameters.

7.22.2 Typedef Documentation

7.22.2.1 Vparam

[Vparam](#)

Declaration of the [Vparam](#) class as the [Vparam](#) structure.

Definition at line 147 of file [vparam.h](#).

7.22.2.2 Vparam_AtomData

```
typedef struct sVparam_AtomData Vparam_AtomData
```

Declaration of the Vparam_AtomData class as the [sVparam_AtomData](#) structure.

Definition at line 106 of file [vparam.h](#).

7.22.2.3 Vparam_ResData

```
Vparam_ResData
```

Declaration of the [Vparam_ResData](#) class as the [Vparam_ResData](#) structure.

Definition at line 127 of file [vparam.h](#).

7.22.3 Function Documentation

7.22.3.1 readFlatFileLine()

```
VPRIVATE int readFlatFileLine (  
    Vio * sock,  
    Vparam_AtomData * atom )
```

Read a single line of the flat file database.

Author

Nathan Baker

Parameters

<i>sock</i>	Socket ready for reading
<i>atom</i>	Atom to hold parsed data

Returns

1 if successful, 0 otherwise

Definition at line 691 of file [vparam.c](#).

7.22.3.2 readXMLFileAtom()

```
VPRIVATE int readXMLFileAtom (  
    Vio * sock,  
    Vparam_AtomData * atom )
```

Read atom information from an XML file.

Author

Todd Dolinsky

Parameters

<i>sock</i>	Socket ready for reading
<i>atom</i>	Atom to hold parsed data

Returns

1 if successful, 0 otherwise

Definition at line 610 of file [vparam.c](#).

7.22.3.3 Vparam_AtomData_copyFrom()

```
VEXTERNC void Vparam_AtomData_copyFrom (
    Vparam_AtomData * thee,
    Vparam_AtomData * src )
```

Copy current atom object from another.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to destination object
<i>src</i>	Pointer to source object

Definition at line 607 of file [vparam.c](#).

7.22.3.4 Vparam_AtomData_copyTo()

```
VEXTERNC void Vparam_AtomData_copyTo (
    Vparam_AtomData * thee,
    Vparam_AtomData * dest )
```

Copy current atom object to destination.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to source object
<i>dest</i>	Pointer to destination object

Definition at line 571 of file [vparam.c](#).

7.22.3.5 Vparam_AtomData_ctor()

```
VEXTERNC Vparam_AtomData * Vparam_AtomData_ctor ( )
```

Construct the object.

Author

Nathan Baker

Returns

Newly allocated object

Definition at line 109 of file [vparam.c](#).

7.22.3.6 Vparam_AtomData_ctor2()

```
EXTERNC int Vparam_AtomData_ctor2 (  
    Vparam_AtomData * thee )
```

FORTTRAN stub to construct the object.

Author

Nathan Baker

Parameters

<i>thee</i>	Allocated memory
-------------	------------------

Returns

1 if successful, 0 otherwise

Definition at line 121 of file [vparam.c](#).

7.22.3.7 Vparam_AtomData_dtor()

```
EXTERNC void Vparam_AtomData_dtor (  
    Vparam_AtomData ** thee )
```

Destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object
-------------	--------------------------------------

Definition at line 123 of file [vparam.c](#).

7.22.3.8 Vparam_AtomData_dtor2()

```
EXTERNC void Vparam_AtomData_dtor2 (  
    Vparam_AtomData * thee )
```

FORTTRAN stub to destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object
-------------	-------------------

Definition at line 133 of file [vparam.c](#).

7.22.3.9 Vparam_ctor()

```
VEXTERNC Vparam * Vparam_ctor ( )
```

Construct the object.

Author

Nathan Baker

Returns

Newly allocated [Vparam](#) object

Definition at line 181 of file [vparam.c](#).

7.22.3.10 Vparam_ctor2()

```
VEXTERNC int Vparam_ctor2 (
    Vparam * thee )
```

FORTTRAN stub to construct the object.

Author

Nathan Baker

Parameters

<i>thee</i>	Allocated Vparam memory
-------------	---

Returns

1 if successful, 0 otherwise

Definition at line 193 of file [vparam.c](#).

7.22.3.11 Vparam_dtor()

```
VEXTERNC void Vparam_dtor (
    Vparam ** thee )
```

Destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object
-------------	--------------------------------------

Definition at line 213 of file [vparam.c](#).

7.22.3.12 Vparam_dtor2()

```
VEXTERNC void Vparam_dtor2 (  
    Vparam * thee )
```

FORTTRAN stub to destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object
-------------	-------------------

Definition at line 223 of file [vparam.c](#).

7.22.3.13 Vparam_getAtomData()

```
VEXTERNC Vparam\_AtomData * Vparam_getAtomData (  
    Vparam * thee,  
    char resName[VMAX_ARGLLEN],  
    char atomName[VMAX_ARGLLEN] )
```

Get atom data.

Author

Nathan Baker

Parameters

<i>thee</i>	Vparam object
<i>resName</i>	Residue name
<i>atomName</i>	Atom name

Returns

Pointer to the desired atom object or VNULL if residue not found

Note

Some method to initialize the database must be called before this method (e.g.,

See also

[Vparam_readFlatFile](#))

Definition at line 267 of file [vparam.c](#).

7.22.3.14 Vparam_getResData()

```
VEXTERNC Vparam_ResData * Vparam_getResData (
    Vparam * thee,
    char resName[VMAX_ARGLLEN] )
```

Get residue data.

Author

Nathan Baker

Parameters

<i>thee</i>	Vparam object
<i>resName</i>	Residue name

Returns

Pointer to the desired residue object or VNULL if residue not found

Note

Some method to initialize the database must be called before this method (e.g.,

See also

[Vparam_readFlatFile](#))

Definition at line 241 of file [vparam.c](#).

7.22.3.15 Vparam_memChk()

```
VEXTERNC unsigned long int Vparam_memChk (
    Vparam * thee )
```

Get number of bytes in this object and its members.

Author

Nathan Baker

Parameters

<i>thee</i>	Vparam object
-------------	---------------

Returns

Number of bytes allocated for object

Definition at line 102 of file [vparam.c](#).

7.22.3.16 Vparam_readFlatFile()

```
VEXTERNC int Vparam_readFlatFile (
    Vparam * thee,
```

```

const char * iodev,
const char * iofmt,
const char * thost,
const char * fname )

```

Read a flat-file format parameter database.

Author

Nathan Baker

Parameters

<i>thee</i>	Vparam object
<i>iodev</i>	Input device type (FILE/BUFF/UNIX/INET)
<i>iofmt</i>	Input device format (ASCII/XDR)
<i>thost</i>	Input hostname (for sockets)
<i>fname</i>	Input FILE/BUFF/UNIX/INET name (see note below for format)

Returns

1 if successful, 0 otherwise

Note

The database file should have the following format:

```
RESIDUE ATOM CHARGE RADIUS EPSILON
```

where RESIDUE is the residue name string, ATOM is the atom name string, CHARGE is the charge in e, RADIUS is the van der Waals radius (σ_i) in Å, and EPSILON is the van der Waals well-depth (ϵ_i) in kJ/mol. See the [Vparam](#) structure documentation for the precise definitions of σ_i and ϵ_i .

ASCII-format flat files are provided with the APBS source code:

tools/conversion/vparam-amber-parm94.dat AMBER parm94 parameters

tools/conversion/vparam-charmm-par_all27.dat CHARMM par_all27_prot_na parameters

Definition at line [445](#) of file [vparam.c](#).

7.22.3.17 Vparam_readXMLFile()

```

VEXTERNC int Vparam_readXMLFile (
    Vparam * thee,
    const char * iodev,
    const char * iofmt,
    const char * thost,
    const char * fname )

```

Read an XML format parameter database.

Author

Todd Dolinsky

Parameters

<i>thee</i>	Vparam object
<i>iodev</i>	Input device type (FILE/BUFF/UNIX/INET)
<i>iofmt</i>	Input device format (ASCII/XDR)
<i>thost</i>	Input hostname (for sockets)
<i>fname</i>	Input FILE/BUFF/UNIX/INET name

Returns

1 if successful, 0 otherwise

Definition at line 306 of file [vparam.c](#).

7.22.3.18 Vparam_ResData_copyTo()

```
VEXTERNC void Vparam_ResData_copyTo (
    Vparam_ResData * thee,
    Vparam_ResData * dest )
```

Copy current residue object to destination.

Author

Todd Dolinsky

Parameters

<i>thee</i>	Pointer to source object
<i>dest</i>	Pointer to destination object

Definition at line 585 of file [vparam.c](#).

7.22.3.19 Vparam_ResData_ctor()

```
VEXTERNC Vparam_ResData * Vparam_ResData_ctor (
    Vmem * mem )
```

Construct the object.

Author

Nathan Baker

Parameters

<i>mem</i>	Memory object of Vparam master class
------------	--

Returns

Newly allocated object

Definition at line 135 of file [vparam.c](#).

7.22.3.20 Vparam_ResData_ctor2()

```
VEXTERNC int Vparam_ResData_ctor2 (
    Vparam_ResData * thee,
    Vmem * mem )
```

FORTTRAN stub to construct the object.

Author

Nathan Baker

Parameters

<i>thee</i>	Allocated memory
<i>mem</i>	Memory object of Vparam master class

Returns

1 if successful, 0 otherwise

Definition at line [147](#) of file [vparam.c](#).

7.22.3.21 Vparam_ResData_dtor()

```
VEXTERNC void Vparam_ResData_dtor (
    Vparam_ResData ** thee )
```

Destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object
-------------	--------------------------------------

Definition at line [160](#) of file [vparam.c](#).

7.22.3.22 Vparam_ResData_dtor2()

```
VEXTERNC void Vparam_ResData_dtor2 (
    Vparam_ResData * thee )
```

FORTTRAN stub to destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object
-------------	-------------------

Definition at line [170](#) of file [vparam.c](#).

7.22.4 Variable Documentation

7.22.4.1 MCcommChars

```
VPRIVATE char* MCcommChars = "#%"
```

Comment characters for socket reads.

Definition at line 71 of file [vparam.c](#).

7.22.4.2 MCwhiteChars

```
VPRIVATE char* MCwhiteChars = " =,;\t\n\r"
```

Whitespace characters for socket reads.

Definition at line 65 of file [vparam.c](#).

7.22.4.3 MCxmlwhiteChars

```
VPRIVATE char* MCxmlwhiteChars = " =,;\t\n\r<>"
```

Whitespace characters for XML socket reads.

Definition at line 77 of file [vparam.c](#).

7.23 Vpbe class

The Poisson-Boltzmann master class.

Files

- file [vpbe.c](#)
Class Vpbe methods.
- file [vpbe.h](#)
Contains declarations for class Vpbe.

Data Structures

- struct [sVpbe](#)
Contains public data members for Vpbe class/module.

Typedefs

- typedef struct [sVpbe](#) [Vpbe](#)
Declaration of the Vpbe class as the Vpbe structure.

Functions

- VEXTERNC [Valist](#) * [Vpbe_getValist](#) ([Vpbe](#) *thee)
Get atom list.
- VEXTERNC [Vacc](#) * [Vpbe_getVacc](#) ([Vpbe](#) *thee)
Get accessibility oracle.
- VEXTERNC double [Vpbe_getBulkIonicStrength](#) ([Vpbe](#) *thee)

- Get bulk ionic strength.*

 - VEXTERNC double [Vpbe_getMaxIonRadius](#) (Vpbe *thee)
- Get maximum radius of ion species.*

 - VEXTERNC double [Vpbe_getTemperature](#) (Vpbe *thee)
- Get temperature.*

 - VEXTERNC double [Vpbe_getSoluteDiel](#) (Vpbe *thee)
- Get solute dielectric constant.*

 - VEXTERNC double [Vpbe_getGamma](#) (Vpbe *thee)
- Get apolar coefficient.*

 - VEXTERNC double [Vpbe_getSoluteRadius](#) (Vpbe *thee)
- Get sphere radius which bounds biomolecule.*

 - VEXTERNC double [Vpbe_getSoluteXlen](#) (Vpbe *thee)
- Get length of solute in x dimension.*

 - VEXTERNC double [Vpbe_getSoluteYlen](#) (Vpbe *thee)
- Get length of solute in y dimension.*

 - VEXTERNC double [Vpbe_getSoluteZlen](#) (Vpbe *thee)
- Get length of solute in z dimension.*

 - VEXTERNC double * [Vpbe_getSoluteCenter](#) (Vpbe *thee)
- Get coordinates of solute center.*

 - VEXTERNC double [Vpbe_getSoluteCharge](#) (Vpbe *thee)
- Get total solute charge.*

 - VEXTERNC double [Vpbe_getSolventDiel](#) (Vpbe *thee)
- Get solvent dielectric constant.*

 - VEXTERNC double [Vpbe_getSolventRadius](#) (Vpbe *thee)
- Get solvent molecule radius.*

 - VEXTERNC double [Vpbe_getXkappa](#) (Vpbe *thee)
- Get Debye-Huckel parameter.*

 - VEXTERNC double [Vpbe_getDeblen](#) (Vpbe *thee)
- Get Debye-Huckel screening length.*

 - VEXTERNC double [Vpbe_getZkappa2](#) (Vpbe *thee)
- Get modified squared Debye-Huckel parameter.*

 - VEXTERNC double [Vpbe_getZmagic](#) (Vpbe *thee)
- Get charge scaling factor.*

 - VEXTERNC double [Vpbe_getzmem](#) (Vpbe *thee)
- Get z position of the membrane bottom.*

 - VEXTERNC double [Vpbe_getLmem](#) (Vpbe *thee)
- Get length of the membrane (A)*
aaauthor Michael Grabe.

 - VEXTERNC double [Vpbe_getmembraneDiel](#) (Vpbe *thee)
- Get membrane dielectric constant.*

 - VEXTERNC double [Vpbe_getmemv](#) (Vpbe *thee)
- Get membrane potential (kT)*

 - VEXTERNC [Vpbe](#) * [Vpbe_ctor](#) (Valist *alist, int ionNum, double *ionConc, double *ionRadii, double *ionQ, double T, double soluteDiel, double solventDiel, double solventRadius, int focusFlag, double sdens, double z_↔mem, double L, double membraneDiel, double V)
- Construct Vpbe object.*

- VEXTERNC int [Vpbe_ctor2](#) ([Vpbe](#) *thee, [Valist](#) *alist, int ionNum, double *ionConc, double *ionRadii, double *ionQ, double T, double soluteDiel, double solventDiel, double solventRadius, int focusFlag, double sdens, double z_mem, double L, double membraneDiel, double V)
FORTRAN stub to construct Vpbe object.
- VEXTERNC int [Vpbe_getIons](#) ([Vpbe](#) *thee, int *nion, double ionConc[[MAXION](#)], double ionRadii[[MAXION](#)], double ionQ[[MAXION](#)])
Get information about the counterion species present.
- VEXTERNC void [Vpbe_dtor](#) ([Vpbe](#) **thee)
Object destructor.
- VEXTERNC void [Vpbe_dtor2](#) ([Vpbe](#) *thee)
FORTRAN stub object destructor.
- VEXTERNC double [Vpbe_getCoulombEnergy1](#) ([Vpbe](#) *thee)
Calculate coulombic energy of set of charges.
- VEXTERNC unsigned long int [Vpbe_memChk](#) ([Vpbe](#) *thee)
Return the memory used by this structure (and its contents) in bytes.

7.23.1 Detailed Description

The Poisson-Boltzmann master class.

Contains objects and parameters used in every PBE calculation, regardless of method.

7.23.2 Typedef Documentation

7.23.2.1 Vpbe

```
typedef struct sVpbe Vpbe
```

Declaration of the Vpbe class as the Vpbe structure.

Definition at line 144 of file [vpbe.h](#).

7.23.3 Function Documentation

7.23.3.1 Vpbe_ctor()

```
VEXTERNC Vpbe * Vpbe_ctor (
    Valist * alist,
    int ionNum,
    double * ionConc,
    double * ionRadii,
    double * ionQ,
    double T,
    double soluteDiel,
    double solventDiel,
    double solventRadius,
    int focusFlag,
    double sdens,
    double z_mem,
    double L,
```

```
double membraneDiel,
double V )
```

Construct Vpbe object.

Author

Nathan Baker and Mike Holst and Michael Grabe

Note

This is partially based on some of Mike Holst's PMG code. Here are a few of the original function comments: kappa is defined as follows:

$$\kappa^2 = \frac{8\pi N_A e_c^2 I_s}{1000 \epsilon_w k_B T}$$

where the units are esu*esu/erg/mol. To obtain cm^{-2} , we multiply by 10^{-16} . Thus, in cm^{-2} , where k_B and e_c are in gaussian rather than mks units, the proper value for kappa is:

$$\kappa^2 = \frac{8\pi N_A e_c^2 I_s}{1000 \epsilon_w k_B T} \times 10^{-16}$$

and the factor of 10^{-16} results from converting cm^2 to angstroms^2 , noting that the 1000 in the denominator has converted m^3 to cm^3 , since the ionic strength I_s is assumed to have been provided in moles per liter, which is moles per 1000 cm^3 .

Returns

Pointer to newly allocated Vpbe object

Parameters

<i>alist</i>	Atom list
<i>ionNum</i>	Number of counterion species
<i>ionConc</i>	Array containing counterion concentrations (M)
<i>ionRadii</i>	Array containing counterion radii (A)
<i>ionQ</i>	Array containing counterion charges (e)
<i>T</i>	Temperature for Boltzmann distribution (K)
<i>soluteDiel</i>	Solute internal dielectric constant
<i>solventDiel</i>	Solvent dielectric constant
<i>solventRadius</i>	Solvent probe radius for surfaces that use it (A)
<i>focusFlag</i>	1 if focusing operation, 0 otherwise
<i>sdens</i>	Vacc sphere density
<i>z_mem</i>	Membrane location (A)
<i>L</i>	Membrane thickness (A)
<i>membraneDiel</i>	Membrane dielectric constant
<i>V</i>	Transmembrane potential (V)

Definition at line 246 of file [vpbe.c](#).

7.23.3.2 Vpbe_ctor2()

```
VEXTERNC int Vpbe_ctor2 (
```

```

Vpbe * thee,
Valist * alist,
int ionNum,
double * ionConc,
double * ionRadii,
double * ionQ,
double T,
double soluteDiel,
double solventDiel,
double solventRadius,
int focusFlag,
double sdens,
double z_mem,
double L,
double membraneDiel,
double V )

```

FORTTRAN stub to construct Vpbe objct.

Author

Nathan Baker and Mike Holst and Michael Grabe

Note

This is partially based on some of Mike Holst's PMG code. Here are a few of the original function comments: kappa is defined as follows:

$$\kappa^2 = \frac{8\pi N_A e_c^2 I_s}{1000 \epsilon \epsilon_w k_B T}$$

where the units are esu*esu/erg/mol. To obtain m^{-2} , we multiply by 10^{-16} . Thus, in m^{-2} , where k_B and e_c are in gaussian rather than mks units, the proper value for kappa is:

$$\kappa^2 = \frac{8\pi N_A e_c^2 I_s}{1000 \epsilon \epsilon_w k_B T} \times 10^{-16}$$

and the factor of 10^{-16} results from converting cm^2 to angstroms^2 , noting that the 1000 in the denominator has converted m^3 to cm^3 , since the ionic strength I_s is assumed to have been provided in moles per liter, which is moles per 1000 cm^3 .

Bug The focusing flag is currently not used!!

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	Pointer to memory allocated for Vpbe object
<i>alist</i>	Atom list
<i>ionNum</i>	Number of counterion species
<i>ionConc</i>	Array containing counterion concentrations (M)
<i>ionRadii</i>	Array containing counterion radii (A)
<i>ionQ</i>	Array containing counterion charges (e)
<i>T</i>	Temperature for Boltzmann distribution (K)
<i>soluteDiel</i>	Solute internal dielectric constant

Parameters

<i>solventDiel</i>	Solvent dielectric constant
<i>solventRadius</i>	Solvent probe radius for surfaces that use it (A)
<i>focusFlag</i>	1 if focusing operation, 0 otherwise
<i>sdens</i>	Vacc sphere density
<i>z_mem</i>	Membrane location (A)
<i>L</i>	Membrane thickness (A)
<i>membraneDiel</i>	Membrane dielectric constant
<i>V</i>	Transmembrane potential (V)

Definition at line 264 of file [vpbe.c](#).

7.23.3.3 Vpbe_dtor()

```
VEXTERNC void Vpbe_dtor (  
    Vpbe ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object to be destroyed
-------------	--

Definition at line 467 of file [vpbe.c](#).

7.23.3.4 Vpbe_dtor2()

```
VEXTERNC void Vpbe_dtor2 (  
    Vpbe * thee )
```

FORTTRAN stub object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object to be destroyed
-------------	-----------------------------------

Definition at line 475 of file [vpbe.c](#).

7.23.3.5 Vpbe_getBulkIonicStrength()

```
VEXTERNC double Vpbe_getBulkIonicStrength (  
    Vpbe * thee )
```

Get bulk ionic strength.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Bulk ionic strength (M)

Definition at line 84 of file [vpbe.c](#).**7.23.3.6 Vpbe_getCoulombEnergy1()**

```
VEXTERNC double Vpbe_getCoulombEnergy1 (  
    Vpbe * thee )
```

Calculate coulombic energy of set of charges.

```
    Perform an inefficient double sum to calculate the Coulombic  
    energy of a set of charges in a homogeneous dielectric (with  
    strength. Result is returned in units of k_B T. The sum can be  
    restriction to charges present in simplices of specified color  
    (pcolor); if (color == -1) no restrictions are used.
```

permittivity equal to the protein interior

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

ReturnsCoulombic energy in units of $k_B T$.Definition at line 481 of file [vpbe.c](#).**7.23.3.7 Vpbe_getDeblen()**

```
VEXTERNC double Vpbe_getDeblen (  
    Vpbe * thee )
```

Get Debye-Huckel screening length.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Debye-Huckel screening length (Å)

Definition at line 141 of file [vpbe.c](#).

7.23.3.8 Vpbe_getGamma()

```
VEXTERNC double Vpbe_getGamma (  
    Vpbe * thee )
```

Get apolar coefficient.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Apolar coefficient (kJ/mol/Å²)

7.23.3.9 Vpbe_getIons()

```
VEXTERNC int Vpbe_getIons (  
    Vpbe * thee,  
    int * nion,  
    double ionConc[MAXION],  
    double ionRadii[MAXION],  
    double ionQ[MAXION] )
```

Get information about the counterion species present.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to Vpbe object
<i>nion</i>	Set to the number of counterion species
<i>ionConc</i>	Array to store counterion species' concentrations (M)
<i>ionRadii</i>	Array to store counterion species' radii (Å)
<i>ionQ</i>	Array to store counterion species' charges (e)

Returns

Number of ions

Definition at line 535 of file [vpbe.c](#).

7.23.3.10 Vpbe_getLmem()

```
VEXTERNC double Vpbe_getLmem (
    Vpbe * thee )
```

Get length of the membrane (A)

author Michael Grabe.

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Length of the membrane (A)

Definition at line 209 of file [vpbe.c](#).

7.23.3.11 Vpbe_getMaxIonRadius()

```
VEXTERNC double Vpbe_getMaxIonRadius (
    Vpbe * thee )
```

Get maximum radius of ion species.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Maximum radius (A)

Definition at line 127 of file [vpbe.c](#).

7.23.3.12 Vpbe_getmembraneDiel()

```
VEXTERNC double Vpbe_getmembraneDiel (
    Vpbe * thee )
```

Get membrane dielectric constant.

Author

Michael Grabe

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Membrane dielectric constant

Definition at line 221 of file [vpbe.c](#).

7.23.3.13 Vpbe_getmemv()

```
VEXTERNC double Vpbe_getmemv (  
    Vpbe * thee )
```

Get membrane potential (kT)

Author

Michael Grabe

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Definition at line 233 of file [vpbe.c](#).

7.23.3.14 Vpbe_getSoluteCenter()

```
VEXTERNC double * Vpbe_getSoluteCenter (  
    Vpbe * thee )
```

Get coordinates of solute center.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Pointer to 3*double array with solute center coordinates (A)

Definition at line 107 of file [vpbe.c](#).

7.23.3.15 Vpbe_getSoluteCharge()

```
VEXTERNC double Vpbe_getSoluteCharge (  
    Vpbe * thee )
```

Get total solute charge.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Total solute charge (e)

Definition at line 186 of file [vpbe.c](#).

7.23.3.16 Vpbe_getSoluteDiel()

```
VEXTERNC double Vpbe_getSoluteDiel (  
    Vpbe * thee )
```

Get solute dielectric constant.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Solute dielectric constant

Definition at line 99 of file [vpbe.c](#).

7.23.3.17 Vpbe_getSoluteRadius()

```
VEXTERNC double Vpbe_getSoluteRadius (  
    Vpbe * thee )
```

Get sphere radius which bounds biomolecule.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Sphere radius which bounds biomolecule (A)

Definition at line 162 of file [vpbe.c](#).

7.23.3.18 Vpbe_getSoluteXlen()

```
VEXTERNC double Vpbe_getSoluteXlen (  
    Vpbe * thee )
```

```
Vpbe * thee )
```

Get length of solute in x dimension.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Length of solute in x dimension (A)

Definition at line 168 of file [vpbe.c](#).

7.23.3.19 Vpbe_getSoluteYlen()

```
VEXTERNC double Vpbe_getSoluteYlen (
```

```
Vpbe * thee )
```

Get length of solute in y dimension.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Length of solute in y dimension (A)

Definition at line 174 of file [vpbe.c](#).

7.23.3.20 Vpbe_getSoluteZlen()

```
VEXTERNC double Vpbe_getSoluteZlen (
```

```
Vpbe * thee )
```

Get length of solute in z dimension.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Length of solute in z dimension (A)

Definition at line 180 of file [vpbe.c](#).

7.23.3.21 Vpbe_getSolventDiel()

```
VEXTERNC double Vpbe_getSolventDiel (  
    Vpbe * thee )
```

Get solvent dielectric constant.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Solvent dielectric constant

Definition at line 113 of file [vpbe.c](#).

7.23.3.22 Vpbe_getSolventRadius()

```
VEXTERNC double Vpbe_getSolventRadius (  
    Vpbe * thee )
```

Get solvent molecule radius.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Solvent molecule radius (A)

Definition at line 120 of file [vpbe.c](#).

7.23.3.23 Vpbe_getTemperature()

```
VEXTERNC double Vpbe_getTemperature (  
    Vpbe * thee )
```

Get temperature.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Temperature (K)

Definition at line 91 of file [vpbe.c](#).

7.23.3.24 Vpbe_getVacc()

```
VEXTERNC Vacc * Vpbe_getVacc (  
    Vpbe * thee )
```

Get accessibility oracle.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Pointer to internal Vacc object

Definition at line 76 of file [vpbe.c](#).

7.23.3.25 Vpbe_getValist()

```
VEXTERNC Valist * Vpbe_getValist (  
    Vpbe * thee )
```

Get atom list.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Pointer to internal Valist object

Definition at line 69 of file [vpbe.c](#).

7.23.3.26 Vpbe_getXkappa()

```
VEXTERNC double Vpbe_getXkappa (
    Vpbe * thee )
```

Get Debye-Huckel parameter.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Bulk Debye-Huckel parameter (Å)

Definition at line 134 of file [vpbe.c](#).

7.23.3.27 Vpbe_getZkappa2()

```
VEXTERNC double Vpbe_getZkappa2 (
    Vpbe * thee )
```

Get modified squared Debye-Huckel parameter.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Modified squared Debye-Huckel parameter ($^{-2}$)

Definition at line 148 of file [vpbe.c](#).

7.23.3.28 Vpbe_getZmagic()

```
VEXTERNC double Vpbe_getZmagic (
    Vpbe * thee )
```

Get charge scaling factor.

Author

Nathan Baker and Mike Holst

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Get factor for scaling charges (in e) to internal units

Definition at line 155 of file [vpbe.c](#).

7.23.3.29 Vpbe_getzmem()

```
VEXTERNC double Vpbe_getzmem (  
    Vpbe * thee )
```

Get z position of the membrane bottom.

Author

Michael Grabe

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

z value of membrane (A)

Definition at line 197 of file [vpbe.c](#).

7.23.3.30 Vpbe_memChk()

```
VEXTERNC unsigned long int Vpbe_memChk (  
    Vpbe * thee )
```

Return the memory used by this structure (and its contents) in bytes.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

The memory used by this structure and its contents in bytes

Definition at line 523 of file [vpbe.c](#).

7.24 Vstring class

Provides a collection of useful non-ANSI string functions.

Files

- file [vstring.c](#)

Class Vstring methods.

- file [vstring.h](#)

Contains declarations for class Vstring.

Functions

- char * [Vstring_wrappedtext](#) (const char *str, int right_margin, int left_padding)
- VEXTERNC int [Vstring_strcasecmp](#) (const char *s1, const char *s2)
Case-insensitive string comparison (BSD standard)
- VEXTERNC int [Vstring_isdigit](#) (const char *tok)
A modified sscanf that examines the complete string.

7.24.1 Detailed Description

Provides a collection of useful non-ANSI string functions.

7.24.2 Function Documentation

7.24.2.1 Vstring_isdigit()

```
VEXTERNC int Vstring_isdigit (
    const char * tok )
```

A modified sscanf that examines the complete string.

Author

Todd Dolinsky

Parameters

<i>tok</i>	The string to examine
------------	-----------------------

Returns

1 if the entire string is an integer, 0 if otherwise.

Definition at line [130](#) of file [vstring.c](#).

7.24.2.2 Vstring_strcasecmp()

```
VEXTERNC int Vstring_strcasecmp (
    const char * s1,
    const char * s2 )
```

Case-insensitive string comparison (BSD standard)

Author

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Note

Copyright (c) 1988-1993 The Regents of the University of California. Copyright (c) 1995-1996 Sun Microsystems, Inc.

Parameters

<i>s1</i>	First string for comparison
<i>s2</i>	Second string for comparison

Returns

An integer less than, equal to, or greater than zero if *s1* is found, respectively, to be less than, to match, or be greater than *s2*. (Source: Linux man pages)

Definition at line 66 of file [vstring.c](#).

7.24.2.3 Vstring_wrappedtext()

```
VEXTERNC char * Vstring_wrappedtext (
    const char * str,
    int right_margin,
    int left_padding )
```

Creates a wrapped and indented string from an input string

Author

Tucker Beck

Note

This function allocates a new string, so be sure to free it!

Creates a wrapped and indented string from an input string

Author

Tucker Beck

Note

This function allocates a new string, so be sure to free it!

Note

: The +2 is for the newline character and the null-terminating character;

Parameters

<i>str</i>	The input string to wrap and indent
<i>right_margin</i>	The number of characters to the right margin
<i>left_padding</i>	The number of characters in the left indent

Definition at line 155 of file [vstring.c](#).

7.25 Vunit class

Collection of constants and conversion factors.

Files

- file [vunit.h](#)
Contains a collection of useful constants and conversion factors.

Macros

- `#define Vunit_J_to_cal 4.1840000e+00`
Multiply by this to convert J to cal.
- `#define Vunit_cal_to_J 2.3900574e-01`
Multiply by this to convert cal to J.
- `#define Vunit_amu_to_kg 1.6605402e-27`
Multiply by this to convert amu to kg.
- `#define Vunit_kg_to_amu 6.0221367e+26`
Multiply by this to convert kg to amu.
- `#define Vunit_ec_to_C 1.6021773e-19`
Multiply by this to convert ec to C.
- `#define Vunit_C_to_ec 6.2415065e+18`
Multiply by this to convert C to ec.
- `#define Vunit_ec 1.6021773e-19`
Charge of an electron in C.
- `#define Vunit_kb 1.3806581e-23`
Boltzmann constant.
- `#define Vunit_Na 6.0221367e+23`
Avogadro's number.
- `#define Vunit_pi VPI`
Pi.
- `#define Vunit_eps0 8.8541878e-12`
Vacuum permittivity.
- `#define Vunit_esu_ec2A 3.3206364e+02`
 e_c^2 / in ESU units => kcal/mol
- `#define Vunit_esu_kb 1.9871913e-03`
 k_b in ESU units => kcal/mol

7.25.1 Detailed Description

Collection of constants and conversion factors.

7.25.2 Macro Definition Documentation

7.25.2.1 Vunit_amu_to_kg

```
#define Vunit_amu_to_kg 1.6605402e-27
```

Multiply by this to convert amu to kg.
Definition at line 76 of file [vunit.h](#).

7.25.2.2 Vunit_C_to_ec

```
#define Vunit_C_to_ec 6.2415065e+18
```

Multiply by this to convert C to ec.
Definition at line 88 of file [vunit.h](#).

7.25.2.3 Vunit_cal_to_J

```
#define Vunit_cal_to_J 2.3900574e-01
```

Multiply by this to convert cal to J.
Definition at line 72 of file [vunit.h](#).

7.25.2.4 Vunit_ec

```
#define Vunit_ec 1.6021773e-19
```

Charge of an electron in C.
Definition at line 92 of file [vunit.h](#).

7.25.2.5 Vunit_ec_to_C

```
#define Vunit_ec_to_C 1.6021773e-19
```

Multiply by this to convert ec to C.
Definition at line 84 of file [vunit.h](#).

7.25.2.6 Vunit_eps0

```
#define Vunit_eps0 8.8541878e-12
```

Vacuum permittivity.
Definition at line 108 of file [vunit.h](#).

7.25.2.7 Vunit_esu_ec2A

```
#define Vunit_esu_ec2A 3.3206364e+02
```

e_c^2 / in ESU units => kcal/mol
Definition at line 112 of file [vunit.h](#).

7.25.2.8 Vunit_esu_kb

```
#define Vunit_esu_kb 1.9871913e-03
```

k_b in ESU units => kcal/mol
Definition at line 116 of file [vunit.h](#).

7.25.2.9 Vunit_J_to_cal

```
#define Vunit_J_to_cal 4.1840000e+00
```

Multiply by this to convert J to cal.
Definition at line 68 of file [vunit.h](#).

7.25.2.10 Vunit_kb

```
#define Vunit_kb 1.3806581e-23
```

Boltzmann constant.
Definition at line 96 of file [vunit.h](#).

7.25.2.11 Vunit_kg_to_amu

```
#define Vunit_kg_to_amu 6.0221367e+26
```

Multiply by this to convert kg to amu.
Definition at line 80 of file [vunit.h](#).

7.25.2.12 Vunit_Na

```
#define Vunit_Na 6.0221367e+23
```

Avogadro's number.
Definition at line 100 of file [vunit.h](#).

7.25.2.13 Vunit_pi

```
#define Vunit_pi VPI
```

Pi.
Definition at line 104 of file [vunit.h](#).

7.26 Vgrid class

Oracle for Cartesian mesh data.

Files

- file [vgrid.c](#)
Class Vgrid methods.
- file [vgrid.h](#)
Potential oracle for Cartesian mesh data.

Data Structures

- struct [sVgrid](#)
Electrostatic potential oracle for Cartesian mesh data.

Macros

- `#define VGRID_DIGITS 6`
Number of decimal places for comparisons and formatting.

Typedefs

- typedef struct [sVgrid](#) Vgrid
Declaration of the Vgrid class as the sVgrid structure.

Functions

- VEXTERNC unsigned long int [Vgrid_memChk](#) ([Vgrid](#) *thee)
Return the memory used by this structure (and its contents) in bytes.
- VEXTERNC [Vgrid](#) * [Vgrid_ctor](#) (int nx, int ny, int nz, double hx, double hy, double hzed, double xmin, double ymin, double zmin, double *data)
Construct Vgrid object with values obtained from Vpmg_readDX (for example)
- VEXTERNC int [Vgrid_ctor2](#) ([Vgrid](#) *thee, int nx, int ny, int nz, double hx, double hy, double hzed, double xmin, double ymin, double zmin, double *data)
Initialize Vgrid object with values obtained from Vpmg_readDX (for example)
- VEXTERNC int [Vgrid_value](#) ([Vgrid](#) *thee, double x[3], double *value)
Get potential value (from mesh or approximation) at a point.
- VEXTERNC void [Vgrid_dtor](#) ([Vgrid](#) **thee)
Object destructor.
- VEXTERNC void [Vgrid_dtor2](#) ([Vgrid](#) *thee)
FORTTRAN stub object destructor.
- VEXTERNC int [Vgrid_curvature](#) ([Vgrid](#) *thee, double pt[3], int cflag, double *curv)
Get second derivative values at a point.
- VEXTERNC int [Vgrid_gradient](#) ([Vgrid](#) *thee, double pt[3], double grad[3])
Get first derivative values at a point.
- VEXTERNC int [Vgrid_readGZ](#) ([Vgrid](#) *thee, const char *fname)
Read in OpenDX data in GZIP format.
- VEXTERNC void [Vgrid_writeUHBD](#) ([Vgrid](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, char *title, double *pvec)
Write out the data in UHBD grid format.
- VEXTERNC void [Vgrid_writeDX](#) ([Vgrid](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, char *title, double *pvec)
Write out the data in OpenDX grid format.
- VEXTERNC int [Vgrid_readDX](#) ([Vgrid](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname)
Read in data in OpenDX grid format.
- VEXTERNC void [Vgrid_writeDXBIN](#) ([Vgrid](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, char *title, double *pvec)
Write out the binary data in OpenDX grid format.
- VEXTERNC int [Vgrid_readDXBIN](#) ([Vgrid](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname)
Read in binary data in OpenDX grid format.
- VEXTERNC double [Vgrid_integrate](#) ([Vgrid](#) *thee)
Get the integral of the data.
- VEXTERNC double [Vgrid_normL1](#) ([Vgrid](#) *thee)
Get the L_1 norm of the data. This returns the integral:
- VEXTERNC double [Vgrid_normL2](#) ([Vgrid](#) *thee)
Get the L_2 norm of the data. This returns the integral:
- VEXTERNC double [Vgrid_normLinf](#) ([Vgrid](#) *thee)
Get the L_∞ norm of the data. This returns the integral:
- VEXTERNC double [Vgrid_seminormH1](#) ([Vgrid](#) *thee)
Get the H_1 semi-norm of the data. This returns the integral:
- VEXTERNC double [Vgrid_normH1](#) ([Vgrid](#) *thee)
Get the H_1 norm (or energy norm) of the data. This returns the integral:

7.26.1 Detailed Description

Oracle for Cartesian mesh data.

7.26.2 Macro Definition Documentation

7.26.2.1 VGRID_DIGITS

```
#define VGRID_DIGITS 6
```

Number of decimal places for comparisons and formatting.

Definition at line 74 of file [vgrid.h](#).

7.26.3 Typedef Documentation

7.26.3.1 Vgrid

```
typedef struct sVgrid Vgrid
```

Declaration of the Vgrid class as the [sVgrid](#) structure.

Definition at line 106 of file [vgrid.h](#).

7.26.4 Function Documentation

7.26.4.1 Vgrid_ctor()

```
VEXTERNC Vgrid * Vgrid_ctor (
    int nx,
    int ny,
    int nz,
    double hx,
    double hy,
    double hzed,
    double xmin,
    double ymin,
    double zmin,
    double * data )
```

Construct Vgrid object with values obtained from Vpmsg_readDX (for example)

Author

Nathan Baker

Parameters

<i>nx</i>	Number grid points in x direction
<i>ny</i>	Number grid points in y direction
<i>nz</i>	Number grid points in z direction
<i>hx</i>	Grid spacing in x direction
<i>hy</i>	Grid spacing in y direction

Parameters

<i>hz</i>	Grid spacing in z direction
<i>xmin</i>	x coordinate of lower grid corner
<i>ymin</i>	y coordinate of lower grid corner
<i>zmin</i>	z coordinate of lower grid corner
<i>data</i>	nx*ny*nz array of data. This can be VNULL if you are planning to read in data later with one of the read routines

Returns

Newly allocated and initialized Vgrid object

Definition at line 86 of file [vgrid.c](#).

7.26.4.2 Vgrid_ctor2()

```

VEXTERNC int Vgrid_ctor2 (
    Vgrid * thee,
    int nx,
    int ny,
    int nz,
    double hx,
    double hy,
    double hzed,
    double xmin,
    double ymin,
    double zmin,
    double * data )

```

Initialize Vgrid object with values obtained from Vpmg_readDX (for example)

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to newly allocated Vgrid object
<i>nx</i>	Number grid points in x direction
<i>ny</i>	Number grid points in y direction
<i>nz</i>	Number grid points in z direction
<i>hx</i>	Grid spacing in x direction
<i>hy</i>	Grid spacing in y direction
<i>hz</i>	Grid spacing in z direction
<i>xmin</i>	x coordinate of lower grid corner
<i>ymin</i>	y coordinate of lower grid corner
<i>zmin</i>	z coordinate of lower grid corner
<i>data</i>	nx*ny*nz array of data. This can be VNULL if you are planning to read in data later with one of the read routines

Returns

Newly allocated and initialized Vgrid object

Definition at line 112 of file [vgrid.c](#).

7.26.4.3 Vgrid_curvature()

```
VEXTERNC int Vgrid_curvature (
    Vgrid * thee,
    double pt[3],
    int cflag,
    double * curv )
```

Get second derivative values at a point.

Author

Steve Bond and Nathan Baker

Parameters

<i>thee</i>	Pointer to Vgrid object
<i>pt</i>	Location to evaluate second derivative
<i>cflag</i>	<ul style="list-style-type: none"> • 0: Reduced Maximal Curvature • 1: Mean Curvature (Laplace) • 2: Gauss Curvature • 3: True Maximal Curvature
<i>curv</i>	Specified curvature value

Returns

1 if successful, 0 if off grid

Definition at line 299 of file [vgrid.c](#).

7.26.4.4 Vgrid_dtor()

```
VEXTERNC void Vgrid_dtor (
    Vgrid ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object to be destroyed
-------------	--

Definition at line 152 of file [vgrid.c](#).

7.26.4.5 Vgrid_dtor2()

```
VEXTERNC void Vgrid_dtor2 (
    Vgrid * thee )
```

FORTTRAN stub object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object to be destroyed
-------------	-----------------------------------

Definition at line 165 of file [vgrid.c](#).

7.26.4.6 Vgrid_gradient()

```
VEXTERNC int Vgrid_gradient (
    Vgrid * thee,
    double pt[3],
    double grad[3] )
```

Get first derivative values at a point.

Author

Nathan Baker and Steve Bond

Parameters

<i>thee</i>	Pointer to Vgrid object
<i>pt</i>	Location to evaluate gradient
<i>grad</i>	Gradient

Returns

1 if successful, 0 if off grid

Definition at line 379 of file [vgrid.c](#).

7.26.4.7 Vgrid_integrate()

```
VEXTERNC double Vgrid_integrate (
    Vgrid * thee )
```

Get the integral of the data.

Author

Nathan Baker

Parameters

<i>thee</i>	Vgrid object
-------------	--------------

Returns

Integral of data

Definition at line 1790 of file [vgrid.c](#).

7.26.4.8 Vgrid_memChk()

```

VEXTERNC unsigned long int Vgrid_memChk (
    Vgrid * thee )

```

Return the memory used by this structure (and its contents) in bytes.

Author

Nathan Baker

Parameters

<i>thee</i>	Vgrid object
-------------	--------------

Returns

The memory used by this structure and its contents in bytes

Definition at line 63 of file [vgrid.c](#).

7.26.4.9 Vgrid_normH1()

```

VEXTERNC double Vgrid_normH1 (
    Vgrid * thee )

```

Get the H_1 norm (or energy norm) of the data. This returns the integral:

Author

Nathan Baker

Parameters

<i>thee</i>	Vgrid object
-------------	--------------

Returns

Integral of data

$$\|u\|_{H_1} = \left(\int_{\Omega} |\nabla u(x)|^2 dx + \int_{\Omega} |u(x)|^2 dx \right)^{1/2}$$

Definition at line 1931 of file [vgrid.c](#).

7.26.4.10 Vgrid_normL1()

```
VEXTERNC double Vgrid_normL1 (
    Vgrid * thee )
```

Get the L_1 norm of the data. This returns the integral:

Author

Nathan Baker

Parameters

<i>thee</i>	Vgrid object
-------------	--------------

Returns

L_1 norm of data

$$\|u\|_{L_1} = \int_{\Omega} |u(x)| dx$$

Definition at line 1828 of file [vgrid.c](#).

7.26.4.11 Vgrid_normL2()

```
VEXTERNC double Vgrid_normL2 (
    Vgrid * thee )
```

Get the L_2 norm of the data. This returns the integral:

Author

Nathan Baker

Parameters

<i>thee</i>	Vgrid object
-------------	--------------

Returns

L_2 norm of data

$$\|u\|_{L_2} = \left(\int_{\Omega} |u(x)|^2 dx \right)^{1/2}$$

Definition at line 1858 of file [vgrid.c](#).

7.26.4.12 Vgrid_normLinf()

```
VEXTERNC double Vgrid_normLinf (
    Vgrid * thee )
```

Get the L_{∞} norm of the data. This returns the integral:

Author

Nathan Baker

Parameters

<i>thee</i>	Vgrid object
-------------	--------------

Returns

L_∞ norm of data

$$\|u\|_{L_\infty} = \sup_{x \in \Omega} |u(x)|$$

Definition at line 1946 of file [vgrid.c](#).

7.26.4.13 Vgrid_readDX()

```

VEXTERNC int Vgrid_readDX (
    Vgrid * thee,
    const char * iodev,
    const char * iofmt,
    const char * thost,
    const char * fname )

```

Read in data in OpenDX grid format.

Note

All dimension information is given in order: z, y, x

Author

Nathan Baker

Parameters

<i>thee</i>	Vgrid object
<i>iodev</i>	Input device type (FILE/BUFF/UNIX/INET)
<i>iofmt</i>	Input device format (ASCII/XDR)
<i>thost</i>	Input hostname (for sockets)
<i>fname</i>	Input FILE/BUFF/UNIX/INET name

Returns

1 if successful, 0 otherwise

Load grid from an input file using sockets.

Author

Nathan Baker

Definition at line 586 of file [vgrid.c](#).

7.26.4.14 Vgrid_readDXBIN()

```

VEXTERNC int Vgrid_readDXBIN (
    Vgrid * thee,

```

```

    const char * iodev,
    const char * iofmt,
    const char * thost,
    const char * fname )

```

Read in binary data in OpenDX grid format.

Note

All dimension information is given in order: z, y, x

Author

Juan Brandi

Parameters

<i>thee</i>	Vgrid object
<i>iodev</i>	Input device type (FILE/BUFF/UNIX/INET)
<i>iofmt</i>	Input device format (ASCII/XDR)
<i>thost</i>	Input hostname (for sockets)
<i>fname</i>	Input FILE/BUFF/UNIX/INET name

Returns

1 if successful, 0 otherwise

Load grid from an input dx binary file.

Author

Juan Brandi

Definition at line 810 of file [vgrid.c](#).

7.26.4.15 Vgrid_readGZ()

```

VEXTERNC int Vgrid_readGZ (
    Vgrid * thee,
    const char * fname )

```

Read in OpenDX data in GZIP format.

Author

Dave Gohara

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	Object with grid data to write
<i>fname</i>	Path to write to

Definition at line 462 of file [vgrid.c](#).

7.26.4.16 Vgrid_seminormH1()

```
VEXTERNC double Vgrid_seminormH1 (
    Vgrid * thee )
```

Get the H_1 semi-norm of the data. This returns the integral:

Author

Nathan Baker

Parameters

<i>thee</i>	Vgrid object
-------------	--------------

Returns

Integral of data

$$|u|_{H_1} = \left(\int_{\Omega} |\nabla u(x)|^2 dx \right)^{1/2}$$

Definition at line 1888 of file [vgrid.c](#).

7.26.4.17 Vgrid_value()

```
VEXTERNC int Vgrid_value (
    Vgrid * thee,
    double x[3],
    double * value )
```

Get potential value (from mesh or approximation) at a point.

Author

Nathan Baker

Parameters

<i>thee</i>	Vgrid obejct
<i>x</i>	Point at which to evaluate potential
<i>value</i>	Value of data at point x

Returns

1 if successful, 0 if off grid

Definition at line 179 of file [vgrid.c](#).

7.26.4.18 Vgrid_writeDX()

```
VEXTERNC void Vgrid_writeDX (
    Vgrid * thee,
```

```

    const char * iodev,
    const char * iofmt,
    const char * thost,
    const char * fname,
    char * title,
    double * pvec )

```

Write out the data in OpenDX grid format.

Author

Nathan Baker

Parameters

<i>thee</i>	Grid object
<i>iodev</i>	Output device type (FILE/BUFF/UNIX/INET)
<i>iofmt</i>	Output device format (ASCII/XDR)
<i>thost</i>	Output hostname (for sockets)
<i>fname</i>	Output FILE/BUFF/UNIX/INET name
<i>title</i>	Title to be inserted in grid file
<i>pvec</i>	Partition weight (if 1: point in current partition, if 0 point not in current partition if > 0 && < 1 point on/near boundary)

Definition at line 1206 of file [vgrid.c](#).

7.26.4.19 Vgrid_writeDXBIN()

```

VEXTERNC void Vgrid_writeDXBIN (
    Vgrid * thee,
    const char * iodev,
    const char * iofmt,
    const char * thost,
    const char * fname,
    char * title,
    double * pvec )

```

Write out the binary data in OpenDX grid format.

Author

Nathan Baker

Parameters

<i>thee</i>	Grid object
<i>iodev</i>	Output device type (FILE/BUFF/UNIX/INET)
<i>iofmt</i>	Output device format (ASCII/XDR)
<i>thost</i>	Output hostname (for sockets)
<i>fname</i>	Output FILE/BUFF/UNIX/INET name
<i>title</i>	Title to be inserted in grid file
<i>pvec</i>	Partition weight (if 1: point in current partition, if 0 point not in current partition if > 0 && < 1 point on/near boundary)

Definition at line 1458 of file [vgrid.c](#).

7.26.4.20 Vgrid_writeUHBD()

```

VEXTERNC void Vgrid_writeUHBD (
    Vgrid * thee,
    const char * iodev,
    const char * iofmt,
    const char * thost,
    const char * fname,
    char * title,
    double * pvec )

```

Write out the data in UHBD grid format.

Note

- The mesh spacing should be uniform
- Format changed from %12.6E to %12.5E

Author

Nathan Baker

Parameters

<i>thee</i>	Grid object
<i>iodev</i>	Output device type (FILE/BUFF/UNIX/INET)
<i>iofmt</i>	Output device format (ASCII/XDR)
<i>thost</i>	Output hostname (for sockets)
<i>fname</i>	Output FILE/BUFF/UNIX/INET name
<i>title</i>	Title to be inserted in grid file
<i>pvec</i>	Partition weight (if 1: point in current partition, if 0 point not in current partition if > 0 && < 1 point on/near boundary)

Bug This routine does not respect partition information

Definition at line 1692 of file [vgrid.c](#).

7.27 Vmgrid class

Oracle for Cartesian mesh data.

Files

- file [vmgrid.c](#)
Class Vmgrid methods.
- file [vmgrid.h](#)
Multiresolution oracle for Cartesian mesh data.

Data Structures

- struct [sVmgrid](#)
Multiresolution oracle for Cartesian mesh data.

Macros

- `#define VMGRIDMAX 20`
The maximum number of levels in the grid hierarchy.

Typedefs

- typedef struct [sVmgrid](#) [Vmgrid](#)
Declaration of the Vmgrid class as the Vmgrid structure.

Functions

- VEXTERNC [Vmgrid](#) * [Vmgrid_ctor](#) ()
Construct Vmgrid object.
- VEXTERNC int [Vmgrid_ctor2](#) ([Vmgrid](#) *thee)
Initialize Vmgrid object.
- VEXTERNC int [Vmgrid_value](#) ([Vmgrid](#) *thee, double x[3], double *value)
Get potential value (from mesh or approximation) at a point.
- VEXTERNC void [Vmgrid_dtor](#) ([Vmgrid](#) **thee)
Object destructor.
- VEXTERNC void [Vmgrid_dtor2](#) ([Vmgrid](#) *thee)
FORTTRAN stub object destructor.
- VEXTERNC int [Vmgrid_addGrid](#) ([Vmgrid](#) *thee, [Vgrid](#) *grid)
Add a grid to the hierarchy.
- VEXTERNC int [Vmgrid_curvature](#) ([Vmgrid](#) *thee, double pt[3], int cflag, double *curv)
Get second derivative values at a point.
- VEXTERNC int [Vmgrid_gradient](#) ([Vmgrid](#) *thee, double pt[3], double grad[3])
Get first derivative values at a point.
- VEXTERNC [Vgrid](#) * [Vmgrid_getGridByNum](#) ([Vmgrid](#) *thee, int num)
Get specific grid in hierarchy.
- VEXTERNC [Vgrid](#) * [Vmgrid_getGridByPoint](#) ([Vmgrid](#) *thee, double pt[3])
Get grid in hierarchy which contains specified point or VNULL.

7.27.1 Detailed Description

Oracle for Cartesian mesh data.

7.27.2 Macro Definition Documentation

7.27.2.1 VMGRIDMAX

```
#define VMGRIDMAX 20
```

The maximum number of levels in the grid hierarchy.

Definition at line 76 of file [vmgrid.h](#).

7.27.3 Typedef Documentation

7.27.3.1 Vmgrid

```
typedef struct sVmgrid Vmgrid
```

Declaration of the Vmgrid class as the Vmgrid structure.

Definition at line 98 of file [vmgrid.h](#).

7.27.4 Function Documentation

7.27.4.1 Vmgrid_addGrid()

```
VEXTERNC int Vmgrid_addGrid (
    Vmgrid * thee,
    Vgrid * grid )
```

Add a grid to the hierarchy.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object to be destroyed
<i>grid</i>	Grid to be added. As mentioned above, we would prefer to have the finest grid added first, next-finest second, ..., coarsest last – this is how the grid will be searched when looking up values for points. However, this is not enforced to provide flexibility for cases where the dataset is decomposed into disjoint partitions, etc.

Returns

1 if successful, 0 otherwise

Definition at line 195 of file [vmgrid.c](#).

7.27.4.2 Vmgrid_ctor()

```
VEXTERNC Vmgrid * Vmgrid_ctor ( )
```

Construct Vmgrid object.

Author

Nathan Baker

Returns

Newly allocated and initialized Vmgrid object

Definition at line 57 of file [vmgrid.c](#).

7.27.4.3 Vmgrid_ctor2()

```
VEXTERNC int Vmgrid_ctor2 (
    Vmgrid * thee )
```

Initialize Vmgrid object.

Author

Nathan Baker

Parameters

<i>thee</i>	Newly allocated Vmgrid object
-------------	-------------------------------

Returns

Newly allocated and initialized Vmgrid object

Definition at line 72 of file [vmgrid.c](#).

7.27.4.4 Vmgrid_curvature()

```
VEXTERNC int Vmgrid_curvature (
    Vmgrid * thee,
    double pt[3],
    int cflag,
    double * curv )
```

Get second derivative values at a point.

Author

Nathan Baker (wrapper for Vgrid routine by Steve Bond)

Parameters

<i>thee</i>	Pointer to Vmgrid object
<i>pt</i>	Location to evaluate second derivative
<i>cflag</i>	<ul style="list-style-type: none"> • 0: Reduced Maximal Curvature • 1: Mean Curvature (Laplace) • 2: Gauss Curvature • 3: True Maximal Curvature
<i>curv</i>	Specified curvature value

Returns

1 if successful, 0 if off grid

Definition at line 138 of file [vmgrid.c](#).

7.27.4.5 Vmgrid_dtor()

```
VEXTERNC void Vmgrid_dtor (  
    Vmgrid ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object to be destroyed
-------------	--

Definition at line 88 of file [vmgrid.c](#).

7.27.4.6 Vmgrid_dtor2()

```
VEXTERNC void Vmgrid_dtor2 (  
    Vmgrid * thee )
```

FORTTRAN stub object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object to be destroyed
-------------	-----------------------------------

Definition at line 101 of file [vmgrid.c](#).

7.27.4.7 Vmgrid_getGridByNum()

```
VEXTERNC Vgrid * Vmgrid_getGridByNum (  
    Vmgrid * thee,  
    int num )
```

Get specific grid in hierarchy.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to Vmgrid object
<i>num</i>	Number of grid in hierarchy

Returns

Pointer to specified grid

7.27.4.8 Vmgrid_getGridByPoint()

```
VEXTERNC Vgrid * Vmgrid_getGridByPoint (
    Vmgrid * thee,
    double pt[3] )
```

Get grid in hierarchy which contains specified point or VNULL.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to Vmgrid object
<i>pt</i>	Point to check

Returns

Pointer to specified grid

7.27.4.9 Vmgrid_gradient()

```
VEXTERNC int Vmgrid_gradient (
    Vmgrid * thee,
    double pt[3],
    double grad[3] )
```

Get first derivative values at a point.

Author

Nathan Baker and Steve Bond

Parameters

<i>thee</i>	Pointer to Vmgrid object
<i>pt</i>	Location to evaluate gradient
<i>grad</i>	Gradient

Returns

1 if successful, 0 if off grid

Definition at line 167 of file [vmgrid.c](#).

7.27.4.10 Vmgrid_value()

```
VEXTERNC int Vmgrid_value (
    Vmgrid * thee,
    double x[3],
    double * value )
```

Get potential value (from mesh or approximation) at a point.

Author

Nathan Baker

Parameters

<i>thee</i>	Vmgrid obejct
<i>x</i>	Point at which to evaluate potential
<i>value</i>	Value of data at point x

Returns

1 if successful, 0 if off grid

Definition at line 107 of file [vmgrid.c](#).

7.28 Vopot class

Potential oracle for Cartesian mesh data.

Files

- file [vopot.c](#)
Class Vopot methods.
- file [vopot.h](#)
Potential oracle for Cartesian mesh data.

Data Structures

- struct [sVopot](#)
Electrostatic potential oracle for Cartesian mesh data.

Typedefs

- typedef struct [sVopot](#) [Vopot](#)
Declaration of the Vopot class as the Vopot structure.

Functions

- VEXTERNC [Vopot](#) * [Vopot_ctor](#) ([Vmgrid](#) *mgrid, [Vpbe](#) *pbe, [Vbcfl](#) bcfl)
Construct Vopot object with values obtained from Vpmg_readDX (for example)
- VEXTERNC int [Vopot_ctor2](#) ([Vopot](#) *thee, [Vmgrid](#) *mgrid, [Vpbe](#) *pbe, [Vbcfl](#) bcfl)
Initialize Vopot object with values obtained from Vpmg_readDX (for example)
- VEXTERNC int [Vopot_pot](#) ([Vopot](#) *thee, double x[3], double *pot)
Get potential value (from mesh or approximation) at a point.
- VEXTERNC void [Vopot_dtor](#) ([Vopot](#) **thee)
Object destructor.
- VEXTERNC void [Vopot_dtor2](#) ([Vopot](#) *thee)
FORTTRAN stub object destructor.
- VEXTERNC int [Vopot_curvature](#) ([Vopot](#) *thee, double pt[3], int cflag, double *curv)

Get second derivative values at a point.

- VEXTERNC int [Vopot_gradient](#) ([Vopot](#) *thee, double pt[3], double grad[3])

Get first derivative values at a point.

7.28.1 Detailed Description

Potential oracle for Cartesian mesh data.

7.28.2 Typedef Documentation

7.28.2.1 Vopot

```
typedef struct sVopot Vopot
```

Declaration of the Vopot class as the Vopot structure.

Definition at line 96 of file [vopot.h](#).

7.28.3 Function Documentation

7.28.3.1 Vopot_ctor()

```
VEXTERNC Vopot * Vopot_ctor (
    Vmgrid * mgrid,
    Vpbe * pbe,
    Vbcfl bcfl )
```

Construct Vopot object with values obtained from Vpmg_readDX (for example)

Author

Nathan Baker

Parameters

<i>mgrid</i>	Multiple grid object containing potential data (in units kT/e)
<i>pbe</i>	Pointer to Vpbe object for parameters
<i>bcfl</i>	Boundary condition to use for potential values off the grid

Returns

Newly allocated and initialized Vopot object

Definition at line 65 of file [vopot.c](#).

7.28.3.2 Vopot_ctor2()

```
VEXTERNC int Vopot_ctor2 (
    Vopot * thee,
    Vmgrid * mgrid,
    Vpbe * pbe,
    Vbcfl bcfl )
```

Initialize Vopot object with values obtained from Vpmg_readDX (for example)

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to newly allocated Vopot object
<i>mgrid</i>	Multiple grid object containing potential data (in units kT/e)
<i>pbe</i>	Pointer to Vpbe object for parameters
<i>bcll</i>	Boundary condition to use for potential values off the grid

Returns

1 if successful, 0 otherwise

Definition at line 80 of file [vopot.c](#).**7.28.3.3 Vopot_curvature()**

```

VEXTERNC int Vopot_curvature (
    Vopot * thee,
    double pt[3],
    int cflag,
    double * curv )

```

Get second derivative values at a point.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to Vopot object
<i>pt</i>	Location to evaluate second derivative
<i>cflag</i>	<ul style="list-style-type: none"> • 0: Reduced Maximal Curvature • 1: Mean Curvature (Laplace) • 2: Gauss Curvature • 3: True Maximal Curvature
<i>curv</i>	Set to specified curvature value

Returns

1 if successful, 0 otherwise

Definition at line 214 of file [vopot.c](#).

7.28.3.4 Vopot_dtor()

```
VEXTERNC void Vopot_dtor (  
    Vopot ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object to be destroyed
-------------	--

Definition at line 94 of file [vopot.c](#).

7.28.3.5 Vopot_dtor2()

```
VEXTERNC void Vopot_dtor2 (  
    Vopot * thee )
```

FORTTRAN stub object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object to be destroyed
-------------	-----------------------------------

Definition at line 107 of file [vopot.c](#).

7.28.3.6 Vopot_gradient()

```
VEXTERNC int Vopot_gradient (  
    Vopot * thee,  
    double pt[3],  
    double grad[3] )
```

Get first derivative values at a point.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to Vopot object
-------------	-------------------------

Parameters

<i>pt</i>	Location to evaluate gradient
<i>grad</i>	Gradient

Returns

1 if successful, 0 otherwise

Definition at line 300 of file [vopot.c](#).

7.28.3.7 Vopot_pot()

```
VEXTERNC int Vopot_pot (
    Vopot * thee,
    double x[3],
    double * pot )
```

Get potential value (from mesh or approximation) at a point.

Author

Nathan Baker

Parameters

<i>thee</i>	Vopot obejct
<i>x</i>	Point at which to evaluate potential
<i>pot</i>	Set to dimensionless potential (units kT/e) at point x

Returns

1 if successful, 0 otherwise

Definition at line 114 of file [vopot.c](#).

7.29 Vpmg class

A wrapper for Mike Holst's PMG multigrid code.

Files

- file [vpmg.c](#)
Class Vpmg methods.
- file [vpmg.h](#)
Contains declarations for class Vpmg.

Data Structures

- struct [sVpmg](#)
Contains public data members for Vpmg class/module.

Typedefs

- typedef struct [sVpmg](#) [Vpmg](#)

Declaration of the Vpmg class as the Vpmg structure.

Functions

- VEXTERNC unsigned long int [Vpmg_memChk](#) ([Vpmg](#) *thee)
Return the memory used by this structure (and its contents) in bytes.
- VEXTERNC [Vpmg](#) * [Vpmg_ctor](#) ([Vpmgp](#) *parms, [Vpbe](#) *pbe, int focusFlag, [Vpmg](#) *pmgOLD, [MGparm](#) *mgparm, [PBEparm_calcEnergy](#) energyFlag)
Constructor for the Vpmg class (allocates new memory)
- VEXTERNC int [Vpmg_ctor2](#) ([Vpmg](#) *thee, [Vpmgp](#) *parms, [Vpbe](#) *pbe, int focusFlag, [Vpmg](#) *pmgOLD, [MGparm](#) *mgparm, [PBEparm_calcEnergy](#) energyFlag)
FORTTRAN stub constructor for the Vpmg class (uses previously-allocated memory)
- VEXTERNC void [Vpmg_dtor](#) ([Vpmg](#) **thee)
Object destructor.
- VEXTERNC void [Vpmg_dtor2](#) ([Vpmg](#) *thee)
FORTTRAN stub object destructor.
- VEXTERNC int [Vpmg_fillco](#) ([Vpmg](#) *thee, [Vsurf_Meth](#) surfMeth, double splineWin, [Vchrg_Meth](#) chargeMeth, int useDielXMap, [Vgrid](#) *dielXMap, int useDielYMap, [Vgrid](#) *dielYMap, int useDielZMap, [Vgrid](#) *dielZMap, int useKappaMap, [Vgrid](#) *kappaMap, int usePotMap, [Vgrid](#) *potMap, int useChargeMap, [Vgrid](#) *chargeMap)
Fill the coefficient arrays prior to solving the equation.
- VEXTERNC int [Vpmg_solve](#) ([Vpmg](#) *thee)
Solve the PBE using PMG.
- VEXTERNC int [Vpmg_solveLaplace](#) ([Vpmg](#) *thee)
Solve Poisson's equation with a homogeneous Laplacian operator using the solvent dielectric constant. This solution is performed by a sine wave decomposition.
- VEXTERNC double [Vpmg_energy](#) ([Vpmg](#) *thee, int extFlag)
Get the total electrostatic energy.
- VEXTERNC double [Vpmg_qfEnergy](#) ([Vpmg](#) *thee, int extFlag)
Get the "fixed charge" contribution to the electrostatic energy.
- VEXTERNC double [Vpmg_qfAtomEnergy](#) ([Vpmg](#) *thee, [Vatom](#) *atom)
Get the per-atom "fixed charge" contribution to the electrostatic energy.
- VEXTERNC double [Vpmg_qmEnergy](#) ([Vpmg](#) *thee, int extFlag)
Get the "mobile charge" contribution to the electrostatic energy.
- VEXTERNC double [Vpmg_dielEnergy](#) ([Vpmg](#) *thee, int extFlag)
Get the "polarization" contribution to the electrostatic energy.
- VEXTERNC double [Vpmg_dielGradNorm](#) ([Vpmg](#) *thee)
Get the integral of the gradient of the dielectric function.
- VEXTERNC int [Vpmg_force](#) ([Vpmg](#) *thee, double *force, int atomID, [Vsurf_Meth](#) srfrm, [Vchrg_Meth](#) chgfm)
Calculate the total force on the specified atom in units of $k_B T/AA$.
- VEXTERNC int [Vpmg_qfForce](#) ([Vpmg](#) *thee, double *force, int atomID, [Vchrg_Meth](#) chgfm)
Calculate the "charge-field" force on the specified atom in units of $k_B T/AA$.
- VEXTERNC int [Vpmg_dbForce](#) ([Vpmg](#) *thee, double *dbForce, int atomID, [Vsurf_Meth](#) srfrm)
Calculate the dielectric boundary forces on the specified atom in units of $k_B T/AA$.
- VEXTERNC int [Vpmg_ibForce](#) ([Vpmg](#) *thee, double *force, int atomID, [Vsurf_Meth](#) srfrm)
Calculate the osmotic pressure on the specified atom in units of $k_B T/AA$.
- VEXTERNC void [Vpmg_setPart](#) ([Vpmg](#) *thee, double lowerCorner[3], double upperCorner[3], int bflags[6])

Set partition information which restricts the calculation of observables to a (rectangular) subset of the problem domain.

- VEXTERNC void `Vpmg_unsetPart` (`Vpmg *thee`)

Remove partition restrictions.

- VEXTERNC int `Vpmg_fillArray` (`Vpmg *thee`, double `*vec`, `Vdata_Type` type, double `parm`, `Vhal_PBEType` pbe-type, `PBEparm *pbeparm`)

Fill the specified array with accessibility values.

- VPUBLIC void `Vpmg_fieldSpline4` (`Vpmg *thee`, int `atomID`, double `field[3]`)

Computes the field at an atomic center using a stencil based on the first derivative of a 5th order B-spline.

- VEXTERNC double `Vpmg_qfPermanentMultipoleEnergy` (`Vpmg *thee`, int `atomID`)

Computes the permanent multipole electrostatic hydration energy (the polarization component of the hydration energy currently computed in TINKER).

- VEXTERNC void `Vpmg_qfPermanentMultipoleForce` (`Vpmg *thee`, int `atomID`, double `force[3]`, double `torque[3]`)

Computes the q-Phi Force for permanent multipoles based on 5th order B-splines.

- VEXTERNC void `Vpmg_ibPermanentMultipoleForce` (`Vpmg *thee`, int `atomID`, double `force[3]`)

Compute the ionic boundary force for permanent multipoles.

- VEXTERNC void `Vpmg_dbPermanentMultipoleForce` (`Vpmg *thee`, int `atomID`, double `force[3]`)

Compute the dielectric boundary force for permanent multipoles.

- VEXTERNC void `Vpmg_qfDirectPolForce` (`Vpmg *thee`, `Vgrid *perm`, `Vgrid *induced`, int `atomID`, double `force[3]`, double `torque[3]`)

q-Phi direct polarization force between permanent multipoles and induced dipoles, which are induced by the sum of the permanent intramolecular field and the permanent reaction field.

- VEXTERNC void `Vpmg_qfNLDirectPolForce` (`Vpmg *thee`, `Vgrid *perm`, `Vgrid *nlInduced`, int `atomID`, double `force[3]`, double `torque[3]`)

q-Phi direct polarization force between permanent multipoles and non-local induced dipoles based on 5th Order B-Splines. Keep in mind that the "non-local" induced dipoles are just a mathematical quantity that result from differentiation of the AMOEBA polarization energy.

- VEXTERNC void `Vpmg_ibDirectPolForce` (`Vpmg *thee`, `Vgrid *perm`, `Vgrid *induced`, int `atomID`, double `force[3]`)

Ionic boundary direct polarization force between permanent multipoles and induced dipoles, which are induced by the sum of the permanent intramolecular field and the permanent reaction field.

- VEXTERNC void `Vpmg_ibNLDirectPolForce` (`Vpmg *thee`, `Vgrid *perm`, `Vgrid *nlInduced`, int `atomID`, double `force[3]`)

Ionic boundary direct polarization force between permanent multipoles and non-local induced dipoles based on 5th order. Keep in mind that the "non-local" induced dipoles are just a mathematical quantity that result from differentiation of the AMOEBA polarization energy.

- VEXTERNC void `Vpmg_dbDirectPolForce` (`Vpmg *thee`, `Vgrid *perm`, `Vgrid *induced`, int `atomID`, double `force[3]`)

Dielectric boundary direct polarization force between permanent multipoles and induced dipoles, which are induced by the sum of the permanent intramolecular field and the permanent reaction field.

- VEXTERNC void `Vpmg_dbNLDirectPolForce` (`Vpmg *thee`, `Vgrid *perm`, `Vgrid *nlInduced`, int `atomID`, double `force[3]`)

Dielectric boundary direct polarization force between permanent multipoles and non-local induced dipoles. Keep in mind that the "non-local" induced dipoles are just a mathematical quantity that result from differentiation of the AMOEBA polarization energy.

- VEXTERNC void `Vpmg_qfMutualPolForce` (`Vpmg *thee`, `Vgrid *induced`, `Vgrid *nlInduced`, int `atomID`, double `force[3]`)

Mutual polarization force for induced dipoles based on 5th order B-Splines. This force arises due to self-consistent convergence of the solute induced dipoles and reaction field.

- VEXTERNC void `Vpmg_ibMutualPolForce` (`Vpmg *thee`, `Vgrid *induced`, `Vgrid *nlInduced`, int `atomID`, double `force[3]`)

Ionic boundary mutual polarization force for induced dipoles based on 5th order B-Splines. This force arises due to self-consistent convergence of the solute induced dipoles and reaction field.

- VEXTERNC void [Vpmg_dbMutualPolForce](#) ([Vpmg](#) *thee, [Vgrid](#) *induced, [Vgrid](#) *nllInduced, int atomID, double force[3])
Dielectric boundary mutual polarization force for induced dipoles based on 5th order B-Splines. This force arises due to self-consistent convergence of the solute induced dipoles and reaction field.
- VEXTERNC void [Vpmg_printColComp](#) ([Vpmg](#) *thee, char path[72], char title[72], char mxtype[3], int flag)
Print out a column-compressed sparse matrix in Harwell-Boeing format.
- VPRIVATE void [bcolcomp](#) (int *iparm, double *rparm, int *iwork, double *rwork, double *values, int *rowind, int *colptr, int *flag)
Build a column-compressed matrix in Harwell-Boeing format.
- VPRIVATE void [bcolcomp2](#) (int *iparm, double *rparm, int *nx, int *ny, int *nz, int *iz, int *ipc, double *rpc, double *ac, double *cc, double *values, int *rowind, int *colptr, int *flag)
Build a column-compressed matrix in Harwell-Boeing format.
- VPRIVATE void [bcolcomp3](#) (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac, double *cc, double *values, int *rowind, int *colptr, int *flag)
Build a column-compressed matrix in Harwell-Boeing format.
- VPRIVATE void [bcolcomp4](#) (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *oC, double *cc, double *oE, double *oN, double *uC, double *values, int *rowind, int *colptr, int *flag)
Build a column-compressed matrix in Harwell-Boeing format.
- VPRIVATE void [pcolcomp](#) (int *nrow, int *ncol, int *nnzero, double *values, int *rowind, int *colptr, char *path, char *title, char *mxtype)
Print a column-compressed matrix in Harwell-Boeing format.
- VEXTERNC void [Vpackmg](#) (int *iparm, double *rparm, size_t *nrwk, int *niwk, int *nx, int *ny, int *nz, int *nlev, int *nu1, int *nu2, int *mgkey, int *itmax, int *istop, int *ipcon, int *nonlin, int *mgsmoo, int *mgprol, int *mgcoar, int *mgsolv, int *mgdisc, int *iinfo, double *errtol, int *ipkey, double *omegal, double *omegan, int *irite, int *iperf)
Print out a column-compressed sparse matrix in Harwell-Boeing format.

7.29.1 Detailed Description

A wrapper for Mike Holst's PMG multigrid code.

Note

Many of the routines and macros are borrowed from the [main.c](#) driver (written by Mike Holst) provided with the PMG code.

7.29.2 Typedef Documentation

7.29.2.1 Vpmg

```
typedef struct sVpmg Vpmg
```

Declaration of the Vpmg class as the Vpmg structure.

Definition at line 195 of file [vpmg.h](#).

7.29.3 Function Documentation

7.29.3.1 bcolcomp()

```
VPRIVATE void bcolcomp (
    int * iparm,
    double * rparm,
    int * iwork,
    double * rwork,
    double * values,
    int * rowind,
    int * colptr,
    int * flag )
```

Build a column-compressed matrix in Harwell-Boeing format.

Author

Tucker Beck [C Translation] Nathan Baker [Original] (mostly ripped off from Harwell-Boeing format documentation)Michael Schnieders)

Parameters

<i>iparm</i>	
<i>rparm</i>	
<i>iwork</i>	
<i>rwork</i>	
<i>values</i>	
<i>rowind</i>	
<i>colptr</i>	
<i>flag</i>	Operation selection parameter 0 = Use Poisson operator only 1 = Use linearization of full operation around current solution.

Definition at line [10741](#) of file [vpmg.c](#).

7.29.3.2 bcolcomp2()

```
VPRIVATE void bcolcomp2 (
    int * iparm,
    double * rparm,
    int * nx,
    int * ny,
    int * nz,
    int * iz,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,
    double * values,
    int * rowind,
    int * colptr,
    int * flag )
```

Build a column-compressed matrix in Harwell-Boeing format.

Author

Tucker Beck [C Translation] Nathan Baker [Original] (mostly ripped off from Harwell-Boeing format documentation)Michael Schnieders)

Parameters

<i>iparm</i>	
<i>rparm</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>iz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>values</i>	
<i>rowind</i>	
<i>colptr</i>	
<i>flag</i>	Operation selection parameter 0 = Use Poisson operator only 1 = Use linearization of full operation around current solution.

Definition at line 10795 of file [vpmg.c](#).

7.29.3.3 bcolcomp3()

```
VPRIVATE void bcolcomp3 (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,
    double * values,
    int * rowind,
    int * colptr,
    int * flag )
```

Build a column-compressed matrix in Harwell-Boeing format.

Author

Tucker Beck [C Translation] Nathan Baker [Original] (mostly ripped off from Harwell-Boeing format documentation)Michael Schnieders)

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	

Parameters

<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>values</i>	
<i>rowind</i>	
<i>colptr</i>	
<i>flag</i>	

Definition at line [10831](#) of file [vpmg.c](#).

7.29.3.4 bcolcomp4()

```
VPRIVATE void bcolcomp4 (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * oC,
    double * cc,
    double * oE,
    double * oN,
    double * uC,
    double * values,
    int * rowind,
    int * colptr,
    int * flag )
```

Build a column-compressed matrix in Harwell-Boeing format.

Author

Tucker Beck [C Translation] Nathan Baker [Original] (mostly ripped off from Harwell-Boeing format documentation)Michael Schnieders)

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>oC</i>	
<i>cc</i>	
<i>oE</i>	
<i>oN</i>	
<i>uC</i>	
<i>values</i>	
<i>rowind</i>	
<i>colptr</i>	
<i>flag</i>	

Definition at line 10858 of file [vpmg.c](#).

7.29.3.5 pcolcomp()

```
VPRIVATE void pcolcomp (
    int * nrow,
    int * ncol,
    int * nnzero,
    double * values,
    int * rowind,
    int * colptr,
    char * path,
    char * title,
    char * mxtype )
```

Print a column-compressed matrix in Harwell-Boeing format.

Author

Tucker Beck [C Translation] Nathan Baker [Original] (mostly ripped off from Harwell-Boeing format documentation)Michael Schnieders)

Parameters

<i>nrow</i>	
<i>ncol</i>	
<i>nnzero</i>	
<i>values</i>	
<i>rowind</i>	
<i>colptr</i>	
<i>path</i>	
<i>title</i>	
<i>mxtype</i>	

Definition at line 11023 of file [vpmg.c](#).

7.29.3.6 Vpackmg()

```
VEXTERNC void Vpackmg (
    int * iparm,
    double * rparm,
    size_t * nrwk,
    int * niwk,
    int * nx,
    int * ny,
    int * nz,
    int * nlev,
    int * nul,
    int * nu2,
    int * mgkey,
    int * itmax,
    int * istop,
    int * ipcon,
```

```

    int * nonlin,
    int * mgsmoo,
    int * mgprol,
    int * mgcoar,
    int * mgsolv,
    int * mgdisc,
    int * iinfo,
    double * errtol,
    int * ipkey,
    double * omegal,
    double * omegan,
    int * irite,
    int * iperf )

```

Print out a column-compressed sparse matrix in Harwell-Boeing format.

Author

Nathan Baker

Bug Can this path variable be replaced with a Vio socket?

Definition at line 555 of file [mgsubd.c](#).

7.29.3.7 Vpmg_ctor()

```

VEXTERNC Vpmg * Vpmg_ctor (
    Vpmgp * parms,
    Vpbe * pbe,
    int focusFlag,
    Vpmg * pmgOLD,
    MGparm * mgparm,
    PBEparm_calcEnergy energyFlag )

```

Constructor for the Vpmg class (allocates new memory)

Author

Nathan Baker

Returns

Pointer to newly allocated Vpmg object

Parameters

<i>parms</i>	PMG parameter object
<i>pbe</i>	PBE-specific variables
<i>focusFlag</i>	1 for focusing, 0 otherwise
<i>pmgOLD</i>	Old Vpmg object to use for boundary conditions
<i>mgparm</i>	MGparm parameter object for boundary conditions
<i>energyFlag</i>	What types of energies to calculate

Definition at line 141 of file [vpmg.c](#).

7.29.3.8 Vpmg_ctor2()

```

VEXTERNC int Vpmg_ctor2 (
    Vpmg * thee,
    Vpmgp * parms,
    Vpbe * pbe,
    int focusFlag,
    Vpmg * pmgOLD,
    MGparm * mgparm,
    PBEparm_calcEnergy energyFlag )

```

FORTRAN stub constructor for the Vpmg class (uses previously-allocated memory)

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Note

this is common to both replace/noreplace options

The fortran replacement functions are run along side the old fortran functions. This is due to the use of common variables in the fortran sub-routines. Once the fortran code has been successfully excised, these functions will no longer need to be called in tandem, and the fortran version may be dropped

Parameters

<i>thee</i>	Memory location for object
<i>parms</i>	PMG parameter object
<i>pbe</i>	PBE-specific variables
<i>focusFlag</i>	1 for focusing, 0 otherwise
<i>pmgOLD</i>	Old Vpmg object to use for boundary conditions (can be VNULL if focusFlag = 0)
<i>mgparm</i>	MGparm parameter object for boundary conditions (can be VNULL if focusFlag = 0)
<i>energyFlag</i>	What types of energies to calculate (ignored if focusFlag = 0)

Definition at line 153 of file [vpmg.c](#).

7.29.3.9 Vpmg_dbDirectPolForce()

```

VEXTERNC void Vpmg_dbDirectPolForce (
    Vpmg * thee,
    Vgrid * perm,
    Vgrid * induced,
    int atomID,
    double force[3] )

```

Dielectric boundary direct polarization force between permanent multipoles and induced dipoles, which are induced by the sum of the permanent intramolecular field and the permanent reaction field.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>perm</i>	Permanent multipole potential
<i>induced</i>	Induced dipole potential
<i>atomID</i>	Atom index
<i>force</i>	(returned) force

7.29.3.10 Vpmg_dbForce()

```
VEXTERNC int Vpmg_dbForce (
    Vpmg * thee,
    double * dbForce,
    int atomID,
    Vsurf_Meth srfm )
```

Calculate the dielectric boundary forces on the specified atom in units of $k_B T/AA$.

Author

Nathan Baker

Note

- Using the force evaluation methods of Im et al (Roux group), Comput Phys Commun, 111, 59–75 (1998). However, this gives the whole (self-interactions included) force – reaction field forces will have to be calculated at higher level.
- No contributions are made from higher levels of focusing.

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	Vpmg object
<i>dbForce</i>	3*sizeof(double) space to hold the dielectric boundary force in units of $k_B T/AA$
<i>atomID</i>	Valist ID of desired atom
<i>srfm</i>	Surface discretization method

Definition at line 6010 of file [vpmg.c](#).

7.29.3.11 Vpmg_dbMutualPolForce()

```
VEXTERNC void Vpmg_dbMutualPolForce (
    Vpmg * thee,
    Vgrid * induced,
```

```

Vgrid * nlInduced,
int atomID,
double force[3] )

```

Dielectric boundary mutual polarization force for induced dipoles based on 5th order B-Splines. This force arises due to self-consistent convergence of the solute induced dipoles and reaction field.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>induced</i>	Induced dipole potential
<i>nlInduced</i>	Non-local induced dipole potential
<i>atomID</i>	Atom index
<i>force</i>	(returned) force

7.29.3.12 Vpmg_dbNLDirectPolForce()

```

VEXTERNC void Vpmg_dbNLDirectPolForce (
    Vpmg * thee,
    Vgrid * perm,
    Vgrid * nlInduced,
    int atomID,
    double force[3] )

```

Dielectric boundary direct polarization force between permanent multipoles and non-local induced dipoles. Keep in mind that the "non-local" induced dipoles are just a mathematical quantity that result from differentiation of the AMOEBA polarization energy.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>perm</i>	Permanent multipole potential
<i>nlInduced</i>	Non-local induced dipole potential
<i>atomID</i>	Atom index
<i>force</i>	(returned) force

7.29.3.13 Vpmg_dbPermanentMultipoleForce()

```

VEXTERNC void Vpmg_dbPermanentMultipoleForce (
    Vpmg * thee,
    int atomID,
    double force[3] )

```

Compute the dielectric boundary force for permanent multipoles.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>atomID</i>	Atom index
<i>force</i>	(returned) force

7.29.3.14 Vpmg_dielEnergy()

```

VEXTERNC double Vpmg_dielEnergy (
    Vpmg * thee,
    int extFlag )

```

Get the "polarization" contribution to the electrostatic energy.

Using the solution at the finest mesh level, get the electrostatic energy due to the interaction of the mobile charges with the potential:

$$\frac{1}{2} \int \epsilon |\nabla u|^2 dx$$

where ϵ is the dielectric parameter and $u(x)$ is the dimensionless electrostatic potential. The energy is scaled to units of $k_B T$.

Author

Nathan Baker

Note

The value of this observable may be modified by setting restrictions on the subdomain over which it is calculated. Such limits can be set via `Vpmg_setPart` and are generally useful for parallel runs.

Returns

The polarization electrostatic energy in units of $k_B T$.

Parameters

<i>thee</i>	Vpmg object
<i>extFlag</i>	If this was a focused calculation, include (1 – for serial calculations) or ignore (0 – for parallel calculations) energy contributions from outside the focusing domain

Definition at line [1279](#) of file [vpmg.c](#).

7.29.3.15 Vpmg_dielGradNorm()

```

VEXTERNC double Vpmg_dielGradNorm (
    Vpmg * thee )

```

Get the integral of the gradient of the dielectric function.

Using the dielectric map at the finest mesh level, calculate the integral of the norm of the dielectric function gradient routines of Im et al (see Vpmg_dbForce for reference):

$$\int |\nabla \epsilon| dx$$
 where ϵ is the dielectric parameter.
 The integral is returned in units of A^2 .

Author

Nathan Baker restrictions on the subdomain over which it is calculated. Such limits can be set via Vpmg_setPart and are generally useful for parallel runs.

Returns

The integral in units of A^2 .

Parameters

<i>thee</i>	Vpmg object
-------------	-------------

Definition at line 1342 of file vpmg.c.

7.29.3.16 Vpmg_dtor()

```
VEXTERNC void Vpmg_dtor (
    Vpmg ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object to be destroyed
-------------	--

Definition at line 561 of file vpmg.c.

7.29.3.17 Vpmg_dtor2()

```
VEXTERNC void Vpmg_dtor2 (
    Vpmg * thee )
```

FORTTRAN stub object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object to be destroyed
-------------	-----------------------------------

Definition at line 571 of file [vpmg.c](#).

7.29.3.18 Vpmg_energy()

```
VEXTERNC double Vpmg_energy (
    Vpmg * thee,
    int extFlag )
```

Get the total electrostatic energy.

Author

Nathan Baker

Note

The value of this observable may be modified by setting restrictions on the subdomain over which it is calculated. Such limits can be set via `Vpmg_setPart` and are generally useful for parallel runs.

Returns

The electrostatic energy in units of $k_B T$.

Parameters

<i>thee</i>	Vpmg object
<i>extFlag</i>	If this was a focused calculation, include (1 – for serial calculations) or ignore (0 – for parallel calculations) energy contributions from outside the focusing domain

Definition at line 1248 of file [vpmg.c](#).

7.29.3.19 Vpmg_fieldSpline4()

```
VPUBLIC void Vpmg_fieldSpline4 (
    Vpmg * thee,
    int atomID,
    double field[3] )
```

Computes the field at an atomic center using a stencil based on the first derivative of a 5th order B-spline.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>atomID</i>	Atom index
<i>field</i>	The (returned) electric field

7.29.3.20 Vpmg_fillArray()

```

VEXTERNC int Vpmg_fillArray (
    Vpmg * thee,
    double * vec,
    Vdata_Type type,
    double parm,
    Vhal_PBEType pbetype,
    PBEparm * pbeparm )

```

Fill the specified array with accessibility values.

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	Vpmg object
<i>vec</i>	A nx*ny*nz*sizeof(double) array to contain the values to be written
<i>type</i>	What to write
<i>parm</i>	Parameter for data type definition (if needed)
<i>pbetype</i>	Parameter for PBE type (if needed)
<i>pbeparm</i>	Pass in the PBE parameters (if needed)

Definition at line 892 of file [vpmg.c](#).

7.29.3.21 Vpmg_fillco()

```

VEXTERNC int Vpmg_fillco (
    Vpmg * thee,
    Vsurf_Meth surfMeth,
    double splineWin,
    Vchrg_Meth chargeMeth,
    int useDielXMap,
    Vgrid * dielXMap,
    int useDielYMap,
    Vgrid * dielYMap,
    int useDielZMap,
    Vgrid * dielZMap,
    int useKappaMap,
    Vgrid * kappaMap,
    int usePotMap,
    Vgrid * potMap,
    int useChargeMap,
    Vgrid * chargeMap )

```

Fill the coefficient arrays prior to solving the equation.

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Bug useDielMap could only be passed once, not three times, to this function - why not just once? that's what the call in [routines.c](#) ends up doing - just passing useDielMap three times. - P. Ellis 11/3/11

Parameters

<i>thee</i>	Vpmg object
<i>surfMeth</i>	Surface discretization method
<i>splineWin</i>	Spline window (in A) for surfMeth = VSM_SPLINE
<i>chargeMeth</i>	Charge discretization method
<i>useDielXMap</i>	Boolean to use dielectric map argument
<i>dielXMap</i>	External dielectric map
<i>useDielYMap</i>	Boolean to use dielectric map argument
<i>dielYMap</i>	External dielectric map
<i>useDielZMap</i>	Boolean to use dielectric map argument
<i>dielZMap</i>	External dielectric map
<i>useKappaMap</i>	Boolean to use kappa map argument
<i>kappaMap</i>	External kappa map
<i>usePotMap</i>	Boolean to use potential map argument
<i>potMap</i>	External potential map
<i>useChargeMap</i>	Boolean to use charge map argument
<i>chargeMap</i>	External charge map

Definition at line 5655 of file [vpmg.c](#).

7.29.3.22 Vpmg_force()

```

VEXTERNC int Vpmg_force (
    Vpmg * thee,
    double * force,
    int atomID,
    Vsurf_Meth srfm,
    Vchrg_Meth chgm )

```

Calculate the total force on the specified atom in units of k_B T/Å.

Author

Nathan Baker

Note

- Using the force evaluation methods of Im et al (Roux group), Comput Phys Commun, 111, 59–75 (1998). However, this gives the whole (self-interactions included) force – reaction field forces will have to be calculated at higher level.
- No contributions are made from higher levels of focusing.

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	Vpmg object
<i>force</i>	3*sizeof(double) space to hold the force in units of k_B T/AA
<i>atomID</i>	Valist ID of desired atom
<i>srfm</i>	Surface discretization method
<i>chgm</i>	Charge discretization method

Definition at line 5822 of file [vpmg.c](#).

7.29.3.23 Vpmg_ibDirectPolForce()

```
VEXTERNC void Vpmg_ibDirectPolForce (
    Vpmg * thee,
    Vgrid * perm,
    Vgrid * induced,
    int atomID,
    double force[3] )
```

Ionic boundary direct polarization force between permanent multipoles and induced dipoles, which are induced by the sum of the permanent intramolecular field and the permanent reaction field.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>perm</i>	Permanent multipole potential
<i>induced</i>	Induced dipole potential
<i>atomID</i>	Atom index
<i>force</i>	(returned) force

7.29.3.24 Vpmg_ibForce()

```
VEXTERNC int Vpmg_ibForce (
    Vpmg * thee,
    double * force,
    int atomID,
    Vsurf_Meth srfm )
```

Calculate the osmotic pressure on the specified atom in units of k_B T/AA.

Author

Nathan Baker

Note

- Using the force evaluation methods of Im et al (Roux group), Comput Phys Commun, 111, 59–75 (1998). However, this gives the whole (self-interactions included) force – reaction field forces will have to be calculated at higher level.
- No contributions are made from higher levels of focusing.

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	Vpmg object
<i>force</i>	3*sizeof(double) space to hold the boundary force in units of $k_B T/AA$
<i>atomID</i>	Valist ID of desired atom
<i>srfm</i>	Surface discretization method

Definition at line 5845 of file [vpmg.c](#).

7.29.3.25 Vpmg_ibMutualPolForce()

```

VEXTERNC void Vpmg_ibMutualPolForce (
    Vpmg * thee,
    Vgrid * induced,
    Vgrid * nlInduced,
    int atomID,
    double force[3] )

```

Ionic boundary mutual polarization force for induced dipoles based on 5th order B-Splines. This force arises due to self-consistent convergence of the solute induced dipoles and reaction field.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>induced</i>	Induced dipole potential
<i>nlInduced</i>	Non-local induced dipole potential
<i>atomID</i>	Atom index
<i>force</i>	(returned) force

7.29.3.26 Vpmg_ibNLDirectPolForce()

```

VEXTERNC void Vpmg_ibNLDirectPolForce (
    Vpmg * thee,
    Vgrid * perm,
    Vgrid * nlInduced,

```

```
int atomID,
double force[3] )
```

Ionic boundary direct polarization force between permanent multipoles and non-local induced dipoles based on 5th order. Keep in mind that the "non-local" induced dipoles are just a mathematical quantity that result from differentiation of the AMOEBA polarization energy.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>perm</i>	Permanent multipole potential
<i>nllInduced</i>	Induced dipole potential
<i>atomID</i>	Atom index
<i>force</i>	(returned) force

7.29.3.27 Vpmg_ibPermanentMultipoleForce()

```
VEXTERNC void Vpmg_ibPermanentMultipoleForce (
    Vpmg * thee,
    int atomID,
    double force[3] )
```

Compute the ionic boundary force for permanent multipoles.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>atomID</i>	Atom index
<i>force</i>	(returned) force

7.29.3.28 Vpmg_memChk()

```
VEXTERNC unsigned long int Vpmg_memChk (
    Vpmg * thee )
```

Return the memory used by this structure (and its contents) in bytes.

Author

Nathan Baker

Returns

The memory used by this structure and its contents in bytes

Parameters

<i>thee</i>	Object for memory check
-------------	-------------------------

Definition at line 79 of file [vpmg.c](#).

7.29.3.29 Vpmg_printColComp()

```

VEXTERNC void Vpmg_printColComp (
    Vpmg * thee,
    char path[72],
    char title[72],
    char mxtype[3],
    int flag )

```

Print out a column-compressed sparse matrix in Harwell-Boeing format.

Author

Nathan Baker

Bug Can this path variable be replaced with a Vio socket?

Parameters

<i>thee</i>	Vpmg object
<i>path</i>	The file to which the matrix is to be written
<i>title</i>	The title of the matrix
<i>mxtype</i>	The type of REAL-valued matrix, a 3-character string of the form "R_A" where the '_' can be one of: <ul style="list-style-type: none"> • S: symmetric matrix • U: unsymmetric matrix • H: Hermitian matrix • Z: skew-symmetric matrix • R: rectangular matrix
<i>flag</i>	The operator to compress: <ul style="list-style-type: none"> • 0: Poisson operator • 1: Linearization of the full Poisson-Boltzmann operator around the current solution

Definition at line 87 of file [vpmg.c](#).

7.29.3.30 Vpmg_qfAtomEnergy()

```

VEXTERNC double Vpmg_qfAtomEnergy (
    Vpmg * thee,
    Vatom * atom )

```

Get the per-atom "fixed charge" contribution to the electrostatic energy.

Using the solution at the finest mesh level, get the electrostatic energy due to the interaction of the fixed charges with the potential:

$$G = qu(r),$$

where q is the charge and r is the location of the atom of interest. The result is returned in units of $k_B T$. Clearly, no self-interaction terms are removed. A factor a 1/2 has to be included to convert this to a real energy.

Author

Nathan Baker

Note

The value of this observable may be modified by setting restrictions on the subdomain over which it is calculated. Such limits can be set via `Vpmg_setPart` and are generally useful for parallel runs.

Returns

The fixed charge electrostatic energy in units of $k_B T$.

Parameters

<i>thee</i>	The Vpmg object
<i>atom</i>	The atom for energy calculations

Definition at line 1791 of file `vpmg.c`.

7.29.3.31 Vpmg_qfDirectPolForce()

```
VEEXTERNC void Vpmg_qfDirectPolForce (
    Vpmg * thee,
    Vgrid * perm,
    Vgrid * induced,
    int atomID,
    double force[3],
    double torque[3] )
```

q-Phi direct polarization force between permanent multipoles and induced dipoles, which are induced by the sum of the permanent intramolecular field and the permanent reaction field.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>perm</i>	Permanent multipole potential
<i>induced</i>	Induced dipole potential
<i>atomID</i>	Atom index
<i>force</i>	(returned) force
<i>torque</i>	(returned) torque

7.29.3.32 Vpmg_qfEnergy()

```

VEXTERNC double Vpmg_qfEnergy (
    Vpmg * thee,
    int extFlag )

```

Get the "fixed charge" contribution to the electrostatic energy.

Using the solution at the finest mesh level, get the electrostatic energy due to the interaction of the fixed charges with the potential: $G = \sum_i q_i u(r_i)$ and return the result in units of $k_B T$. Clearly, no self-interaction terms are removed. A factor a 1/2 has to be included to convert this to a real energy.

Author

Nathan Baker

Note

The value of this observable may be modified by setting restrictions on the subdomain over which it is calculated. Such limits can be set via `Vpmg_setPart` and are generally useful for parallel runs.

Returns

The fixed charge electrostatic energy in units of $k_B T$.

Parameters

<i>thee</i>	Vpmg object
<i>extFlag</i>	If this was a focused calculation, include (1 – for serial calculations) or ignore (0 – for parallel calculations) energy contributions from outside the focusing domain

Definition at line 1687 of file `vpmg.c`.

7.29.3.33 Vpmg_qfForce()

```

VEXTERNC int Vpmg_qfForce (
    Vpmg * thee,
    double * force,
    int atomID,
    Vchrg_Meth chgm )

```

Calculate the "charge-field" force on the specified atom in units of $k_B T/AA$.

Author

Nathan Baker

Note

- Using the force evaluation methods of Im et al (Roux group), Comput Phys Commun, 111, 59–75 (1998). However, this gives the whole (self-interactions included) force – reaction field forces will have to be calculated at higher level.
- No contributions are made from higher levels of focusing.

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	Vpmg object
<i>force</i>	3*sizeof(double) space to hold the force in units of k _B T/Å
<i>atomID</i>	Valist ID of desired atom
<i>chgm</i>	Charge discretization method

Definition at line 6267 of file [vpmg.c](#).

7.29.3.34 Vpmg_qfMutualPolForce()

```
VEXTERNC void Vpmg_qfMutualPolForce (
    Vpmg * thee,
    Vgrid * induced,
    Vgrid * nlInduced,
    int atomID,
    double force[3] )
```

Mutual polarization force for induced dipoles based on 5th order B-Splines. This force arises due to self-consistent convergence of the solute induced dipoles and reaction field.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>induced</i>	Induced dipole potential
<i>nlInduced</i>	Non-local induced dipole potential
<i>atomID</i>	Atom index
<i>force</i>	(returned) force

7.29.3.35 Vpmg_qfNLDirectPolForce()

```
VEXTERNC void Vpmg_qfNLDirectPolForce (
    Vpmg * thee,
    Vgrid * perm,
    Vgrid * nlInduced,
    int atomID,
    double force[3],
    double torque[3] )
```

q-Phi direct polarization force between permanent multipoles and non-local induced dipoles based on 5th Order B-Splines. Keep in mind that the "non-local" induced dipoles are just a mathematical quantity that result from differentiation of the AMOEBA polarization energy.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>perm</i>	Permanent multipole potential
<i>nlInduced</i>	Non-local induced dipole potential
<i>atomID</i>	Atom index
<i>force</i>	(returned) force
<i>torque</i>	(returned) torque

7.29.3.36 Vpmg_qfPermanentMultipoleEnergy()

```
VEXTERNC double Vpmg_qfPermanentMultipoleEnergy (
    Vpmg * thee,
    int atomID )
```

Computes the permanent multipole electrostatic hydration energy (the polarization component of the hydration energy currently computed in TINKER).

Author

Michael Schnieders

Returns

The permanent multipole electrostatic hydration energy

Parameters

<i>thee</i>	Vpmg object
<i>atomID</i>	Atom index

7.29.3.37 Vpmg_qfPermanentMultipoleForce()

```
VEXTERNC void Vpmg_qfPermanentMultipoleForce (
    Vpmg * thee,
    int atomID,
    double force[3],
    double torque[3] )
```

Computes the q-Phi Force for permanent multipoles based on 5th order B-splines.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
-------------	-------------

Parameters

<i>atomID</i>	Atom index
<i>force</i>	(returned) force
<i>torque</i>	(returned) torque

7.29.3.38 Vpmg_qmEnergy()

```

VEXTERNC double Vpmg_qmEnergy (
    Vpmg * thee,
    int extFlag )

```

Get the "mobile charge" contribution to the electrostatic energy.

Using the solution at the finest mesh level, get the electrostatic energy due to the interaction of the mobile charges with the potential:

$$\int \left[G = \frac{1}{4} I_s \sum_i c_i q_i^2 \int \kappa^2(x) e^{-q_i u(x)} dx \right]$$

for the NPBE and

$$\int \left[G = \frac{1}{2} \int \overline{\kappa^2(x)} u^2(x) dx \right]$$

for the LPBE. Here i denotes the counterion species, I_s is the bulk ionic strength, $\kappa^2(x)$ is the modified Debye-Huckel parameter, c_i is the concentration of species i , q_i is the charge of species i , and $u(x)$ is the dimensionless electrostatic potential. The energy is scaled to units of $k_B T$.

Author

Nathan Baker

Note

The value of this observable may be modified by setting restrictions on the subdomain over which it is calculated. Such limits can be set via `Vpmg_setPart` and are generally useful for parallel runs.

Returns

The mobile charge electrostatic energy in units of $k_B T$.

Parameters

<i>thee</i>	Vpmg object
<i>extFlag</i>	If this was a focused calculation, include (1 – for serial calculations) or ignore (0 – for parallel calculations) energy contributions from outside the focusing domain

Definition at line 1386 of file `vpmg.c`.

7.29.3.39 Vpmg_setPart()

```

VEXTERNC void Vpmg_setPart (
    Vpmg * thee,
    double lowerCorner[3],

```

```
double upperCorner[3],
int bflags[6] )
```

Set partition information which restricts the calculation of observables to a (rectangular) subset of the problem domain.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpmg object
<i>lowerCorner</i>	Partition lower corner
<i>upperCorner</i>	Partition upper corner
<i>bflags</i>	Booleans indicating whether a particular processor is on the boundary with another partition. 0 if the face is not bounded (next to) another partition, and 1 otherwise.

Definition at line [627](#) of file [vpmg.c](#).

7.29.3.40 Vpmg_solve()

```
VEEXTERNAL int Vpmg_solve (
    Vpmg * thee )
```

Solve the PBE using PMG.

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	Vpmg object
-------------	-------------

Definition at line [401](#) of file [vpmg.c](#).

7.29.3.41 Vpmg_solveLaplace()

```
VEEXTERNAL int Vpmg_solveLaplace (
    Vpmg * thee )
```

Solve Poisson's equation with a homogeneous Laplacian operator using the solvent dielectric constant. This solution is performed by a sine wave decomposition.

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Note

This function is really only for testing purposes as the PMG multigrid solver can solve the homogeneous system much more quickly. Perhaps we should implement an FFT version at some point...

Parameters

<i>thee</i>	Vpmg object
-------------	-------------

Definition at line 7042 of file [vpmg.c](#).

7.29.3.42 Vpmg_unsetPart()

```
VEXTERNC void Vpmg_unsetPart (
    Vpmg * thee )
```

Remove partition restrictions.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpmg object
-------------	-------------

Definition at line 872 of file [vpmg.c](#).

7.30 Vpmgp class

Parameter structure for Mike Holst's PMGP code.

Files

- file [vpmgp.c](#)
Class Vpmgp methods.
- file [vpmgp.h](#)
Contains declarations for class Vpmgp.

Data Structures

- struct [sVpmgp](#)
Contains public data members for Vpmgp class/module.

Typedefs

- typedef struct [sVpmgp](#) [Vpmgp](#)
Declaration of the Vpmgp class as the [sVpmgp](#) structure.

Functions

- VEXTERNC [Vpmgp](#) * [Vpmgp_ctor](#) ([MGparm](#) *mgparm)

Construct PMG parameter object and initialize to default values.

- VEXTERNC int [Vpmgp_ctor2](#) ([Vpmgp](#) *thee, [MGparm](#) *mgparm)

FORTRAN stub to construct PMG parameter object and initialize to default values.

- VEXTERNC void [Vpmgp_dtor](#) ([Vpmgp](#) **thee)

Object destructor.

- VEXTERNC void [Vpmgp_dtor2](#) ([Vpmgp](#) *thee)

FORTRAN stub for object destructor.

- VEXTERNC void [Vpmgp_size](#) ([Vpmgp](#) *thee)

Determine array sizes and parameters for multigrid solver.

- VEXTERNC void [Vpmgp_makeCoarse](#) (int numLevel, int nxOld, int nyOld, int nzOld, int *nxNew, int *nyNew, int *nzNew)

Coarsen the grid by the desired number of levels and determine the resulting numbers of grid points.

7.30.1 Detailed Description

Parameter structure for Mike Holst's PMGP code.

Note

Variables and many default values taken directly from PMG

7.30.2 Typedef Documentation

7.30.2.1 Vpmgp

```
typedef struct sVpmgp Vpmgp
```

Declaration of the Vpmgp class as the [sVpmgp](#) structure.

Definition at line [204](#) of file [vpmgp.h](#).

7.30.3 Function Documentation

7.30.3.1 Vpmgp_ctor()

```
VEXTERNC Vpmgp * Vpmgp_ctor (
    MGparm * mgparm )
```

Construct PMG parameter object and initialize to default values.

Author

Nathan Baker

Parameters

mgparm	MGParm object containing parameters to be used in setup
------------------------	---

Returns

Newly allocated and initialized Vpmgp object

Definition at line [76](#) of file [vpmgp.c](#).

7.30.3.2 Vpmgp_ctor2()

```
VEXTERNC int Vpmgp_ctor2 (  
    Vpmgp * thee,  
    MGparm * mgparm )
```

FORTTRAN stub to construct PMG parameter object and initialize to default values.

Author

Nathan Baker

Parameters

<i>thee</i>	Newly allocated PMG object
<i>mgparm</i>	MGParm object containing parameters to be used in setup

Returns

1 if successful, 0 otherwise

Definition at line 93 of file [vpmgp.c](#).

7.30.3.3 Vpmgp_dtor()

```
VEXTERNC void Vpmgp_dtor (  
    Vpmgp ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location for Vpmgp object
-------------	---

Definition at line 178 of file [vpmgp.c](#).

7.30.3.4 Vpmgp_dtor2()

```
VEXTERNC void Vpmgp_dtor2 (  
    Vpmgp * thee )
```

FORTTRAN stub for object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to Vpmgp object
-------------	-------------------------

Definition at line 193 of file [vpmgp.c](#).

7.30.3.5 Vpmgp_makeCoarse()

```
VEXTERNC void Vpmgp_makeCoarse (
    int numLevel,
    int nxOld,
    int nyOld,
    int nzOld,
    int * nxNew,
    int * nyNew,
    int * nzNew )
```

Coarsen the grid by the desired number of levels and determine the resulting numbers of grid points.

Author

Mike Holst and Nathan Baker

Parameters

<i>numLevel</i>	Number of levels to coarsen
<i>nxOld</i>	Number of old grid points in this direction
<i>nyOld</i>	Number of old grid points in this direction
<i>nzOld</i>	Number of old grid points in this direction
<i>nxNew</i>	Number of new grid points in this direction
<i>nyNew</i>	Number of new grid points in this direction
<i>nzNew</i>	Number of new grid points in this direction

Definition at line 312 of file [vpmgp.c](#).

7.30.3.6 Vpmgp_size()

```
VEXTERNC void Vpmgp_size (
    Vpmgp * thee )
```

Determine array sizes and parameters for multigrid solver.

Author

Mike Holst and Nathan Baker

Parameters

<i>thee</i>	Object to be sized
-------------	--------------------

Definition at line 196 of file [vpmgp.c](#).

7.31 C translation of Holst group PMG code

C translation of Holst group PMG code.

Macros

- #define **HARMO2**(a, b) $(2.0 * (a) * (b) / ((a) + (b)))$
Multigrid subroutines.
- #define **MAXIONS** 50
Specifies the PDE definition for PMG to solve.

Functions

- VPUBLIC void **VbuildA** (int *nx, int *ny, int *nz, int *ipkey, int *mgdisc, int *numdia, int *ipc, double *rpc, double *ac, double *cc, double *fc, double *xf, double *yf, double *zf, double *gxcf, double *gycf, double *gzcf, double *a1cf, double *a2cf, double *a3cf, double *ccf, double *fcf)
Build the Laplacian.
- VPUBLIC void **Vbuildband** (int *key, int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac, int *ipcb, double *rpcB, double *acB)
Banded matrix builder.
- VEXTERN void **Vbuildband1_7** (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *oC, double *oE, double *oN, double *uC, int *ipcb, double *rpcB, double *acB, int *n, int *m, int *lda)
Build the operator in banded form given the 7-diagonal form.
- VEXTERN void **Vbuildband1_27** (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *oC, double *oE, double *oN, double *uC, double *oNE, double *oNW, double *uE, double *uW, double *uN, double *uS, double *uNE, double *uNW, double *uSE, double *uSW, int *ipcb, double *rpcB, double *acB, int *n, int *m, int *lda)
Build the operator in banded form given the 27-diagonal form.
- VPUBLIC void **VbuildG** (int *nxf, int *nyf, int *nzf, int *nxc, int *nyc, int *nzc, int *numdia, double *pcFF, double *acFF, double *ac)
Build Galerkin matrix structures.
- VEXTERN void **VbuildG_1** (int *nxf, int *nyf, int *nzf, int *nx, int *ny, int *nz, double *oPC, double *oPN, double *oPS, double *oPE, double *oPW, double *oPNE, double *oPNW, double *oPSE, double *oPSW, double *uPC, double *uPN, double *uPS, double *uPE, double *uPW, double *uPNE, double *uPNW, double *uPSE, double *uPSW, double *dPC, double *dPN, double *dPS, double *dPE, double *dPW, double *dPNE, double *dPNW, double *dPSE, double *dPSW, double *oC, double *XoC, double *XoE, double *XoN, double *XuC, double *XoNE, double *XoNW, double *XuE, double *XuW, double *XuN, double *XuS, double *XuNE, double *XuNW, double *XuSE, double *XuSW)
Computes a 27-point galerkin coarse grid matrix from a 1-point (i.e., diagonal) fine grid matrix.
- VEXTERN void **VbuildG_7** (int *nxf, int *nyf, int *nzf, int *nx, int *ny, int *nz, double *oPC, double *oPN, double *oPS, double *oPE, double *oPW, double *oPNE, double *oPNW, double *oPSE, double *oPSW, double *uPC, double *uPN, double *uPS, double *uPE, double *uPW, double *uPNE, double *uPNW, double *uPSE, double *uPSW, double *dPC, double *dPN, double *dPS, double *dPE, double *dPW, double *dPNE, double *dPNW, double *dPSE, double *dPSW, double *oC, double *oE, double *oN, double *uC, double *XoC, double *XoE, double *XoN, double *XuC, double *XoNE, double *XoNW, double *XuE, double *XuW, double *XuN, double *XuS, double *XuNE, double *XuNW, double *XuSE, double *XuSW)
Computes a 27-point galerkin coarse grid matrix from a 7-point fine grid matrix.
- VEXTERN void **VbuildG_27** (int *nxf, int *nyf, int *nzf, int *nx, int *ny, int *nz, double *oPC, double *oPN, double *oPS, double *oPE, double *oPW, double *oPNE, double *oPNW, double *oPSE, double *oPSW, double *uPC, double *uPN, double *uPS, double *uPE, double *uPW, double *uPNE, double *uPNW, double *uPSE, double *uPSW, double *dPC, double *dPN, double *dPS, double *dPE, double *dPW, double *dPNE, double *dPNW, double *dPSE, double *dPSW, double *oC, double *oE, double *oN, double *uC, double *oNE, double *oNW, double *uE, double *uW, double *uN, double *uS, double *uNE, double *uNW, double *uSE, double *uSW, double *XoC, double *XoE, double *XoN, double *XuC, double *XoNE, double *XoNW, double *XuE, double *XuW, double *XuN, double *XuS, double *XuNE, double *XuNW, double *XuSE, double *XuSW)
Compute a 27-point galerkin coarse grid matrix from a 27-point fine grid matrix.

- VPUBLIC void **VbuildP** (int *nxf, int *nyf, int *nzf, int *nxc, int *nyc, int *nzc, int *mgprol, int *ipc, double *rpc, double *pc, double *ac, double *xf, double *yf, double *zf)
Builds prolongation matrix.
- VPUBLIC void **Vcghs** (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac, double *cc, double *fc, double *x, double *p, double *ap, double *r, int *itmax, int *iters, double *errtol, double *omega, int *iresid, int *iadjoint)
A collection of useful low-level routines (timing, etc).
- VPUBLIC void **Vgsrb** (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac, double *cc, double *fc, double *x, double *w1, double *w2, double *r, int *itmax, int *iters, double *errtol, double *omega, int *iresid, int *iadjoint)
Gauss-Seidel solver.
- VPUBLIC void **Vmatvec** (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac, double *cc, double *x, double *y)
Matrix-vector multiplication routines.
- VEXTERNC void **Vnmatvec** (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac, double *cc, double *x, double *y, double *w1)
Break the matrix data-structure into diagonals and then call the matrix-vector routine.
- VEXTERNC void **Vmresid** (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac, double *cc, double *fc, double *x, double *r)
Break the matrix data-structure into diagonals and then call the residual routine.
- VEXTERNC void **Vnmresid** (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac, double *cc, double *fc, double *x, double *r, double *w1)
Break the matrix data-structure into diagonals and then call the residual routine.
- VEXTERNC void **Vrestrc** (int *nxf, int *nyf, int *nzf, int *nxc, int *nyc, int *nzc, double *xin, double *xout, double *pc)
Apply the restriction operator.
- VEXTERNC void **VinterpMG** (int *nxc, int *nyc, int *nzc, int *nxf, int *nyf, int *nzf, double *xin, double *xout, double *pc)
Apply the prolongation operator.
- VEXTERNC void **Vextrac** (int *nxf, int *nyf, int *nzf, int *nxc, int *nyc, int *nzc, double *xin, double *xout)
Simple injection of a fine grid function into coarse grid.
- VEXTERNC void **Vmvcs** (int *nx, int *ny, int *nz, double *x, int *iz, double *w0, double *w1, double *w2, double *w3, int *istop, int *itmax, int *iters, int *ierror, int *nlev, int *ilev, int *nlev_real, int *mgsolv, int *iok, int *iinfo, double *epsiln, double *errtol, double *omega, int *nu1, int *nu2, int *mgsmoo, int *ipc, double *rpc, double *pc, double *ac, double *cc, double *fc, double *tru)
MG helper functions.
- VPUBLIC void **Vmgdriv** (int *iparm, double *rparm, int *iwork, double *rwork, double *u, double *xf, double *yf, double *zf, double *gxcf, double *gycf, double *gzcf, double *a1cf, double *a2cf, double *a3cf, double *ccf, double *fcf, double *tcf)
Multilevel solver driver.
- VEXTERNC void **Vmgdriv2** (int *iparm, double *rparm, int *nx, int *ny, int *nz, double *u, int *iz, int *ipc, double *rpc, double *pc, double *ac, double *cc, double *fc, double *xf, double *yf, double *zf, double *gxcf, double *gycf, double *gzcf, double *a1cf, double *a2cf, double *a3cf, double *ccf, double *fcf, double *tcf)
Solves the pde using the multi-grid method.
- VEXTERNC void **Vmgsz** (int *mgcoar, int *mgdisc, int *mgsolv, int *nx, int *ny, int *nz, int *nlev, int *nxc, int *nyc, int *nzc, int *nf, int *nc, int *narr, int *narrc, int *n_rpc, int *n_iz, int *n_ipc, int *iretot, int *iintot)
This routine computes the required sizes of the real and integer work arrays for the multigrid code. these two sizes are a (complicated) function of input parameters.
- VPUBLIC void **Vfmvfas** (int *nx, int *ny, int *nz, double *x, int *iz, double *w0, double *w1, double *w2, double *w3, double *w4, int *istop, int *itmax, int *iters, int *ierror, int *nlev, int *ilev, int *nlev_real, int *mgsolv, int *iok, int *iinfo, double *epsiln, double *errtol, double *omega, int *nu1, int *nu2, int *mgsmoo, int *ipc, double *rpc, double *pc, double *ac, double *cc, double *fc, double *tru)

Multigrid nonlinear solve iteration routine.

- VEXTERNC void **Vmvmf** (int *nx, int *ny, int *nz, double *x, int *iz, double *w0, double *w1, double *w2, double *w3, double *w4, int *istop, int *itmax, int *iters, int *ierror, int *nlev, int *ilev, int *nlev_real, int *mgsolv, int *iok, int *iinfo, double *epsilon, double *errtol, double *omega, int *nu1, int *nu2, int *mgsmoo, int *ipc, double *rpc, double *pc, double *ac, double *cc, double *fc, double *tru)

Nonlinear multilevel method.

- VPUBLIC void **Vbuildops** (int *nx, int *ny, int *nz, int *nlev, int *ipkey, int *iinfo, int *ido, int *iz, int *mgprol, int *mgcoar, int *mgsolv, int *mgdisc, int *ipc, double *rpc, double *pc, double *ac, double *cc, double *fc, double *xf, double *yf, double *zf, double *gxcf, double *gycf, double *gzc, double *a1cf, double *a2cf, double *a3cf, double *ccf, double *fcf, double *tcf)

Build operators, boundary arrays, modify affine vectors ido==0: do only fine level ido==1: do only coarse levels (including second op at coarsest) ido==2: do all levels ido==3: rebuild the second operator at the coarsest level.

- VEXTERNC void **Vbuildstr** (int *nx, int *ny, int *nz, int *nlev, int *iz)

Build the nexted operator framework in the array iz.

- VEXTERNC void **Vbuildgaler0** (int *nxf, int *nyf, int *nzf, int *nxc, int *nyc, int *nzc, int *ipkey, int *numdia, double *pcFF, int *ipcFF, double *rpcFF, double *acFF, double *ccFF, double *fcFF, int *ipc, double *rpc, double *ac, double *cc, double *fc)

Form the Galerkin coarse grid system.

- VPUBLIC void **Vxcopy** (int *nx, int *ny, int *nz, double *x, double *y)

A collection of useful low-level routines (timing, etc).

- VEXTERNC void **Vxcopy_small** (int *nx, int *ny, int *nz, double *x, double *y)

Copy operation for a grid function with boundary values. Quite simply copies one 3d matrix to another.

- VEXTERNC void **Vxcopy_large** (int *nx, int *ny, int *nz, double *x, double *y)

Copy operation for a grid function with boundary values. Quite simply copies one 3d matrix to another.

- VEXTERNC void **Vxaxpy** (int *nx, int *ny, int *nz, double *alpha, double *x, double *y)

saxpy operation for a grid function with boundary values.

- VEXTERNC double **Vxnrm1** (int *nx, int *ny, int *nz, double *x)

Norm operation for a grid function with boundary values.

- VEXTERNC double **Vxnrm2** (int *nx, int *ny, int *nz, double *x)

Norm operation for a grid function with boundary values.

- VEXTERNC double **Vxdot** (int *nx, int *ny, int *nz, double *x, double *y)

Inner product operation for a grid function with boundary values.

- VEXTERNC void **Vazeros** (int *nx, int *ny, int *nz, double *x)

Zero out operation for a grid function, including boundary values.

- VEXTERNC void **VfboundPMG** (int *ibound, int *nx, int *ny, int *nz, double *x, double *gxc, double *gyc, double *gzc)

Initialize a grid function to have a certain boundary value,.

- VEXTERNC void **VfboundPMG00** (int *nx, int *ny, int *nz, double *x)

Initialize a grid function to have a zero boundary value.

- VEXTERNC void **Vaxrand** (int *nx, int *ny, int *nz, double *x)

Fill grid function with random values, including boundary values.

- VEXTERNC void **Vxscal** (int *nx, int *ny, int *nz, double *fac, double *x)

Scale operation for a grid function with boundary values.

- VEXTERNC void **Vprtmatd** (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac)

- VPUBLIC void **Vdpbsl** (double *abd, int *lda, int *n, int *m, double *b)

LINPACK interface.

- VPUBLIC void **Vmypydefinitpbe** (int *tnion, double *tcharge, double *tsconc)

Set up the ionic species to be used in later calculations. This must be called before any other of the routines in this file.

- VEXTERNC void **Vmypydefinitnpbe** (int *tnion, double *tcharge, double *tsconc)

Set up the ionic species to be used in later calculations. This must be called before any other of the routines in this file.

- VEXTERNC void **Vmypadefinitmpbe** (int *tnion, double *tcharge, double *tsconc, double *smvolume, double *smsize)

Set up the ionic species to be used in later calculations. This must be called before any other of the routines in this file.

- VEXTERNC void **Vc_vec** (double *coef, double *uin, double *uout, int *nx, int *ny, int *nz, int *ipkey)

Define the nonlinearity (vector version)

- VEXTERNC void **Vdc_vec** (double *coef, double *uin, double *uout, int *nx, int *ny, int *nz, int *ipkey)

Define the derivative of the nonlinearity (vector version)

- VEXTERNC void **Vc_vecpmg** (double *coef, double *uin, double *uout, int *nx, int *ny, int *nz, int *ipkey)

Define the nonlinearity (vector version)

- VEXTERNC void **Vc_vecsmpbe** (double *coef, double *uin, double *uout, int *nx, int *ny, int *nz, int *ipkey)

Define the nonlinearity (vector version)

- VEXTERNC void **Vnewdriv** (int *iparm, double *rparm, int *iwork, double *rwork, double *u, double *xf, double *yf, double *zf, double *gxcf, double *gycf, double *gzcf, double *a1cf, double *a2cf, double *a3cf, double *ccf, double *fcf, double *tcf)

Driver for the Newton Solver.

- VEXTERNC void **Vnewdriv2** (int *iparm, double *rparm, int *nx, int *ny, int *nz, double *u, int *iz, double *w1, double *w2, int *ipc, double *rpc, double *pc, double *ac, double *cc, double *fc, double *xf, double *yf, double *zf, double *gxcf, double *gycf, double *gzcf, double *a1cf, double *a2cf, double *a3cf, double *ccf, double *fcf, double *tcf)

Solves using Newton's Method.

- VPUBLIC void **Vfnewton** (int *nx, int *ny, int *nz, double *x, int *iz, double *w0, double *w1, double *w2, double *w3, int *istop, int *itmax, int *iters, int *ierror, int *nlev, int *ilev, int *nlev_real, int *mgsolv, int *iok, int *iinfo, double *epsiln, double *errtol, double *omega, int *nu1, int *nu2, int *mgsmoo, double *cprime, double *rhs, double *xtmp, int *ipc, double *rpc, double *pc, double *ac, double *cc, double *fc, double *tru)

Driver routines for the Newton method.

- VEXTERNC void **Vnewton** (int *nx, int *ny, int *nz, double *x, int *iz, double *w0, double *w1, double *w2, double *w3, int *istop, int *itmax, int *iters, int *ierror, int *nlev, int *ilev, int *nlev_real, int *mgsolv, int *iok, int *iinfo, double *epsiln, double *errtol, double *omega, int *nu1, int *nu2, int *mgsmoo, double *cprime, double *rhs, double *xtmp, int *ipc, double *rpc, double *pc, double *ac, double *cc, double *fc, double *tru)

Inexact-newton-multilevel method.

- VEXTERNC void **Vgetjac** (int *nx, int *ny, int *nz, int *nlev_real, int *iz, int *lev, int *ipkey, double *x, double *r, double *cprime, double *rhs, double *cc, double *pc)

Form the jacobian system.

- VPUBLIC void **Vpower** (int *nx, int *ny, int *nz, int *iz, int *ilev, int *ipc, double *rpc, double *ac, double *cc, double *w1, double *w2, double *w3, double *w4, double *eigmax, double *eigmax_model, double *tol, int *itmax, int *iters, int *iinfo)

Power methods for eigenvalue estimation.

- VEXTERNC void **Vipower** (int *nx, int *ny, int *nz, double *u, int *iz, double *w0, double *w1, double *w2, double *w3, double *w4, double *eigmin, double *eigmin_model, double *tol, int *itmax, int *iters, int *nlev, int *ilev, int *nlev_real, int *mgsolv, int *iok, int *iinfo, double *epsiln, double *errtol, double *omega, int *nu1, int *nu2, int *mgsmoo, int *ipc, double *rpc, double *pc, double *ac, double *cc, double *tru)

Standard inverse power method for minimum eigenvalue estimation.

- VEXTERNC void **Vsmooth** (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac, double *cc, double *fc, double *x, double *w1, double *w2, double *r, int *itmax, int *iters, double *errtol, double *omega, int *iresid, int *iadjoint, int *meth)

Multigrid smoothing functions.

- VEXTERNC void **Vnsmooth** (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac, double *cc, double *fc, double *x, double *w1, double *w2, double *r, int *itmax, int *iters, double *errtol, double *omega, int *iresid, int *iadjoint, int *meth)

call the appropriate non-linear smoothing routine.

7.31.1 Detailed Description

C translation of Holst group PMG code.

7.31.2 Macro Definition Documentation

7.31.2.1 HARMO2

```
#define HARMO2(
    a,
    b ) (2.0 * (a) * (b) / ((a) + (b)))
```

Multigrid subroutines.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

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*
```

Definition at line 65 of file [mgsubd.h](#).

7.31.2.2 MAXIONS

```
#define MAXIONS 50
```

Specifies the PDE definition for PMG to solve.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

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*
*
```

Definition at line 62 of file [mypdec.h](#).

7.31.3 Function Documentation

7.31.3.1 Vaxrand()

```
VEXTERNC void Vaxrand (
    int * nx,
    int * ny,
    int * nz,
    double * x )
```

Fill grid function with random values, including boundary values.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces axrand from mikpckd.f

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the y dimension of the 3d matrix
<i>nz</i>	The size of the z dimension of the 3d matrix
<i>x</i>	The 3d matrix to fill

Definition at line [291](#) of file [mikpckd.c](#).

7.31.3.2 Vazeros()

```
VEXTERNC void Vazeros (
    int * nx,
    int * ny,
    int * nz,
    double * x )
```

Zero out operation for a grid function, including boundary values.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces azeros from mikpckd.f

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the x dimension of the 3d matrix
<i>nz</i>	The size of the x dimension of the 3d matrix
<i>x</i>	The matrix to zero out

Definition at line [195](#) of file [mikpckd.c](#).

7.31.3.3 VbuildA()

```

VEXTERNC void VbuildA (
    int * nx,
    int * ny,
    int * nz,
    int * ipkey,
    int * mgdisc,
    int * numdia,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,
    double * fc,
    double * xf,
    double * yf,
    double * zf,
    double * gxcf,
    double * gycf,
    double * gzcf,
    double * a1cf,
    double * a2cf,
    double * a3cf,
    double * ccf,
    double * fcf )

```

Build the Laplacian.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

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Author

Mike Holst [original], Tucker Beck [translation]

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```

Break the matrix data-structure into diagonals and then call the matrix build routine

Author

Tucker Beck [C Translation], Michael Holst [Original]

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipkey</i>	
<i>mgdisc</i>	
<i>numdia</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>xf</i>	
<i>yf</i>	
<i>zf</i>	
<i>gxcf</i>	
<i>gycf</i>	
<i>gzcf</i>	
<i>a1cf</i>	
<i>a2cf</i>	
<i>a3cf</i>	
<i>ccf</i>	
<i>fcf</i>	

Definition at line 57 of file [buildAd.c](#).

7.31.3.4 Vbuildband()

```

VEXTERNC void Vbuildband (
    int * key,
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * ac,
    int * ipcB,
    double * rpcB,
    double * acB )

```

Banded matrix builder.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

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Author

Mike Holst and Steve Bond [original], Tucker Beck [translation]

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```

Build and factor a banded matrix given a matrix in diagonal form.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces buildband from buildBd.f

Parameters

<i>key</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>ipcB</i>	
<i>rpcB</i>	
<i>acB</i>	

Definition at line 57 of file [buildBd.c](#).

7.31.3.5 Vbuildband1_27()

VEXTERNC void Vbuildband1_27 (

```

int * nx,
int * ny,
int * nz,
int * ipc,
double * rpc,
double * oC,
double * oE,
double * oN,
double * uC,
double * oNE,
double * oNW,
double * uE,
double * uW,
double * uN,
double * uS,
double * uNE,
double * uNW,
double * uSE,
double * uSW,
int * ipcB,
double * rpcB,
double * acB,
int * n,
int * m,
int * lda )

```

Build the operator in banded form given the 27-diagonal form.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces buildband1_7 from buildBd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>oC</i>	
<i>oE</i>	
<i>oN</i>	
<i>uC</i>	
<i>oNE</i>	
<i>oNW</i>	
<i>uE</i>	
<i>uW</i>	
<i>uN</i>	
<i>uS</i>	
<i>uNE</i>	

Parameters

<i>uNW</i>	
<i>uSE</i>	
<i>uSW</i>	
<i>ipcB</i>	
<i>rpcB</i>	
<i>acB</i>	
<i>n</i>	
<i>m</i>	
<i>lda</i>	

Definition at line 183 of file [buildBd.c](#).

7.31.3.6 Vbuildband1_7()

```

VEXTERNC void Vbuildband1_7 (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * oC,
    double * oE,
    double * oN,
    double * uC,
    int * ipcB,
    double * rpcB,
    double * acB,
    int * n,
    int * m,
    int * lda )

```

Build the operator in banded form given the 7-diagonal form.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces buildband1_7 from buildBd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>oC</i>	
<i>oE</i>	
<i>oN</i>	

Parameters

<i>uC</i>	
<i>ipcB</i>	
<i>rpcB</i>	
<i>acB</i>	
<i>n</i>	
<i>m</i>	
<i>lda</i>	

Definition at line 119 of file [buildBd.c](#).

7.31.3.7 VbuildG()

```

VEXTERNC void VbuildG (
    int * nxf,
    int * nyf,
    int * nzf,
    int * nxc,
    int * nyc,
    int * nzc,
    int * numdia,
    double * pcFF,
    double * acFF,
    double * ac )

```

Build Galerkin matrix structures.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

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Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

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```


*
*

Parameters

<i>nx_f</i>	
<i>ny_f</i>	
<i>nz_f</i>	
<i>nx_c</i>	
<i>ny_c</i>	
<i>nz_c</i>	
<i>numdia</i>	
<i>pcFF</i>	
<i>acFF</i>	
<i>ac</i>	

Definition at line 57 of file [buildGd.c](#).

7.31.3.8 VbuildG_1()

```

VEXTERNC void VbuildG_1 (
    int * nxf,
    int * nyf,
    int * nzf,
    int * nx,
    int * ny,
    int * nz,
    double * oPC,
    double * oPN,
    double * oPS,
    double * oPE,
    double * oPW,
    double * oPNE,
    double * oPNW,
    double * oPSE,
    double * oPSW,
    double * uPC,
    double * uPN,
    double * uPS,
    double * uPE,
    double * uPW,
    double * uPNE,
    double * uPNW,
    double * uPSE,
    double * uPSW,
    double * dPC,
    double * dPN,
    double * dPS,
    double * dPE,
    double * dPW,
    double * dPNE,
    double * dPNW,

```

```

double * dPSE,
double * dPSW,
double * oC,
double * XoC,
double * XoE,
double * XoN,
double * XuC,
double * XoNE,
double * XoNW,
double * XuE,
double * XuW,
double * XuN,
double * XuS,
double * XuNE,
double * XuNW,
double * XuSE,
double * XuSW )

```

Computes a 27-point galerkin coarse grid matrix from a 1-point (i.e., diagonal) fine grid matrix.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces buildG_1 from buildGd.f

Expressions for the galerkin coarse grid stencil XA in terms of the fine grid matrix stencil A and the interpolation operator stencil P. these stencils have the form:

```

XA := array([
matrix([ [ -XdNW(i,j,k), -XdN(i,j,k), -XdNE(i,j,k) ], [ -XdW(i,j,k), -XdC(i,j,k), -XdE(i,j,k) ], [ -XdSW(i,j,k), -XdS(i,j,k), -XdSE(i,j,k) ] ]),
matrix([ [ -XoNW(i,j,k), -XoN(i,j,k), -XoNE(i,j,k) ], [ -XoW(i,j,k), XoC(i,j,k), -XoE(i,j,k) ], [ -XoSW(i,j,k), -XoS(i,j,k), -XoSE(i,j,k) ] ]),
matrix([ [ -XuNW(i,j,k), -XuN(i,j,k), -XuNE(i,j,k) ], [ -XuW(i,j,k), -XuC(i,j,k), -XuE(i,j,k) ], [ -XuSW(i,j,k), -XuS(i,j,k), -XuSE(i,j,k) ] ] )]):
A := array([
matrix([ [ 0, 0, 0 ], [ 0, 0, 0 ], [ 0, 0, 0 ] ]),
matrix([ [ 0, 0, 0 ], [ 0, oC(i,j,k), 0 ], [ 0, 0, 0 ] ]),
matrix([ [ 0, 0, 0 ], [ 0, 0, 0 ], [ 0, 0, 0 ] ]))
P := array([
matrix([ [ dPNW(i,j,k), dPN(i,j,k), dPNE(i,j,k) ], [ dPW(i,j,k), dPC(i,j,k), dPE(i,j,k) ], [ dPSW(i,j,k), dPS(i,j,k), dPSE(i,j,k) ] ]),
matrix([ [ oPNW(i,j,k), oPN(i,j,k), oPNE(i,j,k) ], [ oPW(i,j,k), oPC(i,j,k), oPE(i,j,k) ], [ oPSW(i,j,k), oPS(i,j,k), oPSE(i,j,k) ] ]),
matrix([ [ uPNW(i,j,k), uPN(i,j,k), uPNE(i,j,k) ], [ uPW(i,j,k), uPC(i,j,k), uPE(i,j,k) ], [ uPSW(i,j,k), uPS(i,j,k), uPSE(i,j,k) ] ] )]):

```

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>oPC</i>	

Parameters

<i>oPN</i>	
<i>oPS</i>	
<i>oPE</i>	
<i>oPW</i>	
<i>oPNE</i>	
<i>oPNW</i>	
<i>oPSE</i>	
<i>oPSW</i>	
<i>uPC</i>	
<i>uPN</i>	
<i>uPS</i>	
<i>uPE</i>	
<i>uPW</i>	
<i>uPNE</i>	
<i>uPNW</i>	
<i>uPSE</i>	
<i>uPSW</i>	
<i>dPC</i>	
<i>dPN</i>	
<i>dPS</i>	
<i>dPE</i>	
<i>dPW</i>	
<i>dPNE</i>	
<i>dPNW</i>	
<i>dPSE</i>	
<i>dPSW</i>	
<i>oC</i>	
<i>XoC</i>	
<i>XoE</i>	
<i>XoN</i>	
<i>XuC</i>	
<i>XoNE</i>	
<i>XoNW</i>	
<i>XuE</i>	
<i>XuW</i>	
<i>XuN</i>	
<i>XuS</i>	
<i>XuNE</i>	
<i>XuNW</i>	
<i>XuSE</i>	
<i>XuSW</i>	

Definition at line 145 of file [buildGd.c](#).

7.31.3.9 VbuildG_27()

```
VEXTERNC void VbuildG_27 (
```

```
int * nxf,  
int * nyf,  
int * nzf,  
int * nx,  
int * ny,  
int * nz,  
double * oPC,  
double * oPN,  
double * oPS,  
double * oPE,  
double * oPW,  
double * oPNE,  
double * oPNW,  
double * oPSE,  
double * oPSW,  
double * uPC,  
double * uPN,  
double * uPS,  
double * uPE,  
double * uPW,  
double * uPNE,  
double * uPNW,  
double * uPSE,  
double * uPSW,  
double * dPC,  
double * dPN,  
double * dPS,  
double * dPE,  
double * dPW,  
double * dPNE,  
double * dPNW,  
double * dPSE,  
double * dPSW,  
double * oC,  
double * oE,  
double * oN,  
double * uC,  
double * oNE,  
double * oNW,  
double * uE,  
double * uW,  
double * uN,  
double * uS,  
double * uNE,  
double * uNW,  
double * uSE,  
double * uSW,  
double * XoC,  
double * XoE,  
double * XoN,  
double * XuC,  
double * XoNE,  
double * XoNW,  
double * XuE,
```

```

double * XuW,
double * XuN,
double * XuS,
double * XuNE,
double * XuNW,
double * XuSE,
double * XuSW )

```

Compute a 27-point galerkin coarse grid matrix from a 27-point fine grid matrix.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces buildG_27 from buildGd.f

Expressions for the galerkin coarse grid stencil XA in terms of the fine grid matrix stencil A and the interpolation operator stencil P. these stencils have the form:

```

XA := array([
matrix([ [ -XdNW(i,j,k), -XdN(i,j,k), -XdNE(i,j,k) ], [ -XdW(i,j,k), -XdC(i,j,k), -XdE(i,j,k) ], [ -XdSW(i,j,k), -XdS(i,j,k), -XdSE(i,j,k) ] ]),
matrix([ [ -XoNW(i,j,k), -XoN(i,j,k), -XoNE(i,j,k) ], [ -XoW(i,j,k), XoC(i,j,k), -XoE(i,j,k) ], [ -XoSW(i,j,k), -XoS(i,j,k), -XoSE(i,j,k) ] ]),
matrix([ [ -XuNW(i,j,k), -XuN(i,j,k), -XuNE(i,j,k) ], [ -XuW(i,j,k), -XuC(i,j,k), -XuE(i,j,k) ], [ -XuSW(i,j,k), -XuS(i,j,k), -XuSE(i,j,k) ] ] ) ]):

```

```

A := array([
matrix([ [ -dNW(i,j,k), -dN(i,j,k), -dNE(i,j,k) ], [ -dW(i,j,k), -dC(i,j,k), -dE(i,j,k) ], [ -dSW(i,j,k), -dS(i,j,k), -dSE(i,j,k) ] ]),
matrix([ [ -oNW(i,j,k), -oN(i,j,k), -oNE(i,j,k) ], [ -oW(i,j,k), oC(i,j,k), -oE(i,j,k) ], [ -oSW(i,j,k), -oS(i,j,k), -oSE(i,j,k) ] ]),
matrix([ [ -uNW(i,j,k), -uN(i,j,k), -uNE(i,j,k) ], [ -uW(i,j,k), -uC(i,j,k), -uE(i,j,k) ], [ -uSW(i,j,k), -uS(i,j,k), -uSE(i,j,k) ] ] ) ]):

```

```

P := array([
matrix([ [ dPNW(i,j,k), dPN(i,j,k), dPNE(i,j,k) ], [ dPW(i,j,k), dPC(i,j,k), dPE(i,j,k) ], [ dPSW(i,j,k), dPS(i,j,k), dPSE(i,j,k) ] ]),
matrix([ [ oPNW(i,j,k), oPN(i,j,k), oPNE(i,j,k) ], [ oPW(i,j,k), oPC(i,j,k), oPE(i,j,k) ], [ oPSW(i,j,k), oPS(i,j,k), oPSE(i,j,k) ] ]),
matrix([ [ uPNW(i,j,k), uPN(i,j,k), uPNE(i,j,k) ], [ uPW(i,j,k), uPC(i,j,k), uPE(i,j,k) ], [ uPSW(i,j,k), uPS(i,j,k), uPSE(i,j,k) ] ] ) ]):

```

in addition, A is assumed to be symmetric so that:

```

oS := proc(x,y,z) RETURN( oN(x,y-1,z) ): end: oW := proc(x,y,z) RETURN( oE(x-1,y,z) ): end: oSE := proc(x,y,z)
RETURN( oNW(x+1,y-1,z) ): end: oSW := proc(x,y,z) RETURN( oNE(x-1,y-1,z) ): end:

```

```

dC := proc(x,y,z) RETURN( uC(x,y,z-1) ): end: dW := proc(x,y,z) RETURN( uE(x-1,y,z-1) ): end: dE := proc(x,y,z)
RETURN( uW(x+1,y,z-1) ): end:

```

```

dN := proc(x,y,z) RETURN( uS(x,y+1,z-1) ): end: dNW := proc(x,y,z) RETURN( uSE(x-1,y+1,z-1) ): end: dNE := proc(x,y,z)
RETURN( uSW(x+1,y+1,z-1) ): end:

```

```

dS := proc(x,y,z) RETURN( uN(x,y-1,z-1) ): end: dSW := proc(x,y,z) RETURN( uNE(x-1,y-1,z-1) ): end: dSE := proc(x,y,z)
RETURN( uNW(x+1,y-1,z-1) ): end:

```

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>oPC</i>	
<i>oPN</i>	

Parameters

<i>oPS</i>	
<i>oPE</i>	
<i>oPW</i>	
<i>oPNE</i>	
<i>oPNW</i>	
<i>oPSE</i>	
<i>oPSW</i>	
<i>uPC</i>	
<i>uPN</i>	
<i>uPS</i>	
<i>uPE</i>	
<i>uPW</i>	
<i>uPNE</i>	
<i>uPNW</i>	
<i>uPSE</i>	
<i>uPSW</i>	
<i>dPC</i>	
<i>dPN</i>	
<i>dPS</i>	
<i>dPE</i>	
<i>dPW</i>	
<i>dPNE</i>	
<i>dPNW</i>	
<i>dPSE</i>	
<i>dPSW</i>	
<i>oC</i>	
<i>oE</i>	
<i>oN</i>	
<i>uC</i>	
<i>oNE</i>	
<i>oNW</i>	
<i>uE</i>	
<i>uW</i>	
<i>uN</i>	
<i>uS</i>	
<i>uNE</i>	
<i>uNW</i>	
<i>uSE</i>	
<i>uSW</i>	
<i>XoC</i>	
<i>XoE</i>	
<i>XoN</i>	
<i>XuC</i>	
<i>XoNE</i>	
<i>XoNW</i>	
<i>XuE</i>	
<i>XuW</i>	

Parameters

<i>XuN</i>	
<i>XuS</i>	
<i>XuNE</i>	
<i>XuNW</i>	
<i>XuSE</i>	
<i>XuSW</i>	

Definition at line 1252 of file [buildGd.c](#).

7.31.3.10 VbuildG_7()

```

VEXTERNC void VbuildG_7 (
    int * nxf,
    int * nyf,
    int * nzf,
    int * nx,
    int * ny,
    int * nz,
    double * oPC,
    double * oPN,
    double * oPS,
    double * oPE,
    double * oPW,
    double * oPNE,
    double * oPNW,
    double * oPSE,
    double * oPSW,
    double * uPC,
    double * uPN,
    double * uPS,
    double * uPE,
    double * uPW,
    double * uPNE,
    double * uPNW,
    double * uPSE,
    double * uPSW,
    double * dPC,
    double * dPN,
    double * dPS,
    double * dPE,
    double * dPW,
    double * dPNE,
    double * dPNW,
    double * dPSE,
    double * dPSW,
    double * oC,
    double * oE,
    double * oN,
    double * uC,
    double * XoC,
    double * XoE,

```

```

double * XoN,
double * XuC,
double * XoNE,
double * XoNW,
double * XuE,
double * XuW,
double * XuN,
double * XuS,
double * XuNE,
double * XuNW,
double * XuSE,
double * XuSW )

```

Computes a 27-point galerkin coarse grid matrix from a 7-point fine grid matrix.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces buildG_7 from buildGd.f

Expressions for the galerkin coarse grid stencil XA in terms of the fine grid matrix stencil A and the interpolation operator stencil P. these stencils have the form:

```

XA := array([
matrix([ [ -XdNW(i,j,k), -XdN(i,j,k), -XdNE(i,j,k) ], [ -XdW(i,j,k), -XdC(i,j,k), -XdE(i,j,k) ], [ -XdSW(i,j,k), -XdS(i,j,k), -XdSE(i,j,k) ] ]),
matrix([ [ -XoNW(i,j,k), -XoN(i,j,k), -XoNE(i,j,k) ], [ -XoW(i,j,k), XoC(i,j,k), -XoE(i,j,k) ], [ -XoSW(i,j,k), -XoS(i,j,k), -XoSE(i,j,k) ] ]),
matrix([ [ -XuNW(i,j,k), -XuN(i,j,k), -XuNE(i,j,k) ], [ -XuW(i,j,k), -XuC(i,j,k), -XuE(i,j,k) ], [ -XuSW(i,j,k), -XuS(i,j,k), -XuSE(i,j,k) ] ] )]):
A := array([
matrix([ [ 0, 0, 0 ], [ 0, -dC(i,j,k), 0 ], [ 0, 0, 0 ] ]),
matrix([ [ 0, -oN(i,j,k), 0 ], [ -oW(i,j,k), oC(i,j,k), -oE(i,j,k) ], [ 0, -oS(i,j,k), 0 ] ]),
matrix([ [ 0, 0, 0 ], [ 0, -uC(i,j,k), 0 ], [ 0, 0, 0 ] ] )
P := array([
matrix([ [ dPNW(i,j,k), dPN(i,j,k), dPNE(i,j,k) ], [ dPW(i,j,k), dPC(i,j,k), dPE(i,j,k) ], [ dPSW(i,j,k), dPS(i,j,k), dPSE(i,j,k) ] ]),
matrix([ [ oPNW(i,j,k), oPN(i,j,k), oPNE(i,j,k) ], [ oPW(i,j,k), oPC(i,j,k), oPE(i,j,k) ], [ oPSW(i,j,k), oPS(i,j,k), oPSE(i,j,k) ] ]),
matrix([ [ uPNW(i,j,k), uPN(i,j,k), uPNE(i,j,k) ], [ uPW(i,j,k), uPC(i,j,k), uPE(i,j,k) ], [ uPSW(i,j,k), uPS(i,j,k), uPSE(i,j,k) ] ] )
]):

```

in addition, A is assumed to be symmetric so that:

```

oS := proc(x,y,z) RETURN( oN(x,y-1,z) ): end: oW := proc(x,y,z) RETURN( oE(x-1,y,z) ): end: dC := proc(x,y,z) RETURN( uC(x,y,z-1) ): end:

```

Parameters

<i>nx_f</i>	
<i>ny_f</i>	
<i>nz_f</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>oPC</i>	
<i>oPN</i>	
<i>oPS</i>	

Parameters

<i>oPE</i>	
<i>oPW</i>	
<i>oPNE</i>	
<i>oPNW</i>	
<i>oPSE</i>	
<i>oPSW</i>	
<i>uPC</i>	
<i>uPN</i>	
<i>uPS</i>	
<i>uPE</i>	
<i>uPW</i>	
<i>uPNE</i>	
<i>uPNW</i>	
<i>uPSE</i>	
<i>uPSW</i>	
<i>dPC</i>	
<i>dPN</i>	
<i>dPS</i>	
<i>dPE</i>	
<i>dPW</i>	
<i>dPNE</i>	
<i>dPNW</i>	
<i>dPSE</i>	
<i>dPSW</i>	
<i>oC</i>	
<i>oE</i>	
<i>oN</i>	
<i>uC</i>	
<i>XoC</i>	
<i>XoE</i>	
<i>XoN</i>	
<i>XuC</i>	
<i>XoNE</i>	
<i>XoNW</i>	
<i>XuE</i>	
<i>XuW</i>	
<i>XuN</i>	
<i>XuS</i>	
<i>XuNE</i>	
<i>XuNW</i>	
<i>XuSE</i>	
<i>XuSW</i>	

Definition at line 450 of file `buildGd.c`.

7.31.3.11 Vbuildgaler0()

```

VEXTERNC void Vbuildgaler0 (
    int * nxf,
    int * nyf,
    int * nzf,
    int * nxc,
    int * nyc,
    int * nzc,
    int * ipkey,
    int * numdia,
    double * pcFF,
    int * ipcFF,
    double * rpcFF,
    double * acFF,
    double * ccFF,
    double * fcFF,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,
    double * fc )

```

Form the Galerkin coarse grid system.

Note

Although the fine grid matrix may be 7 or 27 diagonal, the coarse grid matrix is always 27 diagonal. (only 14 stored due to symmetry.)

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces buildgaler0 from mgsbnd.f

Parameters

<i>nxf</i>	
<i>nyf</i>	
<i>nzf</i>	
<i>nxc</i>	
<i>nyc</i>	
<i>nzc</i>	
<i>ipkey</i>	
<i>numdia</i>	
<i>pcFF</i>	
<i>ipcFF</i>	
<i>rpcFF</i>	
<i>acFF</i>	
<i>ccFF</i>	
<i>fcFF</i>	
<i>ipc</i>	

Parameters

<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	

Definition at line 341 of file [mgsubd.c](#).

7.31.3.12 Vbuildops()

```

VEXTERNC void Vbuildops (
    int * nx,
    int * ny,
    int * nz,
    int * nlev,
    int * ipkey,
    int * iinfo,
    int * ido,
    int * iz,
    int * mgprol,
    int * mgcoar,
    int * mgsolv,
    int * mgdisc,
    int * ipc,
    double * rpc,
    double * pc,
    double * ac,
    double * cc,
    double * fc,
    double * xf,
    double * yf,
    double * zf,
    double * gxcf,
    double * gycf,
    double * gzcf,
    double * a1cf,
    double * a2cf,
    double * a3cf,
    double * ccf,
    double * fcf,
    double * tcf )

```

Build operators, boundary arrays, modify affine vectors ido==0: do only fine level ido==1: do only coarse levels (including second op at coarsest) ido==2: do all levels ido==3: rebuild the second operator at the coarsest level.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

```

*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
*
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*
*

```

Note

The fine level must be build before any coarse levels.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Replaces buildops from mgsubd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>nlev</i>	
<i>ipkey</i>	
<i>iinfo</i>	

Parameters

<i>ido</i>	
<i>iz</i>	
<i>mgprol</i>	
<i>mgcoar</i>	
<i>mgsolv</i>	
<i>mgdisc</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>pc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>xf</i>	
<i>yf</i>	
<i>zf</i>	
<i>gxcf</i>	
<i>gycf</i>	
<i>gzcf</i>	
<i>a1cf</i>	
<i>a2cf</i>	
<i>a3cf</i>	
<i>ccf</i>	
<i>fcf</i>	
<i>tcf</i>	

Definition at line 57 of file [mgsubd.c](#).

7.31.3.13 VbuildP()

```

VEXTERNC void VbuildP (
    int * nxf,
    int * nyf,
    int * nzf,
    int * nxc,
    int * nyc,
    int * nzc,
    int * mgprol,
    int * ipc,
    double * rpc,
    double * pc,
    double * ac,
    double * xf,
    double * yf,
    double * zf )

```

Builds prolongation matrix.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

```

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Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

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```

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>mgprol</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>pc</i>	
<i>ac</i>	
<i>xf</i>	
<i>yf</i>	
<i>zf</i>	

Definition at line 57 of file [buildPd.c](#).

7.31.3.14 Vbuildstr()

```
VEXTERNC void Vbuildstr (
    int * nx,
    int * ny,
    int * nz,
    int * nlev,
    int * iz )
```

Build the nexted operator framework in the array iz.

Note

iz(50,i) indexes into the gridfn arrays for each level i=(1,...,nlev+1) as follows:

```
fun(i) = fun (iz(1,i)) bndx(i) = bndx(iz(2,i)) bndy(i) = bndy(iz(3,i)) bndz(i) = bndz(iz(4,i)) ipc(i) = ipc(iz(5,i)) rpc(i) =
rpc(iz(6,i)) oper(i) = oper(iz(7,i)) grdx(i) = brdx(iz(8,i)) grdy(i) = brdy(iz(9,i)) grdz(i) = brdz(iz(10,i))
```

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces buildstr from mgsubd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>nlev</i>	
<i>iz</i>	

Definition at line 257 of file [mgsubd.c](#).

7.31.3.15 Vc_vec()

```
VEXTERNC void Vc_vec (
    double * coef,
    double * uin,
    double * uout,
    int * nx,
    int * ny,
    int * nz,
    int * ipkey )
```

Define the nonlinearity (vector version)

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces `c_vec` from `mypde.f`

Parameters

<i>coef</i>	
<i>uin</i>	
<i>uout</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipkey</i>	

Definition at line 121 of file `myppdec.c`.

7.31.3.16 Vc_vecpmg()

```
VEXTERNC void Vc_vecpmg (
    double * coef,
    double * uin,
    double * uout,
    int * nx,
    int * ny,
    int * nz,
    int * ipkey )
```

Define the nonlinearity (vector version)

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces `c_vecpmg` from `mypde.f`

Parameters

<i>coef</i>	
<i>uin</i>	
<i>uout</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipkey</i>	

Definition at line 133 of file `myppdec.c`.

7.31.3.17 Vc_vecsmpbe()

```
VEXTERNC void Vc_vecsmpbe (
```

```

double * coef,
double * uin,
double * uout,
int * nx,
int * ny,
int * nz,
int * ipkey )

```

Define the nonlinearity (vector version)

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces `c_vecpgm` from `mypde.f`

Parameters

<i>coef</i>	
<i>uin</i>	
<i>uout</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipkey</i>	

Definition at line 213 of file `myppdec.c`.

7.31.3.18 Vcghs()

```

VEXTERNC void Vcghs (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,
    double * fc,
    double * x,
    double * p,
    double * ap,
    double * r,
    int * itmax,
    int * iters,
    double * errtol,
    double * omega,
    int * iresid,
    int * iadjoint )

```

A collection of useful low-level routines (timing, etc).

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

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Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

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```

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>x</i>	
<i>p</i>	
<i>ap</i>	
<i>r</i>	
<i>itmax</i>	
<i>iters</i>	
<i>errtol</i>	
<i>omega</i>	
<i>iresid</i>	

Parameters

<i>iadjoint</i>	
-----------------	--

Definition at line 57 of file [cgd.c](#).

7.31.3.19 Vdc_vec()

```
VEXTERNC void Vdc_vec (
    double * coef,
    double * uin,
    double * uout,
    int * nx,
    int * ny,
    int * nz,
    int * ipkey )
```

Define the derivative of the nonlinearity (vector version)

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces dc_vec from mypde.f

Parameters

<i>coef</i>	
<i>uin</i>	
<i>uout</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipkey</i>	

Definition at line 341 of file [mypdec.c](#).

7.31.3.20 Vdpbsl()

```
VEXTERNC void Vdpbsl (
    double * abd,
    int * lda,
    int * n,
    int * m,
    double * b )
```

LINPACK interface.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version**\$Id:****Attention**

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Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

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```

Solves the double precision symmetric positive definite band system $A \cdot X = B$ using the factors computed by `dpbco` or `dpbfa`

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

A division by zero will occur if the input factor contains a zero on the diagonal. Technically this indicates singularity, but it is usually caused by improper subroutine arguments. It will not occur if the subroutines are called correctly and `info == 0`

Replaces `dpbsl` from `mgsubd.f`

Parameters

<i>abd</i>	The output from <code>dpbco</code> or <code>dpbfa</code>
<i>lda</i>	The leading dimension of the array <i>abd</i>
<i>n</i>	The order of the matrix <i>a</i>
<i>m</i>	The number of diagonals above the main diagonal
<i>b</i>	The right hand side vector

Definition at line 57 of file [mlinpckd.c](#).

7.31.3.21 Vextrac()

```

VEXTERNC void Vextrac (
    int * nxf,

```

```

int * nyf,
int * nzf,
int * nxc,
int * ny,
int * nzc,
double * xin,
double * xout )

```

Simple injection of a fine grid function into coarse grid.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces extrac from matvecd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>nxc</i>	
<i>ny</i>	
<i>nzc</i>	
<i>xin</i>	
<i>xout</i>	

Definition at line 1078 of file [matvecd.c](#).

7.31.3.22 VfboundPMG()

```

VEXTERNC void VfboundPMG (
    int * ibound,
    int * nx,
    int * ny,
    int * nz,
    double * x,
    double * gxc,
    double * gyc,
    double * gzc )

```

Initialize a grid function to have a certain boundary value,.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces fboundPMG from mikpckd.f

Parameters

<i>ibound</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>x</i>	
<i>gxc</i>	
<i>gyc</i>	
<i>gzc</i>	

Definition at line 209 of file [mikpckd.c](#).

7.31.3.23 VfboundPMG00()

```

VEXTERNC void VfboundPMG00 (
    int * nx,
    int * ny,
    int * nz,
    double * x )

```

Initialize a grid function to have a zero boundary value.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces fboundPMG00 from mikpckd.f

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the y dimension of the 3d matrix
<i>nz</i>	The size of the z dimension of the 3d matrix
<i>x</i>	The 3d matrix to initialize

Definition at line 258 of file [mikpckd.c](#).

7.31.3.24 Vfmvfas()

```

VEXTERNC void Vfmvfas (
    int * nx,
    int * ny,
    int * nz,
    double * x,
    int * iz,
    double * w0,
    double * w1,
    double * w2,
    double * w3,

```

```

double * w4,
int * istop,
int * itmax,
int * iters,
int * ierror,
int * nlev,
int * ilev,
int * nlev_real,
int * mgsolv,
int * iok,
int * iinfo,
double * epsilon,
double * errtol,
double * omega,
int * nu1,
int * nu2,
int * mgsmoo,
int * ipc,
double * rpc,
double * pc,
double * ac,
double * cc,
double * fc,
double * tru )

```

Multigrid nonlinear solve iteration routine.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

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Author

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```

Nested iteration for a nonlinear multilevel method. Algorithm: nonlinear multigrid iteration (fas)

this routine is the full multigrid front-end for a multigrid v-cycle solver. in other words, it repeatedly calls the v-cycle multigrid solver on successively finer and finer grids.

Note

Author

Tucker Beck [C Translation], Michael Holst [Original]

Replaces fmvmf from mgfasd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>x</i>	
<i>iz</i>	
<i>w0</i>	
<i>w1</i>	
<i>w2</i>	
<i>w3</i>	
<i>w4</i>	
<i>istop</i>	
<i>itmax</i>	
<i>iters</i>	
<i>ierror</i>	
<i>nlev</i>	
<i>ilev</i>	
<i>nlev_real</i>	
<i>mgsovl</i>	
<i>iok</i>	
<i>iinfo</i>	
<i>epsiln</i>	
<i>errtol</i>	
<i>omega</i>	
<i>nu1</i>	
<i>nu2</i>	
<i>mgsmoo</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>pc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>tru</i>	

Definition at line 57 of file [mgfasd.c](#).

7.31.3.25 Vfnewton()

```

VPUBLIC void Vfnewton (
    int * nx,
    int * ny,
    int * nz,
    double * x,
    int * iz,
    double * w0,
    double * w1,
    double * w2,
    double * w3,
    int * istop,
    int * itmax,
    int * iters,
    int * ierror,
    int * nlev,
    int * ilev,
    int * nlev_real,
    int * mgsolv,
    int * iok,
    int * iinfo,
    double * epsiln,
    double * errtol,
    double * omega,
    int * nul,
    int * nu2,
    int * mgsmoo,
    double * cprime,
    double * rhs,
    double * xtmp,
    int * ipc,
    double * rpc,
    double * pc,
    double * ac,
    double * cc,
    double * fc,
    double * tru )

```

Driver routines for the Newton method.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

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*
* APBS -- Adaptive Poisson-Boltzmann Solver
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* Nathan A. Baker (nathan.baker@pnl.gov)
* Pacific Northwest National Laboratory
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Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Attention

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*
```

Nested iteration for an inexact-newton-multilevel method.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces fnewton from newtond.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>x</i>	
<i>iz</i>	
<i>w0</i>	
<i>w1</i>	
<i>w2</i>	
<i>w3</i>	
<i>istop</i>	
<i>itmax</i>	
<i>iters</i>	
<i>ierror</i>	
<i>nlev</i>	
<i>ilev</i>	
<i>nlev_real</i>	
<i>mgsovl</i>	
<i>iok</i>	
<i>iinfo</i>	
<i>epsiln</i>	
<i>errtol</i>	
<i>omega</i>	
<i>nu1</i>	
<i>nu2</i>	
<i>mgsmoo</i>	
<i>cprime</i>	
<i>rhs</i>	

Parameters

<i>xtmp</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>pc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>tru</i>	

Definition at line 58 of file [newtond.c](#).

7.31.3.26 Vgetjac()

```

VEXTERNC void Vgetjac (
    int * nx,
    int * ny,
    int * nz,
    int * nlev_real,
    int * iz,
    int * lev,
    int * ipkey,
    double * x,
    double * r,
    double * cprime,
    double * rhs,
    double * cc,
    double * pc )

```

Form the jacobian system.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces getjac from newtond.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>nlev_real</i>	
<i>iz</i>	
<i>lev</i>	
<i>ipkey</i>	
<i>x</i>	
<i>r</i>	
<i>cprime</i>	
<i>rhs</i>	
<i>cc</i>	
<i>pc</i>	

Definition at line 550 of file [newtond.c](#).

7.31.3.27 Vgsrb()

```
VEXTERNC void Vgsrb (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,
    double * fc,
    double * x,
    double * w1,
    double * w2,
    double * r,
    int * itmax,
    int * iters,
    double * errtol,
    double * omega,
    int * iresid,
    int * iadjoint )
```

Guass-Seidel solver.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

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Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

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*

```

Call the fast diagonal iterative method.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces gsr_b from gsd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>x</i>	
<i>w1</i>	
<i>w2</i>	
<i>r</i>	
<i>itmax</i>	
<i>iters</i>	
<i>errtol</i>	
<i>omega</i>	
<i>iresid</i>	
<i>iadjoint</i>	

Definition at line 57 of file [gsd.c](#).

7.31.3.28 VinterpPMG()

```

VEXTERNC void VinterpPMG (
    int * nxc,
    int * nyc,
    int * nzc,
    int * nxf,
    int * nyf,
    int * nzf,
    double * xin,
    double * xout,
    double * pc )

```

Apply the prolongation operator.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces interpPMG from matvecd.f

Parameters

<i>nxc</i>	
<i>nyc</i>	
<i>nzc</i>	
<i>nx_f</i>	
<i>ny_f</i>	
<i>nz_f</i>	
<i>xin</i>	
<i>xout</i>	
<i>pc</i>	

Definition at line 915 of file [matvecd.c](#).

7.31.3.29 Vipower()

```

VEXTERNC void Vipower (
    int * nx,
    int * ny,
    int * nz,
    double * u,
    int * iz,
    double * w0,
    double * w1,
    double * w2,
    double * w3,
    double * w4,
    double * eigmin,
    double * eigmin_model,
    double * tol,
    int * itmax,
    int * iters,
    int * nlev,
    int * ilev,
    int * nlev_real,
    int * mgsolv,
    int * iok,
    int * iinfo,
    double * epsiln,
    double * errtol,
    double * omega,
    int * nu1,
    int * nu2,
    int * mgsmoo,
    int * ipc,
    double * rpc,
    double * pc,
    double * ac,
    double * cc,
    double * tru )

```

Standard inverse power method for minimum eigenvalue estimation.

Note

To test, note that the 3d laplacean has min/max eigenvalues:

```

lambda_min = 6 - 2*dcos(pi/(nx-1))
              - 2*dcos(pi/(ny-1))
              - 2*dcos(pi/(nz-1))

lambda_max = 6 - 2*dcos((nx-2)*pi/(nx-1))
              - 2*dcos((ny-2)*pi/(ny-1))
              - 2*dcos((nz-2)*pi/(nz-1))

```

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces ipower from powerd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>u</i>	
<i>iz</i>	
<i>w0</i>	
<i>w1</i>	
<i>w2</i>	
<i>w3</i>	
<i>w4</i>	
<i>eigmin</i>	
<i>eigmin_model</i>	
<i>tol</i>	
<i>itmax</i>	
<i>iters</i>	
<i>nlev</i>	
<i>ilev</i>	
<i>nlev_real</i>	
<i>mgsovl</i>	
<i>iok</i>	
<i>iinfo</i>	
<i>epsiln</i>	
<i>errtol</i>	
<i>omega</i>	
<i>nu1</i>	
<i>nu2</i>	
<i>mgsmoo</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>pc</i>	
<i>ac</i>	
<i>cc</i>	
<i>tru</i>	

Definition at line 165 of file [powerd.c](#).

7.31.3.30 Vmatvec()

```
VEXTERNC void Vmatvec (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,
    double * x,
    double * y )
```

Matrix-vector multiplication routines.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

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Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

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*
*
```

Break the matrix data-structure into diagonals and then call the matrix-vector routine.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces matvec from matvecd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>x</i>	
<i>y</i>	

Definition at line 57 of file [matvecd.c](#).

7.31.3.31 Vmgdriv()

```

VEXTERNC void Vmgdriv (
    int * iparm,
    double * rparm,
    int * iwork,
    double * rwork,
    double * u,
    double * xf,
    double * yf,
    double * zf,
    double * gxcf,
    double * gycf,
    double * gzcf,
    double * a1cf,
    double * a2cf,
    double * a3cf,
    double * ccf,
    double * fcf,
    double * tcf )

```

Multilevel solver driver.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

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Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

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```

Author

Tucker Beck [C Translation], Michael Holst [Original]

Replaces mgdriv from mgdrvd.f

Parameters

<i>iparm</i>	
<i>rparm</i>	
<i>iwork</i>	
<i>rwork</i>	
<i>u</i>	
<i>xf</i>	
<i>yf</i>	
<i>zf</i>	
<i>gxcf</i>	
<i>gycf</i>	
<i>gzcf</i>	
<i>a1cf</i>	
<i>a2cf</i>	
<i>a3cf</i>	
<i>ccf</i>	
<i>fcf</i>	
<i>tcf</i>	

Definition at line 57 of file [mgdrvd.c](#).

7.31.3.32 Vmgdriv2()

```

VEXTERNC void Vmgdriv2 (
    int * iparm,
    double * rparm,
    int * nx,
    int * ny,
    int * nz,

```

```

double * u,
int * iz,
int * ipc,
double * rpc,
double * pc,
double * ac,
double * cc,
double * fc,
double * xf,
double * yf,
double * zf,
double * gxcf,
double * gycf,
double * gzcf,
double * a1cf,
double * a2cf,
double * a3cf,
double * ccf,
double * fcf,
double * tcf )

```

Solves the pde using the multi-grid method.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Replaces mgdrv2 from mgdrv.f

This routine uses a multigrid method to solve the following three-dimensional, 2nd order elliptic partial differential equation:

```

lu = f, u in omega
u = g, u on boundary of omega

```

where

```

omega = [xmin,xmax]x[ymin,ymax]x[zmin,zmax]

```

the multigrid code requires the operator in the form:

$$-\nabla \cdot (a \nabla u) + c(u) = f$$

with

$a(x,y,z), f(x,y,z)$, scalar functions (possibly discontinuous) on ω . (discontinuities must be along fine grid lines).
boundary function $g(x,y,z)$ is smooth on boundary of ω .

the function $c(u)$ is a possibly nonlinear function of the unknown u , and varies (possibly discontinuously) with the spatial position also.

user inputs:

the user must provide the coefficients of the differential operator, some initial parameter settings in an integer and a real parameter array, and various work arrays.

Parameters

<i>iparm</i>	
--------------	--

Parameters

<i>rparm</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>u</i>	
<i>iz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>pc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>xf</i>	
<i>yf</i>	
<i>zf</i>	
<i>gxcf</i>	
<i>gycf</i>	
<i>gzcf</i>	
<i>a1cf</i>	
<i>a2cf</i>	
<i>a3cf</i>	
<i>ccf</i>	
<i>fcf</i>	
<i>tcf</i>	

Definition at line 190 of file [mgdrvd.c](#).

7.31.3.33 Vmgsz()

```

VEXTERNC void Vmgsz (
    int * mgcoar,
    int * mgdisc,
    int * mgsolv,
    int * nx,
    int * ny,
    int * nz,
    int * nlev,
    int * nxc,
    int * nyc,
    int * nzc,
    int * nf,
    int * nc,
    int * narr,
    int * narrc,
    int * n_rpc,
    int * n_iz,
    int * n_ipc,
    int * iretot,

```

```
int * iintot )
```

This routine computes the required sizes of the real and integer work arrays for the multigrid code. these two sizes are a (complicated) function of input parameters.

The work arrays must have been declared in the calling program as:

```
double precision rwork(iretot)
integer          iwork(iintot)
```

where:

```
iretot  = function_of(mgcoar,mgdisc,mgssolv,nx,ny,nz,nlev)
iintot  = function_of(mgcoar,mgdisc,mgssolv,nx,ny,nz,nlev)

mgcoar  = coarsening technique:
          0=standard discretization
          1=averaged coefficient + standard discretization
          2=algebraic galerkin coarsening

mgdisc  = discretization technique:
          0=box method
          1=fem method

mgssolv  = coarse grid solver:
           0=conjugate gradients
           1=symmetric banded linpack solver

nx,ny,nz = grid dimensions in each direction,
           including boundary points

nlev     = the number of multigrid levels desired for the
           method.
```

other parameters:

```
nf       = number of unknowns on the finest mesh
          = nx * ny * nz

nc       = number of unknowns on the coarsest mesh

narr     = storage for one vector on all the meshes

narrc    = storage for one vector on all the meshes but the finest
```

the work arrays rwork and iwork will be chopped into smaller pieces according to:

```
double precision ac(STORE)          (system operators on all levels)
double precision pc(27*narrc)       (prol. opers for coarse levels)
double precision cc(narr),fc(narr)  (helmholtz term, rhs -- all levels)
double precision rpc(100*(nlev+1))  (real info for all levels)
integer          ipc(100*(nlev+1))  (integer info for all levels)
integer          iz(50,nlev+1),     (pointers into ac,pc,cc,fc,etc.)
```

where STORE depends on the discretization, coarsening, and coarse grid solver:

```
STORE = 4*nf + 4*narrc + NBAND*nc (mgdisc=box, mgcoar=stan/harm)
       or = 4*nf + 14*narrc + NBAND*nc (mgdisc=box, mgcoar=gal)
       or = 14*nf + 14*narrc + NBAND*nc (mgdisc=fem, mgcoar=stan/harm/gal)

NBAND = 0 (mgssolv=iterative)
       or = 1+(nxc-2)*(nyc-2) (mgssolv=7-pt banded linpack)
       or = 1+(nxc-2)*(nyc-2)+(nxc-2)+1 (mgssolv=27-pt banded linpack)
```

Author

Tucker Beck [C Translation], Michael Holst [Original]

Replaces mgsz from mgdrvd.f

Parameters

<i>mgcoar</i>	
<i>mgdisc</i>	
<i>mgsolv</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>nlev</i>	
<i>nxc</i>	
<i>nyc</i>	
<i>nzc</i>	
<i>nf</i>	
<i>nc</i>	
<i>narr</i>	
<i>narrc</i>	
<i>n_rpc</i>	
<i>n_iz</i>	
<i>n_ipc</i>	
<i>iretot</i>	
<i>iintot</i>	

Definition at line 562 of file [mgdrvd.c](#).

7.31.3.34 Vmresid()

```

VEXTERNC void Vmresid (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,
    double * fc,
    double * x,
    double * r )

```

Break the matrix data-structure into diagonals and then call the residual routine.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces mresid from matvecd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	

Parameters

<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>x</i>	
<i>r</i>	

Definition at line 426 of file [matvecd.c](#).

7.31.3.35 Vmvs()

```
VEXTERNC void Vmvs (
    int * nx,
    int * ny,
    int * nz,
    double * x,
    int * iz,
    double * w0,
    double * w1,
    double * w2,
    double * w3,
    int * istop,
    int * itmax,
    int * iters,
    int * ierror,
    int * nlev,
    int * ilev,
    int * nlev_real,
    int * mgsolv,
    int * iok,
    int * iinfo,
    double * epsiln,
    double * errtol,
    double * omega,
    int * nu1,
    int * nu2,
    int * mgsmoo,
    int * ipc,
    double * rpc,
    double * pc,
    double * ac,
    double * cc,
    double * fc,
    double * tru )
```

MG helper functions.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version**\$Id:****Attention**

```

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```

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version**\$Id:**

Attention

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* Pacific Northwest National Laboratory
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*
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```

Screaming linear multilevel method.

algorithm: linear multigrid iteration (cs)

multigrid v-cycle solver.

input: (1) fine and coarse grid discrete linear operators: L_h , L_H (2) fine grid source function: f_h (3) fine grid approximate solution: u_h

output: (1) fine grid improved solution: u_h

the two-grid algorithm is: (1) pre-smooth: $u1_h = \text{smooth}(L_h, f_h, u_h)$ (2) restrict defect: $d_H = r(L_h(u1_h) - f_h)$ (3) solve for correction: $c_H = L_H^{-1}(d_H)$ (4) prolongate and correct: $u2_h = u1_h - p(c_H)$ (5) post-smooth: $u_h = \text{smooth}(L_h, f_h, u2_h)$

(of course, c_H is determined with another two-grid algorithm)

implementation notes: (0) " $u1_h$ " must be kept on each level until " c_H " is computed, and then both are used to compute " $u2_h$ ". (1) " u_h " (and then " $u1_h$ ") on all levels is stored in the "x" array. (2) " d_H " is identically " f_h " for f_h on the next coarser grid. (3) " c_h " is identically " u_h " for u_h on the next coarser grid. (4) " d_H " is stored in the "r" array (must be kept for post-smooth). (5) " f_h " is stored in the "fc" array. (6) " L_h " on all levels is stored in the "ac" array. (7) signs may be reversed; i.e., residual is used in place of the defect in places, etc.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces mvcs from mgcsd.f

New grid size

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>x</i>	
<i>iz</i>	
<i>w0</i>	
<i>w1</i>	
<i>w2</i>	
<i>w3</i>	
<i>istop</i>	
<i>itmax</i>	
<i>iters</i>	
<i>ierror</i>	
<i>nlev</i>	
<i>ilev</i>	
<i>nlev_real</i>	
<i>mgssolv</i>	
<i>iok</i>	
<i>iinfo</i>	
<i>epsiln</i>	
<i>errtol</i>	
<i>omega</i>	
<i>nu1</i>	
<i>nu2</i>	
<i>mgsmoo</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>pc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>tru</i>	

Definition at line 57 of file [mgcsd.c](#).

7.31.3.36 Vmvas()

```

VEXTERNC void Vmvas (
    int * nx,
    int * ny,
    int * nz,
    double * x,
    int * iz,

```

```

double * w0,
double * w1,
double * w2,
double * w3,
double * w4,
int * istop,
int * itmax,
int * iters,
int * ierror,
int * nlev,
int * ilev,
int * nlev_real,
int * mgsolv,
int * iok,
int * iinfo,
double * epsilon,
double * errtol,
double * omega,
int * nul,
int * nu2,
int * mgsmoo,
int * ipc,
double * rpc,
double * pc,
double * ac,
double * cc,
double * fc,
double * tru )

```

Nonlinear multilevel method.

Note

Replaces mvfas from mgfasd.f

Author

Tucker Beck [C Translation], Michael Holst [Original]

Algorithm: nonlinear multigrid iteration (fas)

multigrid v-cycle solver.

input: (1) fine and coarse grid discrete nonlinear operators: L_h , L_H (2) fine grid source function: f_h (3) fine grid approximate solution: u_h

output: (1) fine grid improved solution: u_h

the two-grid algorithm is: (1) pre-smooth: $u1_h = \text{smooth}(L_h, f_h, u_h)$ (2) restrict defect: $d_H = r(L_h(u1_h) - f_h)$

restrict solution: $u_H = r(u1_h)$ (3) form coarse grid rhs: $f_H = L_H(u_H) - d_H$ solve for correction: $c_H = L_H^{-1}\{f_H - L_H(u_H)\}$ (4) prolongate and correct: $u2_h = u1_h - p(c_H - u_H)$ (5) post-smooth: $u_h = \text{smooth}(L_h, f_h, u2_h)$

(of course, c_H is determined with another two-grid algorithm)

implementation notes: (0) " $u1_h$ " and " u_H " must be kept on each level until " c_H " is computed, and then all three are used to compute " $u2_h$ ". (1) " u_h " (and then " $u1_h$ ") on all levels is stored in the " x " array. (2) " u_H " on all levels is stored in the " e " array. (3) " c_h " is identically " u_h " for u_h on the next coarser grid. (4) " d_H " is stored in the " r " array. (5) " f_h " and " f_H " are stored in the " fc " array. (6) " L_h " on all levels is stored in the " ac " array. (7) signs may be reversed; i.e., residual is used in place of the defect in places, etc.

Parameters

n_x	
-------	--

Parameters

<i>ny</i>	
<i>nz</i>	
<i>x</i>	
<i>iz</i>	
<i>w0</i>	
<i>w1</i>	
<i>w2</i>	
<i>w3</i>	
<i>w4</i>	
<i>istop</i>	
<i>itmax</i>	
<i>iters</i>	
<i>ierror</i>	
<i>nlev</i>	
<i>ilev</i>	
<i>nlev_real</i>	
<i>mgsolv</i>	
<i>iok</i>	
<i>iinfo</i>	
<i>epsiln</i>	
<i>errtol</i>	
<i>omega</i>	
<i>nu1</i>	
<i>nu2</i>	
<i>mgsmoo</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>pc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>tru</i>	

Definition at line 157 of file [mgfasd.c](#).

7.31.3.37 Vmypdefinitlpbe()

```

VEXTERNC void Vmypdefinitlpbe (
    int * tnion,
    double * tcharge,
    double * tsconc )

```

Set up the ionic species to be used in later calculations. This must be called before any other of the routines in this file.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

```

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```

Author

Tucker Beck [C Translation], Nathan Baker [Original]

Note

Replaces mypdefinitlpbe from mypde.f

Parameters

<i>tnion</i>	The number if ionic species
<i>tcharge</i>	The charge in electrons
<i>tsconc</i>	Prefactor for conterion Boltzmann distribution terms. Basically a scaled concentration $-(ion\ concentration/bulkIonicStrength)/2$

Definition at line 57 of file [mypdec.c](#).

7.31.3.38 Vmypdefinitnpbe()

```
VEXTERNC void Vmypdefinitnpbe (
    int * tnion,
    double * tcharge,
    double * tsconc )
```

Set up the ionic species to be used in later calculations. This must be called before any other of the routines in this file.

Author

Tucker Beck [C Translation], Nathan Baker [Original]

Note

Replaces mypdefinitnpbe from mypde.f

Parameters

<i>tnion</i>	The number if ionic species
<i>tcharge</i>	The charge in electrons
<i>tsconc</i>	Prefactor for conterion Boltzmann distribution terms. Basically a scaled concentration $-(ion\ concentration/bulkIonicStrength)/2$

Definition at line 75 of file [mypdec.c](#).

7.31.3.39 Vmypdefinitmpbe()

```
VEXTERNC void Vmypdefinitmpbe (
    int * tnion,
    double * tcharge,
    double * tsconc,
    double * smvolume,
    double * smsize )
```

Set up the ionic species to be used in later calculations. This must be called before any other of the routines in this file.

Author

Tucker Beck [C Translation], Nathan Baker [Original]

Note

Replaces mypdefinitmpbe from mypde.f

Parameters

<i>tnion</i>	The number if ionic species
<i>tcharge</i>	The charge in electrons
<i>tsconc</i>	Prefactor for conterion Boltzmann distribution terms. Basically a scaled concentration $-(ion\ concentration/bulkIonicStrength)/2$
<i>smvolume</i>	
<i>smsize</i>	

Definition at line 93 of file [myppdec.c](#).

7.31.3.40 Vnewdriv()

```
VEXTERNC void Vnewdriv (
    int * iparm,
    double * rparm,
    int * iwork,
    double * rwork,
    double * u,
    double * xf,
    double * yf,
    double * zf,
    double * gxcf,
    double * gycf,
    double * gzcf,
    double * a1cf,
    double * a2cf,
    double * a3cf,
    double * ccf,
    double * fcf,
    double * tcf )
```

Driver for the Newton Solver.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

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```

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

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*
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```


Driver for a screaming inexact-newton-multilevel solver.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces newdriv from newdrvd.f

Parameters

<i>iparm</i>	
<i>rparm</i>	
<i>iwork</i>	
<i>rwork</i>	
<i>u</i>	
<i>xf</i>	
<i>yf</i>	
<i>zf</i>	
<i>gxcf</i>	
<i>gycf</i>	
<i>gzcf</i>	
<i>a1cf</i>	
<i>a2cf</i>	
<i>a3cf</i>	
<i>ccf</i>	
<i>fcf</i>	
<i>tcf</i>	

Definition at line 57 of file [newdrvd.c](#).

7.31.3.41 Vnewdriv2()

```

VEXTERNC void Vnewdriv2 (
    int * iparm,
    double * rparm,
    int * nx,
    int * ny,
    int * nz,
    double * u,
    int * iz,
    double * w1,
    double * w2,
    int * ipc,
    double * rpc,
    double * pc,
    double * ac,
    double * cc,
    double * fc,
    double * xf,

```

```

double * yf,
double * zf,
double * gxcf,
double * gycf,
double * gzcf,
double * a1cf,
double * a2cf,
double * a3cf,
double * ccf,
double * fcf,
double * tcf )

```

Solves using Newton's Method.

Author

Tucker Beck [C Translation], Michael Holst [Original]

This routine uses a newton's method, combined with a linear multigrid iteration, to solve the following three-dimensional, 2nd order elliptic partial differential equation:

```

lu = f, u in omega
u = g, u on boundary of omega

```

where

```
omega = [xmin,xmax]x[ymin,ymax]x[zmin,zmax]
```

the multigrid code requires the operator in the form:

```
- \nabla \cdot (a \nabla u) + c(u) = f
```

with

$a(x,y,z)$, $f(x,y,z)$, scalar functions (possibly discontinuous) on ω . (discontinuities must be along fine grid lines).
boundary function $g(x,y,z)$ is smooth on boundary of ω .

the function $c(u)$ is a possibly nonlinear function of the unknown u , and varies (possibly discontinuously) with the spatial position also.

User inputs:

the user must provide the coefficients of the differential operator, some initial parameter settings in an integer and a real parameter array, and various work arrays.

Note

Replaces newdriv2 from newdrvd.f

Parameters

<i>iparm</i>	
<i>rparm</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>u</i>	
<i>iz</i>	
<i>w1</i>	

Parameters

<i>w2</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>pc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>xf</i>	
<i>yf</i>	
<i>zf</i>	
<i>gxcf</i>	
<i>gycf</i>	
<i>gzcf</i>	
<i>a1cf</i>	
<i>a2cf</i>	
<i>a3cf</i>	
<i>ccf</i>	
<i>fcf</i>	
<i>tcf</i>	

Definition at line 169 of file [newdrvd.c](#).

7.31.3.42 Vnewton()

```

VEXTERNC void Vnewton (
    int * nx,
    int * ny,
    int * nz,
    double * x,
    int * iz,
    double * w0,
    double * w1,
    double * w2,
    double * w3,
    int * istop,
    int * itmax,
    int * iters,
    int * ierror,
    int * nlev,
    int * ilev,
    int * nlev_real,
    int * mgsolv,
    int * iok,
    int * iinfo,
    double * epsiln,
    double * ertol,
    double * omega,
    int * nu1,
    int * nu2,

```

```

    int * mgsmoo,
    double * cprime,
    double * rhs,
    double * xtmp,
    int * ipc,
    double * rpc,
    double * pc,
    double * ac,
    double * cc,
    double * fc,
    double * tru )

```

Inexact-newton-multilevel method.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces newton from newtond.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>x</i>	
<i>iz</i>	
<i>w0</i>	
<i>w1</i>	
<i>w2</i>	
<i>w3</i>	
<i>istop</i>	
<i>itmax</i>	
<i>iters</i>	
<i>ierror</i>	
<i>nlev</i>	
<i>ilev</i>	
<i>nlev_real</i>	
<i>mgsovl</i>	
<i>iok</i>	
<i>iinfo</i>	
<i>epsiln</i>	
<i>errtol</i>	
<i>omega</i>	
<i>nu1</i>	
<i>nu2</i>	
<i>mgsmoo</i>	
<i>cprime</i>	
<i>rhs</i>	
<i>xtmp</i>	
<i>ipc</i>	

Parameters

<i>rpc</i>	
<i>pc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>tru</i>	

Definition at line 162 of file [newtond.c](#).

7.31.3.43 Vnmatvec()

```

VEXTERNC void Vnmatvec (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,
    double * x,
    double * y,
    double * w1 )

```

Break the matrix data-structure into diagonals and then call the matrix-vector routine.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces nmatvec from matvecd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>x</i>	
<i>y</i>	
<i>w1</i>	

Definition at line 232 of file [matvecd.c](#).

7.31.3.44 Vnmresid()

```

VEXTERNC void Vnmresid (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,
    double * fc,
    double * x,
    double * r,
    double * w1 )

```

Break the matrix data-structure into diagonals and then call the residual routine.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces nmresid from matvecd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>x</i>	
<i>r</i>	
<i>w1</i>	

Definition at line [598](#) of file [matvecd.c](#).

7.31.3.45 Vnsmooth()

```

VEXTERNC void Vnsmooth (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,
    double * fc,
    double * x,
    double * w1,

```

```

double * w2,
double * r,
int * itmax,
int * iters,
double * errtol,
double * omega,
int * iresid,
int * iadjoint,
int * meth )

```

call the appropriate non-linear smoothing routine.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces nsmooth from nsmoothd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>x</i>	
<i>w1</i>	
<i>w2</i>	
<i>r</i>	
<i>itmax</i>	
<i>iters</i>	
<i>errtol</i>	
<i>omega</i>	
<i>iresid</i>	
<i>iadjoint</i>	
<i>meth</i>	

Definition at line 98 of file [smoothd.c](#).

7.31.3.46 Vpower()

```

VEXTERNC void Vpower (
    int * nx,
    int * ny,
    int * nz,
    int * iz,
    int * ilev,
    int * ipc,

```

```

double * rpc,
double * ac,
double * cc,
double * w1,
double * w2,
double * w3,
double * w4,
double * eigmax,
double * eigmax_model,
double * tol,
int * itmax,
int * iters,
int * iinfo )

```

Power methods for eigenvalue estimation.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

```

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*
```

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Attention

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* Nathan A. Baker (nathan.baker@pnl.gov)
* Pacific Northwest National Laboratory
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*
*
```

Standard power method for maximum eigenvalue estimation of a matrix $c * c *$

Note

To test, note that the 3d laplacean has min/max eigenvalues: $c * c * \lambda_{\min} = 6 - 2 * \text{dcos}(\pi / (n_x - 1))$ $c * c * \lambda_{\max} = 6 - 2 * \text{dcos}(\pi / (n_y - 1))$ $c * c * \lambda_{\min} = 6 - 2 * \text{dcos}(\pi / (n_z - 1))$ $c * c * \lambda_{\max} = 6 - 2 * \text{dcos}((n_x - 2) * \pi / (n_x - 1))$ $c * c * \lambda_{\min} = 6 - 2 * \text{dcos}((n_y - 2) * \pi / (n_y - 1))$ $c * c * \lambda_{\max} = 6 - 2 * \text{dcos}((n_z - 2) * \pi / (n_z - 1))$

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces power from powerd.f

Vpower is yet untested as a call stack including it hasn't been found

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>iz</i>	
<i>ilev</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>w1</i>	
<i>w2</i>	
<i>w3</i>	
<i>w4</i>	
<i>eigmax</i>	
<i>eigmax_model</i>	
<i>tol</i>	
<i>itmax</i>	
<i>iters</i>	
<i>iinfo</i>	

Definition at line 57 of file [powerd.c](#).

7.31.3.47 Vprtmatd()

```

VEXTERNC void Vprtmatd (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * ac )

```

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces prtmatd from mikpckd.f

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the y dimension of the 3d matrix
<i>nz</i>	The size of the z dimension of the 3d matrix
<i>ipc</i>	Integer parameters
<i>rpc</i>	Double parameters
<i>ac</i>	

Definition at line [332](#) of file [mikpckd.c](#).

7.31.3.48 Vrestrc()

```
VEXTERNC void Vrestrc (
    int * nxf,
    int * nyf,
    int * nzf,
    int * nxc,
    int * nyc,
    int * nzc,
    double * xin,
    double * xout,
    double * pc )
```

Apply the restriction operator.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces restrc from matvecd.f

Parameters

<i>nxf</i>	
<i>nyf</i>	
<i>nzf</i>	
<i>nxc</i>	
<i>nyc</i>	
<i>nzc</i>	
<i>xin</i>	
<i>xout</i>	
<i>pc</i>	

Definition at line [782](#) of file [matvecd.c](#).

7.31.3.49 Vsmooth()

```
VEXTERNC void Vsmooth (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,
    double * fc,
    double * x,
    double * w1,
    double * w2,
```

```

double * r,
int * itmax,
int * iters,
double * errtol,
double * omega,
int * iresid,
int * iadjoint,
int * meth )

```

Multigrid smoothing functions.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

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Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

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*
*
```

call the appropriate linear smoothing routine.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces smooth from smoothd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	

Parameters

<i>cc</i>	
<i>fc</i>	
<i>x</i>	
<i>w1</i>	
<i>w2</i>	
<i>r</i>	
<i>itmax</i>	
<i>iters</i>	
<i>errtol</i>	
<i>omega</i>	
<i>iresid</i>	
<i>iadjoint</i>	
<i>meth</i>	

Definition at line 58 of file [smoothd.c](#).

7.31.3.50 Vxaxpy()

```
VEXTERNC void Vxaxpy (
    int * nx,
    int * ny,
    int * nz,
    double * alpha,
    double * x,
    double * y )
```

saxpy operation for a grid function with boundary values.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces xaxpy from mikpckd.f

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the y dimension of the 3d matrix
<i>nz</i>	The size of the z dimension of the 3d matrix
<i>alpha</i>	
<i>x</i>	The source matrix from which to copy data
<i>y</i>	The destination matrix to receive copied data

Definition at line 112 of file [mikpckd.c](#).

7.31.3.51 Vxcopy()

```
VEXTERNC void Vxcopy (
    int * nx,
    int * ny,
    int * nz,
    double * x,
    double * y )
```

A collection of useful low-level routines (timing, etc).

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

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Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

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```

Copy operation for a grid function with boundary values. Quite simply copies one 3d matrix to another

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces xcopy from mikpckd.f

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the y dimension of the 3d matrix
<i>nz</i>	The size of the z dimension of the 3d matrix
<i>Generated by Doxygen</i>	The source matrix from which to copy data
<i>y</i>	The destination matrix to receive copied data

Definition at line 57 of file [mikpckd.c](#).

7.31.3.52 Vxcopy_large()

```
VEXTERNC void Vxcopy_large (
    int * nx,
    int * ny,
    int * nz,
    double * x,
    double * y )
```

Copy operation for a grid function with boundary values. Quite simply copies one 3d matrix to another.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces xcopy_large from mikpckd.f

Note

This function is exactly equivalent to calling xcopy_small with the matrix arguments reversed.

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the y dimension of the 3d matrix
<i>nz</i>	The size of the z dimension of the 3d matrix
<i>x</i>	The source matrix from which to copy data
<i>y</i>	The destination matrix to receive copied data

Definition at line 91 of file [mikpckd.c](#).

7.31.3.53 Vxcopy_small()

```
VEXTERNC void Vxcopy_small (
    int * nx,
    int * ny,
    int * nz,
    double * x,
    double * y )
```

Copy operation for a grid function with boundary values. Quite simply copies one 3d matrix to another.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces xcopy_small from mikpckd.f

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the y dimension of the 3d matrix
<i>nz</i>	The size of the z dimension of the 3d matrix
<i>x</i>	The source matrix from which to copy data
<i>y</i>	The destination matrix to receive copied data

Definition at line 75 of file [mikpckd.c](#).

7.31.3.54 Vxdot()

```
VEXTERNC double Vxdot (  
    int * nx,  
    int * ny,  
    int * nz,  
    double * x,  
    double * y )
```

Inner product operation for a grid function with boundary values.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces xdot from mikpckd.f

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the y dimension of the 3d matrix
<i>nz</i>	The size of the z dimension of the 3d matrix
<i>x</i>	The first vector
<i>y</i>	The second vector

Definition at line 173 of file [mikpckd.c](#).

7.31.3.55 Vxnrml()

```
VEXTERNC double Vxnrml (  
    int * nx,  
    int * ny,  
    int * nz,  
    double * x )
```

Norm operation for a grid function with boundary values.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces xnm1 from mikpckd.f

< Accumulates the calculated normal value

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the y dimension of the 3d matrix
<i>nz</i>	The size of the z dimension of the 3d matrix
<i>x</i>	The matrix to normalize

Definition at line 131 of file [mikpckd.c](#).

7.31.3.56 Vxnm2()

```
VEXTERNC double Vxnm2 (
    int * nx,
    int * ny,
    int * nz,
    double * x )
```

Norm operation for a grid function with boundary values.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces xnm2 from mikpckd.f

< Accumulates the calculated normal value

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the y dimension of the 3d matrix
<i>nz</i>	The size of the z dimension of the 3d matrix
<i>x</i>	The matrix to normalize

Definition at line 152 of file [mikpckd.c](#).

7.31.3.57 Vxscal()

```
VEXTERNC void Vxscal (
    int * nx,
    int * ny,
    int * nz,
    double * fac,
    double * x )
```

Scale operation for a grid function with boundary values.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces xscal from mikpckd.f

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the y dimension of the 3d matrix
<i>nz</i>	The size of the z dimension of the 3d matrix
<i>fac</i>	The scaling factor
<i>x</i>	The 3d matrix to scale

Definition at line 318 of file [mikpckd.c](#).

7.32 High-level front-end routines

Files

- file [apbs.h](#)
Header file for header dependencies.
- file [main.c](#)
APBS "front end" program using formatted input files.
- file [routines.h](#)
Header file for front end auxiliary routines.

Data Structures

- struct [AtomForce](#)
Structure to hold atomic forces.

Macros

- #define [APBSRC](#) 13
Return code for APBS during failure.

Typedefs

- typedef struct [AtomForce](#) [AtomForce](#)
Define [AtomForce](#) type.

Functions

- int [main](#) (int argc, char **argv)
The main APBS function.
- VPUBLIC Vrc_Codes [initFE](#) (int icalc, [NOSH](#) *nosh, [FEMparm](#) *feparm, [PBEparm](#) *pbeparm, [Vpbe](#) *pbe[[NOSH_MAXCALC](#)], [Valist](#) *alist[[NOSH_MAXMOL](#)], [Vfetk](#) *fetk[[NOSH_MAXCALC](#)])
Initialize FE solver objects.

- VEXTERNC `Vparam * loadParameter (NOsh *nosh)`
Loads and returns parameter object.
- VEXTERNC `int loadMolecules (NOsh *nosh, Vparam *param, Valist *alist[NOSH_MAXMOL])`
Load the molecules given in NOsh into atom lists.
- VEXTERNC `void killMolecules (NOsh *nosh, Valist *alist[NOSH_MAXMOL])`
Destroy the loaded molecules.
- VEXTERNC `int loadDielMaps (NOsh *nosh, Vgrid *dielXMap[NOSH_MAXMOL], Vgrid *dielYMap[NOSH_MAXMOL], Vgrid *dielZMap[NOSH_MAXMOL])`
Load the dielectric maps given in NOsh into grid objects.
- VEXTERNC `void killDielMaps (NOsh *nosh, Vgrid *dielXMap[NOSH_MAXMOL], Vgrid *dielYMap[NOSH_MAXMOL], Vgrid *dielZMap[NOSH_MAXMOL])`
Destroy the loaded dielectric.
- VEXTERNC `int loadKappaMaps (NOsh *nosh, Vgrid *kappa[NOSH_MAXMOL])`
Load the kappa maps given in NOsh into grid objects.
- VEXTERNC `void killKappaMaps (NOsh *nosh, Vgrid *kappa[NOSH_MAXMOL])`
Destroy the loaded kappa maps.
- VEXTERNC `int loadPotMaps (NOsh *nosh, Vgrid *pot[NOSH_MAXMOL])`
Load the potential maps given in NOsh into grid objects.
- VEXTERNC `void killPotMaps (NOsh *nosh, Vgrid *pot[NOSH_MAXMOL])`
Destroy the loaded potential maps.
- VEXTERNC `int loadChargeMaps (NOsh *nosh, Vgrid *charge[NOSH_MAXMOL])`
Load the charge maps given in NOsh into grid objects.
- VEXTERNC `void killChargeMaps (NOsh *nosh, Vgrid *charge[NOSH_MAXMOL])`
Destroy the loaded charge maps.
- VEXTERNC `void printPBEPARM (PBEparm *pbeparm)`
Print out generic PBE params loaded from input.
- VEXTERNC `void printMGPARAM (MGparm *mgparm, double realCenter[3])`
Print out MG-specific params loaded from input.
- VEXTERNC `int initMG (int icalc, NOsh *nosh, MGparm *mgparm, PBEparm *pbeparm, double realCenter[3], Vpbe *pbe[NOSH_MAXCALC], Valist *alist[NOSH_MAXMOL], Vgrid *dielXMap[NOSH_MAXMOL], Vgrid *dielYMap[NOSH_MAXMOL], Vgrid *dielZMap[NOSH_MAXMOL], Vgrid *kappaMap[NOSH_MAXMOL], Vgrid *chargeMap[NOSH_MAXMOL], Vpmgp *pmgp[NOSH_MAXCALC], Vpmg *pmg[NOSH_MAXCALC], Vgrid *potMap[NOSH_MAXMOL])`
Initialize an MG calculation.
- VEXTERNC `void killMG (NOsh *nosh, Vpbe *pbe[NOSH_MAXCALC], Vpmgp *pmgp[NOSH_MAXCALC], Vpmg *pmg[NOSH_MAXCALC])`
Kill structures initialized during an MG calculation.
- VEXTERNC `int solveMG (NOsh *nosh, Vpmg *pmg, MGparm_CalcType type)`
Solve the PBE with MG.
- VEXTERNC `int setPartMG (NOsh *nosh, MGparm *mgparm, Vpmg *pmg)`
Set MG partitions for calculating observables and performing I/O.
- VEXTERNC `int energyMG (NOsh *nosh, int icalc, Vpmg *pmg, int *nenergy, double *totEnergy, double *qf↔Energy, double *qmEnergy, double *dielEnergy)`
Calculate electrostatic energies from MG solution.
- VEXTERNC `void killEnergy ()`
Kill arrays allocated for energies.
- VEXTERNC `int forceMG (Vmem *mem, NOsh *nosh, PBEparm *pbeparm, MGparm *mgparm, Vpmg *pmg, int *nforce, AtomForce **atomForce, Valist *alist[NOSH_MAXMOL])`

Calculate forces from MG solution.

- VEXTERNC void `killForce` (Vmem *mem, NOSH *nosh, int nforce[NOSH_MAXCALC], AtomForce *atom← Force[NOSH_MAXCALC])

Free memory from MG force calculation.

- VEXTERNC void `storeAtomEnergy` (Vpmg *pmg, int icalc, double **atomEnergy, int *nenergy)

Store energy in arrays for future use.

- VEXTERNC int `writedataFlat` (NOSH *nosh, Vcom *com, const char *fname, double totEnergy[NOSH_MAXCALC], double qfEnergy[NOSH_MAXCALC], double qmEnergy[NOSH_MAXCALC], double dielEnergy[NOSH_MAXCALC], int nenergy[NOSH_MAXCALC], double *atomEnergy[NOSH_MAXCALC], int nforce[NOSH_MAXCALC], AtomForce *atomForce[NOSH_MAXCALC])

Write out information to a flat file.

- VEXTERNC int `writedataXML` (NOSH *nosh, Vcom *com, const char *fname, double totEnergy[NOSH_MAXCALC], double qfEnergy[NOSH_MAXCALC], double qmEnergy[NOSH_MAXCALC], double dielEnergy[NOSH_MAXCALC], int nenergy[NOSH_MAXCALC], double *atomEnergy[NOSH_MAXCALC], int nforce[NOSH_MAXCALC], AtomForce *atomForce[NOSH_MAXCALC])

Write out information to an XML file.

- VEXTERNC int `writedataMG` (int rank, NOSH *nosh, PBEparm *pbeparm, Vpmg *pmg)

Write out observables from MG calculation to file.

- VEXTERNC int `writematMG` (int rank, NOSH *nosh, PBEparm *pbeparm, Vpmg *pmg)

Write out operator matrix from MG calculation to file.

- VEXTERNC double `returnEnergy` (Vcom *com, NOSH *nosh, double totEnergy[NOSH_MAXCALC], int iprint)

Access net local energy.

- VEXTERNC int `printEnergy` (Vcom *com, NOSH *nosh, double totEnergy[NOSH_MAXCALC], int iprint)

Combine and pretty-print energy data (deprecated...see printElecEnergy)

- VEXTERNC int `printElecEnergy` (Vcom *com, NOSH *nosh, double totEnergy[NOSH_MAXCALC], int iprint)

Combine and pretty-print energy data.

- VEXTERNC int `printApolEnergy` (NOSH *nosh, int iprint)

Combine and pretty-print energy data.

- VEXTERNC int `printForce` (Vcom *com, NOSH *nosh, int nforce[NOSH_MAXCALC], AtomForce *atom← Force[NOSH_MAXCALC], int i)

Combine and pretty-print force data (deprecated...see printElecForce)

- VEXTERNC int `printElecForce` (Vcom *com, NOSH *nosh, int nforce[NOSH_MAXCALC], AtomForce *atom← Force[NOSH_MAXCALC], int i)

Combine and pretty-print force data.

- VEXTERNC int `printApolForce` (Vcom *com, NOSH *nosh, int nforce[NOSH_MAXCALC], AtomForce *atom← Force[NOSH_MAXCALC], int i)

Combine and pretty-print force data.

- VEXTERNC void `startVio` ()

Wrapper to start MALOC Vio layer.

- VEXTERNC int `energyAPOL` (APOLparm *apolparm, double sasa, double sav, double atomsasa[], double atomwcaEnergy[], int numatoms)

Calculate non-polar energies.

- VEXTERNC int `forceAPOL` (Vacc *acc, Vmem *mem, APOLparm *apolparm, int *nforce, AtomForce **atom← Force, Valist *alist, Vclist *clist)

Calculate non-polar forces.

- VEXTERNC int `initAPOL` (NOSH *nosh, Vmem *mem, Vparam *param, APOLparm *apolparm, int *nforce, AtomForce **atomForce, Valist *alist)

Upperlevel routine to the non-polar energy and force routines.

- VEXTERNC void `printFEPARM` (int icalc, NOSH *nosh, FEParm *feparm, Vfetc *fetc[NOSH_MAXCALC])

Print out FE-specific params loaded from input.

- VEXTERNC int [energyFE](#) (NOsh *nosh, int icalc, Vfetk *fetc[NOSH_MAXCALC], int *nenergy, double *totEnergy, double *qfEnergy, double *qmEnergy, double *dielEnergy)

Calculate electrostatic energies from FE solution.

- VEXTERNC void [killFE](#) (NOsh *nosh, Vpbe *pbe[NOSH_MAXCALC], Vfetk *fetc[NOSH_MAXCALC], Gem *gem[NOSH_MAXMOL])

Kill structures initialized during an FE calculation.

- VEXTERNC int [preRefineFE](#) (int i, FEMparm *feparm, Vfetk *fetc[NOSH_MAXCALC])

Pre-refine mesh before solve.

- VEXTERNC int [partFE](#) (int i, NOsh *nosh, FEMparm *feparm, Vfetk *fetc[NOSH_MAXCALC])

Partition mesh (if applicable)

- VEXTERNC int [solveFE](#) (int i, PBEparm *pbeparm, FEMparm *feparm, Vfetk *fetc[NOSH_MAXCALC])

Solve-estimate-refine.

- VEXTERNC int [postRefineFE](#) (int icalc, FEMparm *feparm, Vfetk *fetc[NOSH_MAXCALC])

Estimate error, mark mesh, and refine mesh after solve.

- VEXTERNC int [writedataFE](#) (int rank, NOsh *nosh, PBEparm *pbeparm, Vfetk *fetc)

Write FEM data to files.

- VEXTERNC Vrc_Codes [loadMeshes](#) (NOsh *nosh, Gem *gm[NOSH_MAXMOL])

Load the meshes given in NOsh into geometry objects.

- VEXTERNC void [killMeshes](#) (NOsh *nosh, Gem *alist[NOSH_MAXMOL])

Destroy the loaded meshes.

7.32.1 Detailed Description

7.32.2 Macro Definition Documentation

7.32.2.1 APBSRC

```
#define APBSRC 13
```

Return code for APBS during failure.

Definition at line 93 of file [routines.h](#).

7.32.3 Typedef Documentation

7.32.3.1 AtomForce

```
typedef struct AtomForce AtomForce
```

Define [AtomForce](#) type.

Definition at line 111 of file [routines.h](#).

7.32.4 Function Documentation

7.32.4.1 energyAPOL()

```
VEXTERNC int energyAPOL (
    APOLparm * apolparm,
    double sasa,
    double sav,
    double atomsasa[],
    double atomwcaEnergy[],
    int numatoms )
```

Calculate non-polar energies.

Author

David Gohara

Returns

1 if successful, 0 otherwise

Parameters

<i>sasa</i>	APOLparm object
<i>sav</i>	Solvent accessible surface area
<i>atomsasa</i>	Solvent accessible volume
<i>atomwcaEnergy</i>	Array for SASA per atom *
<i>numatoms</i>	Array for WCA energy per atom * Number of atoms (or size of the above arrays) *

Definition at line [4674](#) of file [routines.c](#).

7.32.4.2 energyFE()

```
VEXTERNC int energyFE (
    NOSH * nosh,
    int icalc,
    Vfetk * fetk[NOSH_MAXCALC],
    int * nenergy,
    double * totEnergy,
    double * qfEnergy,
    double * qmEnergy,
    double * dielEnergy )
```

Calculate electrostatic energies from FE solution.

Author

Nathan Baker

Parameters

<i>nosh</i>	Object with parsed input file parameters
<i>icalc</i>	Index of calculation
<i>fetk</i>	FE object array
<i>nenergy</i>	Set to number of entries in energy arrays
<i>totEnergy</i>	Set to total energy (in kT)

Parameters

<i>qfEnergy</i>	Set to charge-potential energy (in kT)
<i>qmEnergy</i>	Set to mobile ion energy (in kT)
<i>dielEnergy</i>	Set to polarization energy (in kT)

Bug "calcenergy 2" does not work

Returns

1 if successful, 0 otherwise

Calculates the electrostatic energies from an FE calculation. < FE-specific parameters

< PBE-specific parameters

If we're not ignoring this particular NOsh object because it has been rendered invalid, call the Vfetc object's energy calculation function. The flag differences specified have to do with setting specific calculation restrictions (see color variable documentation in function code).

Parameters

<i>nosh</i>	Object with parsed input file parameters
<i>icalc</i>	Calculation index
<i>fetc</i>	FE object array
<i>nenergy</i>	Set to number of entries in energy arrays
<i>totEnergy</i>	Set to total energy (in kT)
<i>qfEnergy</i>	Set to charge-potential energy (in kT)
<i>qmEnergy</i>	Set to mobile ion energy (in kT)
<i>dielEnergy</i>	Set to polarization energy (in kT)

Definition at line 4179 of file [routines.c](#).

7.32.4.3 energyMG()

```

VEXTERNC int energyMG (
    NOsh * nosh,
    int icalc,
    Vpmg * pmg,
    int * nenergy,
    double * totEnergy,
    double * qfEnergy,
    double * qmEnergy,
    double * dielEnergy )

```

Calculate electrostatic energies from MG solution.

Author

Nathan Baker

Parameters

<i>nosh</i>	Object with parsed input file parameters
-------------	--

Parameters

<i>icalc</i>	Index of calculation
<i>pmg</i>	MG object
<i>nenergy</i>	Set to number of entries in energy arrays
<i>totEnergy</i>	Set to total energy (in kT)
<i>qfEnergy</i>	Set to charge-potential energy (in kT)
<i>qmEnergy</i>	Set to mobile ion energy (in kT)
<i>dielEnergy</i>	Set to polarization energy (in kT)

Returns

1 if successful, 0 otherwise

Definition at line 1569 of file [routines.c](#).

7.32.4.4 forceAPOL()

```

VEXTERNC int forceAPOL (
    Vacc * acc,
    Vmem * mem,
    APOLparm * apolparm,
    int * nforce,
    AtomForce ** atomForce,
    Valist * alist,
    Vclist * clist )

```

Calculate non-polar forces.

Author

David Gohara

Returns

1 if successful, 0 otherwise

Parameters

<i>acc</i>	Accessibility object
<i>mem</i>	Memory manager
<i>apolparm</i>	Apolar calculation parameter object
<i>nforce</i>	Number of atomic forces to calculate statements for
<i>atomForce</i>	Object for storing atom forces
<i>alist</i>	Atom list
<i>clist</i>	Cell list for accessibility object

Definition at line 4729 of file [routines.c](#).

7.32.4.5 forceMG()

```

VEXTERNC int forceMG (
    Vmem * mem,
    NOsh * nosh,
    PBEparm * pbeparm,
    MGparm * mgparm,
    Vpmg * pmg,
    int * nforce,
    AtomForce ** atomForce,
    Valist * alist[NOSH_MAXMOL] )

```

Calculate forces from MG solution.

Author

Nathan Baker

Parameters

<i>mem</i>	Memory management object
<i>nosh</i>	Parameters from input file
<i>pbeparm</i>	Generic PBE parameters
<i>mgparm</i>	MG-specific parameters
<i>pmg</i>	MG object
<i>nforce</i>	Set to number of forces in arrays
<i>atomForce</i>	List of atom forces
<i>alist</i>	List of atom lists

Returns

1 if successful, 0 otherwise

Definition at line 1636 of file [routines.c](#).

7.32.4.6 initAPOL()

```

VEXTERNC int initAPOL (
    NOsh * nosh,
    Vmem * mem,
    Vparam * param,
    APOLparm * apolparm,
    int * nforce,
    AtomForce ** atomForce,
    Valist * alist )

```

Upperlevel routine to the non-polar energy and force routines.

Author

David Gohara

1 if successful, 0 otherwise

Parameters

<i>nosh</i>	Input parameter object
<i>mem</i>	Memory manager
<i>param</i>	Atom parameters
<i>apolparm</i>	Apolar calculation parameters
<i>nforce</i>	Number of force calculations
<i>atomForce</i>	Atom force storage object
<i>alist</i>	Atom list

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7.32.4.7 initFE()

```
VEXTERNC Vrc_Codes initFE (
    int icalc,
    NOsh * nosh,
    FEMparm * feparm,
    PBEparm * pbeparm,
    Vpbe * pbe[NOSH_MAXCALC],
    Valist * alist[NOSH_MAXMOL],
    Vfetk * fetk[NOSH_MAXCALC] )
```

Initialize FE solver objects.

Author

Nathan Baker

Bug THIS FUNCTION IS HARD-CODED TO SOLVE LRPBE

Author

Nathan Baker

Bug THIS FUNCTION IS HARD-CODED TO SOLVE LRPBE

< Loop counter
< Mesh ID
< Loop counter
< Loop counter
< Molecule ID
<
< I/O socket for reading MCSF mesh data
< Total bytes used by this operation
< High-water memory usage for this operation
< The type of mesh being used (see struct for enum values)
<
<
<
<
<
< Return codes for function calls (see struct for enum value)
< List of atoms being operated on
< Atom/molecule being operated on

Parameters

<i>icalc</i>	Index in pb, fetk to initialize (calculation index)
<i>nosh</i>	Master parmaeter object
<i>feparm</i>	FE-specific parameters
<i>pbeparm</i>	Generic PBE parameters
<i>pbe</i>	Array of PBE objects
<i>alist</i>	Array of atom lists
<i>fetk</i>	Array of finite element objects

Definition at line 3711 of file [routines.c](#).

7.32.4.8 initMG()

```

VEXTERNC int initMG (
    int icalc,
    NOsh * nosh,
    MGparm * mgparm,
    PBEparm * pbeparm,
    double realCenter[3],
    Vpbe * pbe[NOSH_MAXCALC],
    Valist * alist[NOSH_MAXMOL],
    Vgrid * dielXMap[NOSH_MAXMOL],
    Vgrid * dielYMap[NOSH_MAXMOL],
    Vgrid * dielZMap[NOSH_MAXMOL],
    Vgrid * kappaMap[NOSH_MAXMOL],
    Vgrid * chargeMap[NOSH_MAXMOL],
    Vpmgp * pmgp[NOSH_MAXCALC],
    Vpmg * pmg[NOSH_MAXCALC],
    Vgrid * potMap[NOSH_MAXMOL] )

```

Initialize an MG calculation.

Author

Nathan Baker

Returns

1 if succesful, 0 otherwise

Initialize a multigrid calculation.

Parameters

<i>icalc</i>	Index of calculation in pmg/pmpg arrays
<i>nosh</i>	Object with parsed input file parameters
<i>mgparm</i>	Object with MG-specific parameters
<i>pbeparm</i>	Object with generic PBE parameters
<i>realCenter</i>	The actual center of the current mesh
<i>pbe</i>	Array of Vpbe objects (one for each calc)
<i>alist</i>	Array of atom lists
<i>dielXMap</i>	Array of x-shifted dielectric maps
<i>dielYMap</i>	Array of y-shifted dielectric maps
<i>dielZMap</i>	Array of z-shifted dielectric maps
<i>kappaMap</i>	Array of kappa maps
<i>chargeMap</i>	Array of charge maps
<i>pmgp</i>	Array of MG parameter objects (one for each calc)
<i>pmg</i>	Array of MG objects (one for each calc)
<i>potMap</i>	Array of potential maps

Definition at line 1212 of file [routines.c](#).

7.32.4.9 killChargeMaps()

```

VEXTERNC void killChargeMaps (
    NOsh * nosh,
    Vgrid * charge[NOSH_MAXMOL] )

```

Destroy the loaded charge maps.

Author

Nathan Baker

Parameters

<i>nosh</i>	NOsh object with input file information
<i>charge</i>	List of charge maps

Definition at line 984 of file [routines.c](#).

7.32.4.10 killDielMaps()

```

VEXTERNC void killDielMaps (
    NOsh * nosh,
    Vgrid * dielXMap[NOSH_MAXMOL],
    Vgrid * dielYMap[NOSH_MAXMOL],
    Vgrid * dielZMap[NOSH_MAXMOL] )

```

Destroy the loaded dielectric.

Author

Nathan Baker

Parameters

<i>nosh</i>	NOsh object with input file information
<i>dielXMap</i>	List of x-shifted dielectric maps
<i>dielYMap</i>	List of y-shifted dielectric maps
<i>dielZMap</i>	List of z-shifted dielectric maps

Definition at line 639 of file [routines.c](#).

7.32.4.11 killEnergy()

```

VEXTERNC void killEnergy ( )

```

Kill arrays allocated for energies.

Author

Nathan Baker

Definition at line 1774 of file [routines.c](#).

7.32.4.12 killFE()

```

VEXTERNC void killFE (
    NOsh * nosh,
    Vpbe * pbe[NOSH_MAXCALC],
    Vfetk * fetk[NOSH_MAXCALC],
    Gem * gem[NOSH_MAXMOL] )

```

Kill structures initialized during an FE calculation.

Author

Nathan Baker

Parameters

<i>pbe</i>	Object with parsed input file parameters
<i>fetk</i>	Array of Vpbe objects for each calc
<i>gem</i>	Array of FEtk objects for each calc Array of geometry manager objects for each calc

Definition at line [3683](#) of file [routines.c](#).

7.32.4.13 killForce()

```

VEXTERNC void killForce (
    Vmem * mem,
    NOsh * nosh,
    int nforce[NOSH_MAXCALC],
    AtomForce * atomForce[NOSH_MAXCALC] )

```

Free memory from MG force calculation.

Author

Nathan Baker

Parameters

<i>mem</i>	Memory management object
<i>nosh</i>	Parameters from input file
<i>nforce</i>	Number of forces in arrays
<i>atomForce</i>	List of atom forces

Definition at line [1782](#) of file [routines.c](#).

7.32.4.14 killKappaMaps()

```

VEXTERNC void killKappaMaps (
    NOsh * nosh,
    Vgrid * kappa[NOSH_MAXMOL] )

```

Destroy the loaded kappa maps.

Author

Nathan Baker

Parameters

<i>nosh</i>	NOsh object with input file information
<i>kappa</i>	List of kappa maps

Definition at line 776 of file [routines.c](#).**7.32.4.15 killMeshes()**

```

VEXTERNC void killMeshes (
    NOsh * nosh,
    Gem * alist[NOSH_MAXMOL] )

```

Destroy the loaded meshes.

Author

Nathan Baker

Parameters

<i>nosh</i>	NOsh object with input file information
<i>alist</i>	Populated list of geometry objects to be destroyed

7.32.4.16 killMG()

```

VEXTERNC void killMG (
    NOsh * nosh,
    Vpbe * pbe[NOSH_MAXCALC],
    Vpmgp * pmgp[NOSH_MAXCALC],
    Vpmg * pmg[NOSH_MAXCALC] )

```

Kill structures initialized during an MG calculation.

Author

Nathan Baker

Parameters

<i>pbe</i>	Object with parsed input file parameters
<i>pmgp</i>	Array of Vpbe objects for each calc
<i>pmg</i>	Array of MG parameter objects for each calc Array of MG objects for each calc

Definition at line 1461 of file [routines.c](#).

7.32.4.17 killMolecules()

```
VEXTERNC void killMolecules (
    NOsh * nosh,
    Valist * alist[NOSH_MAXMOL] )
```

Destroy the loaded molecules.

Author

Nathan Baker

Parameters

<i>nosh</i>	NOsh object with input file information
<i>alist</i>	List of atom list objects

Definition at line 233 of file [routines.c](#).

7.32.4.18 killPotMaps()

```
VEXTERNC void killPotMaps (
    NOsh * nosh,
    Vgrid * pot[NOSH_MAXMOL] )
```

Destroy the loaded potential maps.

Author

David Gohara

Parameters

<i>nosh</i>	NOsh object with input file information
<i>pot</i>	List of potential maps

Definition at line 865 of file [routines.c](#).

7.32.4.19 loadChargeMaps()

```
VEXTERNC int loadChargeMaps (
    NOsh * nosh,
    Vgrid * map[NOSH_MAXMOL] )
```

Load the charge maps given in NOsh into grid objects.

Author

Nathan Baker

Parameters

<i>nosh</i>	NOsh object with input file information
<i>charge</i>	List of kappa maps

Returns

1 if successful, 0 otherwise
 0 on failure, 1 on success

Definition at line 884 of file [routines.c](#).

7.32.4.20 loadDielMaps()

```

VEXTERNC int loadDielMaps (
    NOsh * nosh,
    Vgrid * dielXMap[NOSH_MAXMOL],
    Vgrid * dielYMap[NOSH_MAXMOL],
    Vgrid * dielZMap[NOSH_MAXMOL] )

```

Load the dielectric maps given in NOsh into grid objects.

Author

Nathan Baker

Parameters

<i>nosh</i>	NOsh object with input file information
<i>dielXMap</i>	List of x-shifted dielectric maps
<i>dielYMap</i>	List of y-shifted dielectric maps
<i>dielZMap</i>	List of x-shifted dielectric maps

Returns

1 if successful, 0 otherwise

Loads dielectric map path data into NOsh object

Returns

1 on success, 0 on error

Definition at line 250 of file [routines.c](#).

7.32.4.21 loadKappaMaps()

```

VEXTERNC int loadKappaMaps (
    NOsh * nosh,
    Vgrid * map[NOSH_MAXMOL] )

```

Load the kappa maps given in NOsh into grid objects.

Author

Nathan Baker

Parameters

<i>nosh</i>	NOsh object with input file information
<i>kappa</i>	List of kappa maps

Returns

1 if successful, 0 otherwise
0 on failure, 1 on success

Definition at line 664 of file [routines.c](#).

7.32.4.22 loadMeshes()

```
VEXTERNC Vrc_Codes loadMeshes (
    NOsh * nosh,
    Gem * gm[NOSH_MAXMOL] )
```

Load the meshes given in NOsh into geometry objects.

Author

Nathan Baker

Returns

Error code on success/failure

Parameters

<i>nosh</i>	NOsh object with input file information
<i>gm</i>	List of geometry objects (to be populated)

7.32.4.23 loadMolecules()

```
VEXTERNC int loadMolecules (
    NOsh * nosh,
    Vparam * param,
    Valist * alist[NOSH_MAXMOL] )
```

Load the molecules given in NOsh into atom lists.

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Parameters

<i>nosh</i>	NOsh object with input file information
<i>param</i>	NULL (if PQR files only) or pointer to parameter object
<i>alist</i>	List of atom list objects (to be populated)

Definition at line 95 of file [routines.c](#).

7.32.4.24 loadParameter()

```
VEXTERNC Vparam * loadParameter (
    NOsh * nosh )
```

Loads and returns parameter object.

Author

Nathan Baker

Returns

Pointer to parameter object or NULL

Parameters

<i>nosh</i>	Pointer to NOsh object with input file information
-------------	--

Definition at line 60 of file [routines.c](#).

7.32.4.25 loadPotMaps()

```
VEXTERNC int loadPotMaps (
    NOsh * nosh,
    Vgrid * map[NOSH_MAXMOL] )
```

Load the potential maps given in NOsh into grid objects.

Author

David Gohara

Parameters

<i>nosh</i>	NOsh object with input file information
<i>pot</i>	List of potential maps

Returns

1 if successful, 0 otherwise

0 on failure, 1 on success

Definition at line 793 of file [routines.c](#).

7.32.4.26 main()

```
int main (
    int argc,
    char ** argv )
```

The main APBS function.

Author

Nathan Baker, Dave Gohara, Todd Dolinsky

Returns

Status code (0 for success)

Parameters

<i>argc</i>	Number of arguments
<i>argv</i>	Argument strings

Definition at line 80 of file [main.c](#).

7.32.4.27 partFE()

```
VEXTERNC int partFE (
    int i,
    NOsh * nosh,
    FEMparm * feparm,
    Vfetk * fetk[NOSH_MAXCALC] )
```

Partition mesh (if applicable)

Author

Nathan Baker

Parameters

<i>i</i>	Calculation index
<i>nosh</i>	Master parameter object
<i>feparm</i>	FE-specific parameters
<i>fetk</i>	Array of FE solver objects

Returns

1 if successful, 0 otherwise

Definition at line 4039 of file [routines.c](#).

7.32.4.28 postRefineFE()

```
VEXTERNC int postRefineFE (
    int icalc,
    FEMparm * feparm,
    Vfetk * fetk[NOSH_MAXCALC] )
```

Estimate error, mark mesh, and refine mesh after solve.

Author

Nathan Baker

Parameters

<i>icalc</i>	Calculation index
<i>feparm</i>	FE-specific parameters
<i>fetk</i>	Array of FE solver objects

Returns

1 if successful, 0 otherwise – note that a 0 will likely imply that either the max number of vertices have been met or no vertices were marked for refinement. In either case, this should not be treated as a fatal error.

Estimates the error, marks the mesh, and refines the mesh after solving.

Returns

1 if successful, 0 otherwise – note that a 0 will likely imply that either the max number of vertices have been met or no vertices were marked for refinement. In either case, this should not be treated as a fatal error.

< Number of vertices in the molecular geometry

< Whether vertices are marked for refinement

Parameters

<i>icalc</i>	Calculation index
<i>feparm</i>	FE-specific parameters
<i>fetk</i>	Array of FE solver objects

Definition at line 4239 of file [routines.c](#).

7.32.4.29 preRefineFE()

```

VEXTERNC int preRefineFE (
    int i,
    FEMparm * feparm,
    Vfetk * fetk[NOSH_MAXCALC] )

```

Pre-refine mesh before solve.

Author

Nathan Baker

Parameters

<i>i</i>	Calculation index
<i>nosh</i>	Master parameter object
<i>feparm</i>	FE-specific parameters
<i>fetk</i>	Array of FE solver objects

Returns

1 if successful, 0 otherwise

< Number of vertices in the mesh geometry

< Essentially a boolean; indicates whether further refinement is required after running MC's refinement algorithm.

TODO: could this be optimized by moving nverts out of the loop to just above this initial printout? This depends heavily on whether the number of vertices can change during the calculation. - PCE

Definition at line 4046 of file [routines.c](#).

7.32.4.30 printApolEnergy()

```

VEXTERNC int printApolEnergy (
    NOsh * nosh,
    int iprint )

```

Combine and pretty-print energy data.

Author

David Gohara

Returns

1 if successful, 0 otherwise

Parameters

<i>nosh</i>	Parameters from input file
<i>iprint</i>	Index of energy statement to print

Definition at line 2918 of file [routines.c](#).

7.32.4.31 printApolForce()

```

VEXTERNC int printApolForce (
    Vcom * com,
    NOsh * nosh,
    int nforce[NOSH_MAXCALC],
    AtomForce * atomForce[NOSH_MAXCALC],
    int i )

```

Combine and pretty-print force data.

Author

David Gohara

Returns

1 if successful, 0 otherwise

Parameters

<i>nosh</i>	Communications object
<i>nforce</i>	Parameters from input file
<i>atomForce</i>	Number of forces calculated
<i>i</i>	Array of force structures Index of force statement to print

Definition at line 3471 of file [routines.c](#).

7.32.4.32 printElecEnergy()

```

VEXTERNC int printElecEnergy (

```

```

Vcom * com,
NOSH * nosh,
double totEnergy[NOSH_MAXCALC],
int iprint )

```

Combine and pretty-print energy data.

Author

David Gohara

Returns

1 if successful, 0 otherwise

Parameters

<i>nosh</i>	Communications object
<i>totEnergy</i>	Parameters from input file
<i>iprint</i>	Array of energies from different calculations Index of energy statement to print

Definition at line [2853](#) of file [routines.c](#).

7.32.4.33 printElecForce()

```

VEXTERNC int printElecForce (
    Vcom * com,
    NOSH * nosh,
    int nforce[NOSH_MAXCALC],
    AtomForce * atomForce[NOSH_MAXCALC],
    int i )

```

Combine and pretty-print force data.

Author

David Gohara

Returns

1 if successful, 0 otherwise

Parameters

<i>nosh</i>	Communications object
<i>nforce</i>	Parameters from input file
<i>atomForce</i>	Number of forces calculated
<i>i</i>	Array of force structures Index of force statement to print

Definition at line [3228](#) of file [routines.c](#).

7.32.4.34 printEnergy()

```

VEXTERNC int printEnergy (

```

```

Vcom * com,
NOsh * nosh,
double totEnergy[NOSH_MAXCALC],
int iprint )

```

Combine and pretty-print energy data (deprecated...see printElecEnergy)

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Parameters

<i>nosh</i>	Communications object
<i>totEnergy</i>	Parameters from input file
<i>iprint</i>	Array of energies from different calculations Index of energy statement to print

Definition at line 2785 of file [routines.c](#).

7.32.4.35 printFEPARM()

```

VEXTERNC void printFEPARM (
    int icalc,
    NOsh * nosh,
    FEMparm * feparm,
    Vfetk * fetk[NOSH_MAXCALC] )

```

Print out FE-specific params loaded from input.

Author

Nathan Baker

Parameters

<i>icalc</i>	Calculation index
<i>nosh</i>	Master parameter object
<i>feparm</i>	FE-specific parameters
<i>fetk</i>	Array of FE solver objects

Definition at line 3903 of file [routines.c](#).

7.32.4.36 printForce()

```

VEXTERNC int printForce (
    Vcom * com,
    NOsh * nosh,
    int nforce[NOSH_MAXCALC],

```

```

    AtomForce * atomForce[NOSH_MAXCALC],
    int i )

```

Combine and pretty-print force data (deprecated...see printElecForce)

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Parameters

<i>nosh</i>	Communications object
<i>nforce</i>	Parameters from input file
<i>atomForce</i>	Number of forces calculated
<i>i</i>	Array of force structures Index of force statement to print

Definition at line 2980 of file [routines.c](#).

7.32.4.37 printMGPARAM()

```

VEXTERNC void printMGPARAM (
    MGparm * mgparm,
    double realCenter[3] )

```

Print out MG-specific params loaded from input.

Author

Nathan Baker

Parameters

<i>realCenter</i>	Center of mesh for actual calculation
<i>mgparm</i>	MGparm object

Definition at line 1179 of file [routines.c](#).

7.32.4.38 printPBEPARM()

```

VEXTERNC void printPBEPARM (
    PBEParm * pbeparm )

```

Print out generic PBE params loaded from input.

Author

Nathan Baker

Parameters

<i>pbeparm</i>	PBEParm object
----------------	----------------

Definition at line 1002 of file [routines.c](#).

7.32.4.39 returnEnergy()

```
VEXTERNC double returnEnergy (
    Vcom * com,
    NOsh * nosh,
    double totEnergy[NOSH_MAXCALC],
    int iprint )
```

Access net local energy.

Author

Justin Xiang

Parameters

<i>com</i>	Communications object
<i>nosh</i>	Parameters from input file
<i>totEnergy</i>	Array of energies from different calculations
<i>iprint</i>	Index of energy statement to print

Returns

Net local energy

Definition at line 2753 of file [routines.c](#).

7.32.4.40 setPartMG()

```
VEXTERNC int setPartMG (
    NOsh * nosh,
    MGparm * mgparm,
    Vpmg * pmg )
```

Set MG partitions for calculating observables and performing I/O.

Author

Nathan Baker

Parameters

<i>nosh</i>	Object with parsed input file parameters
<i>mgparm</i>	MG parameters from input file
<i>pmg</i>	MG object

Returns

1 if successful, 0 otherwise

Definition at line 1523 of file [routines.c](#).

7.32.4.41 solveFE()

```

VEXTERNC int solveFE (
    int icalc,
    PBEparm * pbeparm,
    FEMparm * feparm,
    Vfetk * fetk[NOSH_MAXCALC] )

```

Solve-estimate-refine.

Author

Nathan Baker

Parameters

<i>i</i>	Calculation index
<i>feparm</i>	FE-specific parameters
<i>pbeparm</i>	Generic PBE parameters
<i>fetk</i>	Array of FE solver objects

Returns

1 if successful, 0 otherwise

Call MC's mesh solving equations depending upon the type of PBE we're dealing with. < AM_hPcg

< Coarse-grid solver; 0 = SLU, 1 = MG, 2 = CG, 3 = BCG, 4 = PCG, 5 = PBCG

< Primal problem

< Preconditioner; 0 = identity.

Parameters

<i>icalc</i>	Calculation index
<i>pbeparm</i>	PBE-specific parameters
<i>feparm</i>	FE-specific parameters
<i>fetk</i>	Array of FE solver objects

Definition at line [4116](#) of file [routines.c](#).

7.32.4.42 solveMG()

```

VEXTERNC int solveMG (
    NOsh * nosh,
    Vpmg * pmg,
    MGparm_CalcType type )

```

Solve the PBE with MG.

Author

Nathan Baker

Parameters

<i>nosh</i>	Object with parsed input file parameters
-------------	--

Parameters

<i>pmg</i>	MG objects for this calculation
<i>type</i>	Type of MG calculation

Returns

1 if successful, 0 otherwise

Definition at line 1487 of file [routines.c](#).

7.32.4.43 startVio()

```
VEXTERNC void startVio ( )
```

Wrapper to start MALOC Vio layer.

Author

Nathan Baker and Robert Konecny

Definition at line 58 of file [routines.c](#).

7.32.4.44 storeAtomEnergy()

```
VEXTERNC void storeAtomEnergy (
    Vpmg * pmg,
    int icalc,
    double ** atomEnergy,
    int * nenergy )
```

Store energy in arrays for future use.

Author

Todd Dolinsky

Parameters

<i>pmg</i>	MG object
<i>icalc</i>	Calculation number
<i>atomEnergy</i>	Pointer to storage array of doubles
<i>nenergy</i>	Stores number of atoms per calc

Definition at line 1870 of file [routines.c](#).

7.32.4.45 writedataFE()

```
VEXTERNC int writedataFE (
    int rank,
    NOsh * nosh,
    PBEparm * pbeparm,
    Vfetk * fetk )
```

Write FEM data to files.

Author

Nathan Baker

Parameters

<i>rank</i>	Rank of processor (for parallel runs)
<i>nosh</i>	NOsh object
<i>pbeparm</i>	PBEparm object
<i>fetk</i>	FEtk object (with solution)

Returns

1 if successful, 0 otherwise

Write FEM data to file. <

<

< Loop counter

< Flag indicating whether data can be written to output

<

<

Parameters

<i>rank</i>	Rank of processor (for parallel runs)
<i>nosh</i>	NOsh object
<i>pbeparm</i>	PBE-specific parameters
<i>fetk</i>	FEtk object (with solution)

Definition at line 4300 of file [routines.c](#).**7.32.4.46 writedataFlat()**

```

VEXTERNC int writedataFlat (
    NOsh * nosh,
    Vcom * com,
    const char * fname,
    double totEnergy[NOSH_MAXCALC],
    double qfEnergy[NOSH_MAXCALC],
    double qmEnergy[NOSH_MAXCALC],
    double dielEnergy[NOSH_MAXCALC],
    int nenergy[NOSH_MAXCALC],
    double * atomEnergy[NOSH_MAXCALC],
    int nforce[NOSH_MAXCALC],
    AtomForce * atomForce[NOSH_MAXCALC] )

```

Write out information to a flat file.

Author

Todd Dolinsky

Parameters

<i>nosh</i>	Parameters from input file
<i>com</i>	The communications object
<i>fname</i>	The target XML file name
<i>totEnergy</i>	An array with per-calc total energies (in kT)
<i>qtEnergy</i>	An array with per-calc charge-potential energies (in kT)
<i>qmEnergy</i>	An array with per-calc mobile energies (in kT)
<i>dielEnergy</i>	An array with per-calc polarization energies (in kT)
<i>nenergy</i>	An array containing the number of atoms per-calc
<i>atomEnergy</i>	An array containing per-atom energies (in KT) per calc
<i>nforce</i>	An array containing the number of forces calculated per-calc
<i>atomForce</i>	An array containing per-atom forces per calc

Returns

1 if successful, 0 otherwise

Definition at line 1887 of file [routines.c](#).

7.32.4.47 writedataMG()

```

VEXTERNC int writedataMG (
    int rank,
    NOsh * nosh,
    PBEparm * pbeparm,
    Vpmg * pmg )

```

Write out observables from MG calculation to file.

Author

Nathan Baker

Parameters

<i>rank</i>	Processor rank (if parallel calculation)
<i>nosh</i>	Parameters from input file
<i>pbeparm</i>	Generic PBE parameters
<i>pmg</i>	MG object

Returns

1 if successful, 0 otherwise

Definition at line 2383 of file [routines.c](#).

7.32.4.48 writedataXML()

```

VEXTERNC int writedataXML (
    NOsh * nosh,

```

```

Vcom * com,
const char * fname,
double totEnergy[NOSH_MAXCALC],
double qfEnergy[NOSH_MAXCALC],
double qmEnergy[NOSH_MAXCALC],
double dielEnergy[NOSH_MAXCALC],
int nenergy[NOSH_MAXCALC],
double * atomEnergy[NOSH_MAXCALC],
int nforce[NOSH_MAXCALC],
AtomForce * atomForce[NOSH_MAXCALC] )

```

Write out information to an XML file.

Author

Todd Dolinsky

Parameters

<i>nosh</i>	Parameters from input file
<i>com</i>	The communications object
<i>fname</i>	The target XML file name
<i>totEnergy</i>	An array with per-calc total energies (in kT)
<i>qfEnergy</i>	An array with per-calc charge-potential energies (in kT)
<i>qmEnergy</i>	An array with per-calc mobile energies (in kT)
<i>dielEnergy</i>	An array with per-calc polarization energies (in kT)
<i>nenergy</i>	An array containing the number of atoms per-calc
<i>atomEnergy</i>	An array containing per-atom energies (in KT) per calc
<i>nforce</i>	An array containing the number of forces calculated per-calc
<i>atomForce</i>	An array containing per-atom forces per calc

Returns

1 if successful, 0 otherwise

Definition at line 2123 of file [routines.c](#).

7.32.4.49 writematMG()

```

VEXTERNC int writematMG (
    int rank,
    NOsh * nosh,
    PBEparm * pbeparm,
    Vpmg * pmg )

```

Write out operator matrix from MG calculation to file.

Author

Nathan Baker

Parameters

<i>rank</i>	Processor rank (if parallel calculation)
-------------	--

Parameters

<i>nosh</i>	Parameters from input file
<i>pbeparm</i>	Generic PBE parameters
<i>pmg</i>	MG object

Returns

1 if successful, 0 otherwise

Definition at line [1799](#) of file [routines.c](#).

Chapter 8

Data Structure Documentation

8.1 AtomForce Struct Reference

Structure to hold atomic forces.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/routines.h>
```

Data Fields

- double [ibForce](#) [3]
- double [qfForce](#) [3]
- double [dbForce](#) [3]
- double [sasaForce](#) [3]
- double [savForce](#) [3]
- double [wcaForce](#) [3]

8.1.1 Detailed Description

Structure to hold atomic forces.

Author

Nathan Baker

Definition at line 99 of file [routines.h](#).

8.1.2 Field Documentation

8.1.2.1 dbForce

```
double dbForce[3]
```

Dielectric boundary force

Definition at line 102 of file [routines.h](#).

8.1.2.2 ibForce

```
double ibForce[3]
```

Ion-boundary force

Definition at line 100 of file [routines.h](#).

8.1.2.3 qfForce

```
double qfForce[3]
```

Charge-field force

Definition at line 101 of file [routines.h](#).

8.1.2.4 sasaForce

```
double sasaForce[3]
```

SASA force (coupled to gamma)

Definition at line 103 of file [routines.h](#).

8.1.2.5 savForce

```
double savForce[3]
```

SAV force (coupled to press)

Definition at line 104 of file [routines.h](#).

8.1.2.6 wcaForce

```
double wcaForce[3]
```

WCA integral force (coupled to bconc)

Definition at line 105 of file [routines.h](#).

The documentation for this struct was generated from the following file:

- [src/routines.h](#)

8.2 sAPOLparm Struct Reference

Parameter structure for APOL-specific variables from input files.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/apolparm.h>
```

Data Fields

- int [parsed](#)
- double [grid](#) [3]
- int [setgrid](#)
- int [molid](#)
- int [setmolid](#)
- double [bconc](#)
- int [setbconc](#)
- double [sdens](#)
- int [setsdens](#)
- double [dpos](#)
- int [setdpos](#)
- double [press](#)
- int [setpress](#)
- [Vsurf_Meth](#) [srfm](#)
- int [setsrfm](#)
- double [srad](#)

- int [setsrad](#)
- double [swin](#)
- int [setswin](#)
- double [temp](#)
- int [settemp](#)
- double [gamma](#)
- int [setgamma](#)
- [APOLparm_calcEnergy](#) [calcenergy](#)
- int [setcalcenergy](#)
- [APOLparm_calcForce](#) [calcforce](#)
- int [setcalcforce](#)
- double [watsigma](#)
- double [watepsilon](#)
- double [sasa](#)
- double [sav](#)
- double [wcaEnergy](#)
- double [totForce](#) [3]
- int [setwat](#)

8.2.1 Detailed Description

Parameter structure for APOL-specific variables from input files.

Author

David Gohara

Definition at line 129 of file [apolparm.h](#).

8.2.2 Field Documentation

8.2.2.1 bconc

`double bconc`

Vacc sphere density

Definition at line 139 of file [apolparm.h](#).

8.2.2.2 calcenergy

`APOLparm_calcEnergy calcenergy`

Energy calculation flag

Definition at line 167 of file [apolparm.h](#).

8.2.2.3 calcforce

`APOLparm_calcForce calcforce`

Atomic forces calculation

Definition at line 170 of file [apolparm.h](#).

8.2.2.4 dpos

double dpos

Atom position offset

Definition at line 145 of file [apolparm.h](#).

8.2.2.5 gamma

double gamma

Surface tension for apolar energies/forces (in kJ/mol/A²)

Definition at line 163 of file [apolparm.h](#).

8.2.2.6 grid

double grid[3]

Grid spacing

Definition at line 133 of file [apolparm.h](#).

8.2.2.7 molid

int molid

Molecule ID to perform calculation on

Definition at line 136 of file [apolparm.h](#).

8.2.2.8 parsed

int parsed

Flag: Has this structure been filled with anything other than the default values? (0 = no, 1 = yes)

Definition at line 131 of file [apolparm.h](#).

8.2.2.9 press

double press

Solvent pressure

Definition at line 148 of file [apolparm.h](#).

8.2.2.10 sasa

double sasa

Solvent accessible surface area for this calculation

Definition at line 175 of file [apolparm.h](#).

8.2.2.11 sav

double sav

Solvent accessible volume for this calculation

Definition at line 176 of file [apolparm.h](#).

8.2.2.12 sdens

`double sdens`

Vacc sphere density

Definition at line 142 of file [apolparm.h](#).

8.2.2.13 setbconc

`int setbconc`

Flag,

See also

[bconc](#)

Definition at line 140 of file [apolparm.h](#).

8.2.2.14 setcalcenergy

`int setcalcenergy`

Flag,

See also

[calcenergy](#)

Definition at line 168 of file [apolparm.h](#).

8.2.2.15 setcalcforce

`int setcalcforce`

Flag,

See also

[calcforce](#)

Definition at line 171 of file [apolparm.h](#).

8.2.2.16 setdpos

`int setdpos`

Flag,

See also

[dpos](#)

Definition at line 146 of file [apolparm.h](#).

8.2.2.17 setgamma

`int setgamma`

Flag,

See also

[gamma](#)

Definition at line 165 of file [apolparm.h](#).

8.2.2.18 setgrid

```
int setgrid
```

Flag,

See also

[grid](#)

Definition at line 134 of file [apolparm.h](#).

8.2.2.19 setmolid

```
int setmolid
```

Flag,

See also

[molid](#)

Definition at line 137 of file [apolparm.h](#).

8.2.2.20 setpress

```
int setpress
```

Flag,

See also

[press](#)

Definition at line 149 of file [apolparm.h](#).

8.2.2.21 setsdens

```
int setsdens
```

Flag,

See also

[sdens](#)

Definition at line 143 of file [apolparm.h](#).

8.2.2.22 setsrad

```
int setsrad
```

Flag,

See also

[srad](#)

Definition at line 155 of file [apolparm.h](#).

8.2.2.23 setsrfm

```
int setsrfm
```

Flag,

See also

[srfm](#)

Definition at line 152 of file [apolparm.h](#).

8.2.2.24 setswin

```
int setswin
```

Flag,

See also

[swin](#)

Definition at line 158 of file [apolparm.h](#).

8.2.2.25 settemp

```
int settemp
```

Flag,

See also

[temp](#)

Definition at line 161 of file [apolparm.h](#).

8.2.2.26 setwat

```
int setwat
```

Boolean for determining if a water parameter is supplied. Yes = 1, No = 0

Definition at line 180 of file [apolparm.h](#).

8.2.2.27 srad

```
double srad
```

Solvent radius

Definition at line 154 of file [apolparm.h](#).

8.2.2.28 srfm

```
Vsurf_Meth srfm
```

Surface calculation method

Definition at line 151 of file [apolparm.h](#).

8.2.2.29 swin

double swin

Cubic spline window

Definition at line 157 of file [apolparm.h](#).

8.2.2.30 temp

double temp

Temperature (in K)

Definition at line 160 of file [apolparm.h](#).

8.2.2.31 totForce

double totForce[3]

Total forces on x, y, z

Definition at line 178 of file [apolparm.h](#).

8.2.2.32 watepsilon

double watepsilon

Water oxygen Lennard-Jones well depth (kJ/mol)

Definition at line 174 of file [apolparm.h](#).

8.2.2.33 watsigma

double watsigma

Water oxygen Lennard-Jones radius (A)

Definition at line 173 of file [apolparm.h](#).

8.2.2.34 wcaEnergy

double wcaEnergy

wcaEnergy

Definition at line 177 of file [apolparm.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/apolparm.h](#)

8.3 sBEMparm Struct Reference

Parameter structure for BEM-specific variables from input files.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/bemparm.h>
```

Data Fields

- [BEMparm_CalcType](#) type
- int [parsed](#)
- [Vchrg_Src](#) chgs
- int [tree_order](#)

- int [settree_order](#)
- int [tree_n0](#)
- int [settree_n0](#)
- double [mac](#)
- int [setmac](#)
- int [nonlintype](#)
- int [setnonlintype](#)
- int [mesh](#)
- int [setmesh](#)
- int [outdata](#)
- int [setoutdata](#)

8.3.1 Detailed Description

Parameter structure for BEM-specific variables from input files.

Author

Nathan Baker and Todd Dolinsky and Weihua Geng

Note

If you add/delete/change something in this class, the member functions – especially `BEMparm_copy` – must be modified accordingly

Definition at line 96 of file [bemparm.h](#).

8.3.2 Field Documentation

8.3.2.1 chgs

`Vchrg_Src` `chgs`

Charge source (Charge, Multipole, Induced Dipole, NL Induced. Not currently implemented but should be relatively easy to add in the future (cf Pengyu Ren)

Definition at line 102 of file [bemparm.h](#).

8.3.2.2 mac

`double` `mac`

Multipole acceptance criterion (should be between 0 and 1)

Definition at line 108 of file [bemparm.h](#).

8.3.2.3 mesh

`int` `mesh`

0 for msms, 1 for NanoShaper SES, 2 for NanoShaper Skin

Definition at line 113 of file [bemparm.h](#).

8.3.2.4 nonlintage

`int nonlintage`

Linearity Type Method to be used

Definition at line 110 of file [bemparm.h](#).

8.3.2.5 outdata

`int outdata`

0 does not output vtk, 1 outputs vtk

Definition at line 116 of file [bemparm.h](#).

8.3.2.6 parsed

`int parsed`

Has this structure been filled? (0 = no, 1 = yes)

Definition at line 99 of file [bemparm.h](#).

8.3.2.7 setmac

`int setmac`

Flag,

See also

[mac](#)

Definition at line 109 of file [bemparm.h](#).

8.3.2.8 setmesh

`int setmesh`

Flag,

See also

[mesh](#)

Definition at line 114 of file [bemparm.h](#).

8.3.2.9 setnonlintage

`int setnonlintage`

Flag,

See also

[nonlintage](#)

Definition at line 111 of file [bemparm.h](#).

8.3.2.10 setoutdata

`int setoutdata`

Flag,

See also

[outdata](#)

Definition at line 117 of file [bemparm.h](#).

8.3.2.11 settree_n0

`int settree_n0`

Flag,

See also

[tree_npart](#)

Definition at line 107 of file [bemparm.h](#).

8.3.2.12 settree_order

`int settree_order`

Flag,

See also

[tree_order](#)

Definition at line 105 of file [bemparm.h](#).

8.3.2.13 tree_n0

`int tree_n0`

Number of particles per leaf of the tree

Definition at line 106 of file [bemparm.h](#).

8.3.2.14 tree_order

`int tree_order`

User-defined order for the treecode expansion

Definition at line 104 of file [bemparm.h](#).

8.3.2.15 type

[BEMparm_CalcType](#) type

What type of BEM calculation?

Definition at line 98 of file [bemparm.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/bemparm.h](#)

8.4 sFEMparm Struct Reference

Parameter structure for FEM-specific variables from input files.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/femparm.h>
```

Data Fields

- int [parsed](#)
- [FEMparm_CalcType](#) type
- int [settype](#)
- double [glen](#) [3]
- int [setglen](#)
- double [etol](#)
- int [setetol](#)
- [FEMparm_EtolType](#) ekey
- int [setekey](#)
- [FEMparm_EstType](#) akeyPRE
- int [setakeyPRE](#)
- [FEMparm_EstType](#) akeySOLVE
- int [setakeySOLVE](#)
- int [targetNum](#)
- int [settargetNum](#)
- double [targetRes](#)
- int [settargetRes](#)
- int [maxsolve](#)
- int [setmaxsolve](#)
- int [maxvert](#)
- int [setmaxvert](#)
- int [pkey](#)
- int [useMesh](#)
- int [meshID](#)

8.4.1 Detailed Description

Parameter structure for FEM-specific variables from input files.

Author

Nathan Baker

Definition at line 133 of file [femparm.h](#).

8.4.2 Field Documentation

8.4.2.1 akeyPRE

[FEMparm_EstType](#) akeyPRE

Adaptive refinement error estimator method for pre-solution refine. Note, this should either be FRT_UNIF or FRT_GEOM.

Definition at line 148 of file [femparm.h](#).

8.4.2.2 akeySOLVE

`FEMparm_EstType` akeySOLVE

Adaptive refinement error estimator method for a posteriori solution-based refinement.

Definition at line 152 of file [femparm.h](#).

8.4.2.3 ekey

`FEMparm_EtolType` ekey

Adaptive refinement interpretation of error tolerance

Definition at line 145 of file [femparm.h](#).

8.4.2.4 etol

`double` etol

Error tolerance for refinement; interpretation depends on the adaptive refinement method chosen

Definition at line 142 of file [femparm.h](#).

8.4.2.5 glen

`double` glen[3]

Domain side lengths (in Å)

Definition at line 140 of file [femparm.h](#).

8.4.2.6 maxsolve

`int` maxsolve

Maximum number of solve-estimate-refine cycles

Definition at line 165 of file [femparm.h](#).

8.4.2.7 maxvert

`int` maxvert

Maximum number of vertices in mesh (ignored if less than zero)

Definition at line 167 of file [femparm.h](#).

8.4.2.8 meshID

`int` meshID

External finite element mesh ID (if used)

Definition at line 174 of file [femparm.h](#).

8.4.2.9 parsed

`int` parsed

Flag: Has this structure been filled with anything other than * the default values? (0 = no, 1 = yes)

Definition at line 135 of file [femparm.h](#).

8.4.2.10 pkey

`int pkey`

Boolean sets the pkey type for going into AM_R refine pkey = 0 for non-HB based methods pkey = 1 for HB based methods

Definition at line 170 of file [femparm.h](#).

8.4.2.11 setakeyPRE

`int setakeyPRE`

Boolean

Definition at line 151 of file [femparm.h](#).

8.4.2.12 setakeySOLVE

`int setakeySOLVE`

Boolean

Definition at line 154 of file [femparm.h](#).

8.4.2.13 setekey

`int setekey`

Boolean

Definition at line 147 of file [femparm.h](#).

8.4.2.14 setetol

`int setetol`

Boolean

Definition at line 144 of file [femparm.h](#).

8.4.2.15 setglen

`int setglen`

Boolean

Definition at line 141 of file [femparm.h](#).

8.4.2.16 setmaxsolve

`int setmaxsolve`

Boolean

Definition at line 166 of file [femparm.h](#).

8.4.2.17 setmaxvert

`int setmaxvert`

Boolean

Definition at line 169 of file [femparm.h](#).

8.4.2.18 settargetNum

int settargetNum

Boolean

Definition at line 159 of file [femparm.h](#).

8.4.2.19 settargetRes

int settargetRes

Boolean

Definition at line 164 of file [femparm.h](#).

8.4.2.20 settype

int settype

Boolean

Definition at line 139 of file [femparm.h](#).

8.4.2.21 targetNum

int targetNum

Initial mesh will continue to be marked and refined with the method specified by akeyPRE until the mesh contains this many vertices or until targetRes is reached.

Definition at line 155 of file [femparm.h](#).

8.4.2.22 targetRes

double targetRes

Initial mesh will continue to be marked and refined with the method specified by akeyPRE until the mesh contains no markable simplices with longest edges above this size or until targetNum is reached.

Definition at line 160 of file [femparm.h](#).

8.4.2.23 type

[FEMparm_CalcType](#) type

Calculation type

Definition at line 138 of file [femparm.h](#).

8.4.2.24 useMesh

int useMesh

Indicates whether we use external finite element mesh

Definition at line 173 of file [femparm.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/femparm.h](#)

8.5 sGEOFLOWparm Struct Reference

Parameter structure for GEOFLOW-specific variables from input files.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/geoflowparm.h>
```

Data Fields

- [GEOFLOWparm_CalcType](#) type
- int [parsed](#)
- int [vdw](#)
- int [setvdw](#)
- double [etol](#)

8.5.1 Detailed Description

Parameter structure for GEOFLOW-specific variables from input files.

Author

Andrew Stevens, Kyle Monson

Note

If you add/delete/change something in this class, the member functions – especially `GEOFLOWparm_copy` – must be modified accordingly

Definition at line 98 of file [geoflowparm.h](#).

8.5.2 Field Documentation

8.5.2.1 etol

```
double etol
```

user defined error tolerance

Definition at line 106 of file [geoflowparm.h](#).

8.5.2.2 parsed

```
int parsed
```

Has this structure been filled? (0 = no, 1 = yes)

Definition at line 101 of file [geoflowparm.h](#).

8.5.2.3 setvdw

```
int setvdw
```

Definition at line 105 of file [geoflowparm.h](#).

8.5.2.4 type

```
GEOFLOWparm_CalcType type
```

What type of GEOFLOW calculation?

Definition at line 100 of file [geoflowparm.h](#).

8.5.2.5 vdw

int vdw

Definition at line 104 of file [geoflowparm.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/geoflowparm.h](#)

8.6 sMGparm Struct Reference

Parameter structure for MG-specific variables from input files.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/mgparm.h>
```

Data Fields

- [MGparm_CalcType](#) type
- int [parsed](#)
- int [dime](#) [3]
- int [setdime](#)
- [Vchrg_Meth](#) chgm
- int [setchgm](#)
- [Vchrg_Src](#) chgs
- int [nlev](#)
- int [setnlev](#)
- double [etol](#)
- int [setetol](#)
- double [grid](#) [3]
- int [setgrid](#)
- double [glen](#) [3]
- int [setglen](#)
- [MGparm_CentMeth](#) cmeth
- double [center](#) [3]
- int [centmol](#)
- int [setgcent](#)
- double [cglen](#) [3]
- int [setcglen](#)
- double [fglen](#) [3]
- int [setfglen](#)
- [MGparm_CentMeth](#) ccmeth
- double [ccenter](#) [3]
- int [ccentmol](#)
- int [setcgcent](#)
- [MGparm_CentMeth](#) fcmeth
- double [fcenter](#) [3]
- int [fcentmol](#)
- int [setfgcent](#)
- double [partDisjCenter](#) [3]
- double [partDisjLength](#) [3]
- int [partDisjOwnSide](#) [6]
- int [pdime](#) [3]
- int [setpdime](#)
- int [proc_rank](#)

- int [setrank](#)
- int [proc_size](#)
- int [setsize](#)
- double [ofrac](#)
- int [setofrac](#)
- int [async](#)
- int [setasync](#)
- int [nonlotype](#)
- int [setnonlotype](#)
- int [method](#)
- int [setmethod](#)
- int [useAqua](#)
- int [setUseAqua](#)

8.6.1 Detailed Description

Parameter structure for MG-specific variables from input files.

Author

Nathan Baker and Todd Dolinsky

Note

If you add/delete/change something in this class, the member functions – especially `MGparm_copy` – must be modified accordingly

Definition at line [114](#) of file [mgparm.h](#).

8.6.2 Field Documentation

8.6.2.1 `async`

```
int async
```

Processor ID for asynchronous calculation

Definition at line [186](#) of file [mgparm.h](#).

8.6.2.2 `ccenter`

```
double ccenter[3]
```

Coarse grid center.

Definition at line [157](#) of file [mgparm.h](#).

8.6.2.3 `ccentmol`

```
int ccentmol
```

Particular molecule on which we want to center the grid. This should be the appropriate index in an array of molecules, not the positive definite integer specified by the user.

Definition at line [158](#) of file [mgparm.h](#).

8.6.2.4 ccmeth

`MGparm_CentMeth` ccmeth

Coarse grid centering method

Definition at line 156 of file `mgparm.h`.

8.6.2.5 center

`double` center[3]

Grid center. If `ispart = 0`, then this is only meaningful if `cmeth = 0`. However, if `ispart = 1` and `cmeth = MCM_PNT`, then this is the center of the non-disjoint (overlapping) partition. If `ispart = 1` and `cmeth = MCM_MOL`, then this is the vector that must be added to the center of the molecule to give the center of the non-disjoint partition.

Definition at line 138 of file `mgparm.h`.

8.6.2.6 centmol

`int` centmol

Particular molecule on which we want to center the grid. This should be the appropriate index in an array of molecules, not the positive definite integer specified by the user.

Definition at line 146 of file `mgparm.h`.

8.6.2.7 cglen

`double` cglen[3]

Coarse grid side lengths

Definition at line 152 of file `mgparm.h`.

8.6.2.8 chgm

`Vchrg_Meth` chgm

Charge discretization method

Definition at line 122 of file `mgparm.h`.

8.6.2.9 chgs

`Vchrg_Src` chgs

Charge source (Charge, Multipole, Induced Dipole, NL Induced

Definition at line 124 of file `mgparm.h`.

8.6.2.10 cmeth

`MGparm_CentMeth` cmeth

Centering method

Definition at line 137 of file `mgparm.h`.

8.6.2.11 dime

```
int dime[3]
```

Grid dimensions

Definition at line 120 of file [mgparm.h](#).

8.6.2.12 etol

```
double etol
```

User-defined error tolerance

Definition at line 131 of file [mgparm.h](#).

8.6.2.13 fcenter

```
double fcenter[3]
```

Fine grid center.

Definition at line 163 of file [mgparm.h](#).

8.6.2.14 fcentmol

```
int fcentmol
```

Particular molecule on which we want to center the grid. This should be the appropriate index in an array of molecules, not the positive definite integer specified by the user.

Definition at line 164 of file [mgparm.h](#).

8.6.2.15 fcmeth

```
MGparm_CentMeth fcmeth
```

Fine grid centering method

Definition at line 162 of file [mgparm.h](#).

8.6.2.16 fglen

```
double fglen[3]
```

Fine grid side lengths

Definition at line 154 of file [mgparm.h](#).

8.6.2.17 glen

```
double glen[3]
```

Grid side lengths.

Definition at line 135 of file [mgparm.h](#).

8.6.2.18 grid

```
double grid[3]
```

Grid spacings

Definition at line 133 of file [mgparm.h](#).

8.6.2.19 method

`int method`

Solver Method

Definition at line 192 of file [mgparm.h](#).

8.6.2.20 nlev

`int nlev`

Levels in multigrid hierarchy

Deprecated Just ignored now

Definition at line 128 of file [mgparm.h](#).

8.6.2.21 nonlntype

`int nonlntype`

Linearity Type Method to be used

Definition at line 189 of file [mgparm.h](#).

8.6.2.22 ofrac

`double ofrac`

Overlap fraction between procs

Definition at line 184 of file [mgparm.h](#).

8.6.2.23 parsed

`int parsed`

Has this structure been filled? (0 = no, 1 = yes)

Definition at line 117 of file [mgparm.h](#).

8.6.2.24 partDisjCenter

`double partDisjCenter[3]`

This gives the center of the disjoint partitions

Definition at line 171 of file [mgparm.h](#).

8.6.2.25 partDisjLength

`double partDisjLength[3]`

This gives the lengths of the disjoint partitions

Definition at line 173 of file [mgparm.h](#).

8.6.2.26 `partDisjOwnSide`

```
int partDisjOwnSide[6]
```

Tells whether the boundary points are ours (1) or not (0)

Definition at line 175 of file [mgparm.h](#).

8.6.2.27 `pdime`

```
int pdime[3]
```

Grid of processors to be used in calculation

Definition at line 178 of file [mgparm.h](#).

8.6.2.28 `proc_rank`

```
int proc_rank
```

Rank of this processor

Definition at line 180 of file [mgparm.h](#).

8.6.2.29 `proc_size`

```
int proc_size
```

Total number of processors

Definition at line 182 of file [mgparm.h](#).

8.6.2.30 `setasynch`

```
int setasynch
```

Flag,

See also

[asynch](#)

Definition at line 187 of file [mgparm.h](#).

8.6.2.31 `setcgcent`

```
int setcgcent
```

Flag,

See also

[ccmeth](#)

Definition at line 161 of file [mgparm.h](#).

8.6.2.32 `setcglen`

```
int setcglen
```

Flag,

See also

[cglen](#)

Definition at line 153 of file [mgparm.h](#).

8.6.2.33 setchgm

```
int setchgm
```

Flag,

See also

[chgm](#)

Definition at line 123 of file [mgparm.h](#).

8.6.2.34 setdime

```
int setdime
```

Flag,

See also

[dime](#)

Definition at line 121 of file [mgparm.h](#).

8.6.2.35 setetol

```
int setetol
```

Flag,

See also

[etol](#)

Definition at line 132 of file [mgparm.h](#).

8.6.2.36 setfgcent

```
int setfgcent
```

Flag,

See also

[fcmeth](#)

Definition at line 167 of file [mgparm.h](#).

8.6.2.37 setfglen

```
int setfglen
```

Flag,

See also

[fglen](#)

Definition at line 155 of file [mgparm.h](#).

8.6.2.38 setgcent

`int setgcent`
Flag,

See also

[cmeth](#)

Definition at line 149 of file [mgparm.h](#).

8.6.2.39 setglen

`int setglen`
Flag,

See also

[glen](#)

Definition at line 136 of file [mgparm.h](#).

8.6.2.40 setgrid

`int setgrid`
Flag,

See also

[grid](#)

Definition at line 134 of file [mgparm.h](#).

8.6.2.41 setmethod

`int setmethod`
Flag,

See also

[method](#)

Definition at line 193 of file [mgparm.h](#).

8.6.2.42 setnlev

`int setnlev`
Flag,

See also

[nlev](#)

Definition at line 130 of file [mgparm.h](#).

8.6.2.43 setnonlotype

`int setnonlotype`
Flag,

See also

[nonlotype](#)

Definition at line 190 of file [mgparm.h](#).

8.6.2.44 setofrac

`int setofrac`
Flag,

See also

[ofrac](#)

Definition at line 185 of file [mgparm.h](#).

8.6.2.45 setpdime

`int setpdime`
Flag,

See also

[pdime](#)

Definition at line 179 of file [mgparm.h](#).

8.6.2.46 setrank

`int setrank`
Flag,

See also

[proc_rank](#)

Definition at line 181 of file [mgparm.h](#).

8.6.2.47 setsize

`int setsize`
Flag,

See also

[proc_size](#)

Definition at line 183 of file [mgparm.h](#).

8.6.2.48 `setUseAqua`

`int setUseAqua`
Flag,

See also

[useAqua](#)

Definition at line 196 of file [mgparm.h](#).

8.6.2.49 `type`

`MGparm_CalcType` type

What type of MG calculation?

Definition at line 116 of file [mgparm.h](#).

8.6.2.50 `useAqua`

`int useAqua`

Enable use of lpbe/aqua

Definition at line 195 of file [mgparm.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/mgparm.h](#)

8.7 sNOsh Struct Reference

Class for parsing fixed format input files.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/nosh.h>
```

Data Fields

- `NOsh_calc * calc` [`NOSH_MAXCALC`]
- `int ncalc`
- `NOsh_calc * elec` [`NOSH_MAXCALC`]
- `int nelec`
- `NOsh_calc * apol` [`NOSH_MAXCALC`]
- `int napol`
- `int ispara`
- `int proc_rank`
- `int proc_size`
- `int bogus`
- `int elec2calc` [`NOSH_MAXCALC`]
- `int apol2calc` [`NOSH_MAXCALC`]
- `int nmol`
- `char molpath` [`NOSH_MAXMOL`][`VMAX_ARGLEN`]
- `NOsh_MolFormat molfmt` [`NOSH_MAXMOL`]
- `Valist * alist` [`NOSH_MAXMOL`]
- `int gotparm`
- `char parmpath` [`VMAX_ARGLEN`]
- `NOsh_ParmFormat parmfmt`

- int [ndiel](#)
- char [dielXpath](#) [NOSH_MAXMOL][VMAX_ARGLEN]
- char [dielYpath](#) [NOSH_MAXMOL][VMAX_ARGLEN]
- char [dielZpath](#) [NOSH_MAXMOL][VMAX_ARGLEN]
- [Vdata_Format](#) [dielfmt](#) [NOSH_MAXMOL]
- int [nkappa](#)
- char [kappapath](#) [NOSH_MAXMOL][VMAX_ARGLEN]
- [Vdata_Format](#) [kappafmt](#) [NOSH_MAXMOL]
- int [npot](#)
- char [potpath](#) [NOSH_MAXMOL][VMAX_ARGLEN]
- [Vdata_Format](#) [potfmt](#) [NOSH_MAXMOL]
- int [ncharge](#)
- char [chargepath](#) [NOSH_MAXMOL][VMAX_ARGLEN]
- [Vdata_Format](#) [chargefmt](#) [NOSH_MAXMOL]
- int [nmesh](#)
- char [meshpath](#) [NOSH_MAXMOL][VMAX_ARGLEN]
- [Vdata_Format](#) [meshfmt](#) [NOSH_MAXMOL]
- int [nprint](#)
- [NOSH_PrintType](#) [printwhat](#) [NOSH_MAXPRINT]
- int [printnarg](#) [NOSH_MAXPRINT]
- int [printcalc](#) [NOSH_MAXPRINT][NOSH_MAXPOP]
- int [printop](#) [NOSH_MAXPRINT][NOSH_MAXPOP]
- int [parsed](#)
- char [elecname](#) [NOSH_MAXCALC][VMAX_ARGLEN]
- char [apolname](#) [NOSH_MAXCALC][VMAX_ARGLEN]

8.7.1 Detailed Description

Class for parsing fixed format input files.

Author

Nathan Baker

Definition at line 195 of file [nosh.h](#).

8.7.2 Field Documentation

8.7.2.1 alist

[Valist*](#) [alist](#) [NOSH_MAXMOL]

Molecules for calculation (can be used in setting mesh centers)

Definition at line 234 of file [nosh.h](#).

8.7.2.2 apol

[NOSH_calc*](#) [apol](#) [NOSH_MAXCALC]

The array of calculation objects corresponding to APOLAR statements read in the input file. Compare to [sNosh::calc](#)

Definition at line 208 of file [nosh.h](#).

8.7.2.3 apol2calc

```
int apol2calc[NOSH_MAXCALC]
```

(see elec2calc)

Definition at line 229 of file [nosh.h](#).

8.7.2.4 apolname

```
char apolname[NOSH_MAXCALC][VMAX_ARGLEN]
```

Optional user-specified name for APOLAR statement

Definition at line 269 of file [nosh.h](#).

8.7.2.5 bogus

```
int bogus
```

A flag which tells routines using NOsh that this particular NOsh is broken – useful for parallel focusing calculations where the user gave us too many processors (1 => ignore this NOsh; 0 => this NOsh is OK)

Definition at line 217 of file [nosh.h](#).

8.7.2.6 calc

```
NOSH_calc* calc[NOSH_MAXCALC]
```

The array of calculation objects corresponding to actual calculations performed by the code. Compare to [sNOsh::elec](#)

Definition at line 197 of file [nosh.h](#).

8.7.2.7 chargefmt

```
Vdata_Format chargefmt[NOSH_MAXMOL]
```

Charge maps fileformats

Definition at line 255 of file [nosh.h](#).

8.7.2.8 chargepath

```
char chargepath[NOSH_MAXMOL][VMAX_ARGLEN]
```

Paths to charge map files

Definition at line 254 of file [nosh.h](#).

8.7.2.9 dielfmt

```
Vdata_Format dielfmt[NOSH_MAXMOL]
```

Dielectric maps file formats

Definition at line 246 of file [nosh.h](#).

8.7.2.10 dielXpath

```
char dielXpath[NOSH_MAXMOL][VMAX_ARGLEN]
```

Paths to x-shifted dielectric map files

Definition at line 240 of file [nosh.h](#).

8.7.2.11 dielYpath

```
char dielYpath[NOSH_MAXMOL][VMAX_ARGLEN]
```

Paths to y-shifted dielectric map files

Definition at line 242 of file [nosh.h](#).

8.7.2.12 dielZpath

```
char dielZpath[NOSH_MAXMOL][VMAX_ARGLEN]
```

Paths to z-shifted dielectric map files

Definition at line 244 of file [nosh.h](#).

8.7.2.13 elec

```
NOSH_calc* elec[NOSH_MAXCALC]
```

The array of calculation objects corresponding to ELEC statements read in the input file. Compare to [sNOsh::calc](#)

Definition at line 202 of file [nosh.h](#).

8.7.2.14 elec2calc

```
int elec2calc[NOSH_MAXCALC]
```

A mapping between ELEC statements which appear in the input file and calc objects stored above. Since we allow both normal and focused multigrid, there isn't a 1-to-1 correspondence between ELEC statements and actual calculations. This can really confuse operations which work on specific calculations further down the road (like PRINT). Therefore this array is the initial point of entry for any calculation-specific operation. It points to a specific entry in the calc array.

Definition at line 221 of file [nosh.h](#).

8.7.2.15 elecname

```
char elecname[NOSH_MAXCALC][VMAX_ARGLEN]
```

Optional user-specified name for ELEC statement

Definition at line 267 of file [nosh.h](#).

8.7.2.16 gotparm

```
int gotparm
```

Either have (1) or don't have (0) parm

Definition at line 236 of file [nosh.h](#).

8.7.2.17 ispara

```
int ispara
```

1 => is a parallel calculation, 0 => is not

Definition at line 214 of file [nosh.h](#).

8.7.2.18 kappafmt

```
Vdata_Format kappafmt[NOSH_MAXMOL]
```

Kappa maps file formats

Definition at line 249 of file [nosh.h](#).

8.7.2.19 kappapath

```
char kappapath[NOSH_MAXMOL] [VMAX_ARGLEN]
```

Paths to kappa map files

Definition at line 248 of file [nosh.h](#).

8.7.2.20 meshfmt

```
Vdata_Format meshfmt[NOSH_MAXMOL]
```

Mesh fileformats

Definition at line 258 of file [nosh.h](#).

8.7.2.21 meshpath

```
char meshpath[NOSH_MAXMOL] [VMAX_ARGLEN]
```

Paths to mesh files

Definition at line 257 of file [nosh.h](#).

8.7.2.22 molfmt

```
NOSH_MolFormat molfmt[NOSH_MAXMOL]
```

Mol files formats

Definition at line 233 of file [nosh.h](#).

8.7.2.23 molpath

```
char molpath[NOSH_MAXMOL] [VMAX_ARGLEN]
```

Paths to mol files

Definition at line 232 of file [nosh.h](#).

8.7.2.24 napol

```
int napol
```

The number of apolar statements in the input file and in the apolar array

Definition at line 211 of file [nosh.h](#).

8.7.2.25 ncalc

```
int ncalc
```

The number of calculations in the calc array

Definition at line 200 of file [nosh.h](#).

8.7.2.26 ncharge

```
int ncharge
```

Number of charge maps

Definition at line 253 of file [nosh.h](#).

8.7.2.27 ndiel

```
int ndiel
```

Number of dielectric maps

Definition at line 239 of file [nosh.h](#).

8.7.2.28 nelec

```
int nelec
```

The number of elec statements in the input file and in the elec array

Definition at line 205 of file [nosh.h](#).

8.7.2.29 nkappa

```
int nkappa
```

Number of kappa maps

Definition at line 247 of file [nosh.h](#).

8.7.2.30 nmesh

```
int nmesh
```

Number of meshes

Definition at line 256 of file [nosh.h](#).

8.7.2.31 nmol

```
int nmol
```

Number of molecules

Definition at line 231 of file [nosh.h](#).

8.7.2.32 npot

```
int npot
```

Number of potential maps

Definition at line 250 of file [nosh.h](#).

8.7.2.33 nprint

```
int nprint
```

How many print sections?

Definition at line 259 of file [nosh.h](#).

8.7.2.34 parmfmt

`Nosh_ParmFormat` parmfmt

Parm file format

Definition at line 238 of file [nosh.h](#).

8.7.2.35 parmpath

`char parmpath[VMAX_ARGLEN]`

Paths to parm file

Definition at line 237 of file [nosh.h](#).

8.7.2.36 parsed

`int parsed`

Have we parsed an input file yet?

Definition at line 266 of file [nosh.h](#).

8.7.2.37 potfmt

`Vdata_Format` potfmt [`NOSH_MAXMOL`]

Potential maps file formats

Definition at line 252 of file [nosh.h](#).

8.7.2.38 potpath

`char potpath[NOSH_MAXMOL][VMAX_ARGLEN]`

Paths to potential map files

Definition at line 251 of file [nosh.h](#).

8.7.2.39 printcalc

`int printcalc[NOSH_MAXPRINT][NOSH_MAXPOP]`

ELEC id (see `elec2calc`)

Definition at line 263 of file [nosh.h](#).

8.7.2.40 printnarg

`int printnarg[NOSH_MAXPRINT]`

How many arguments in energy list

Definition at line 262 of file [nosh.h](#).

8.7.2.41 printop

`int printop[NOSH_MAXPRINT][NOSH_MAXPOP]`

Operation id (0 = add, 1 = subtract)

Definition at line 264 of file [nosh.h](#).

8.7.2.42 printwhat

`NOsh_PrintType printwhat[NOSH_MAXPRINT]`

What do we print:

- 0 = energy,
- 1 = force

Definition at line 260 of file [nosh.h](#).

8.7.2.43 proc_rank

`int proc_rank`

Processor rank in parallel calculation

Definition at line 215 of file [nosh.h](#).

8.7.2.44 proc_size

`int proc_size`

Number of processors in parallel calculation

Definition at line 216 of file [nosh.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/nosh.h](#)

8.8 sNOsh_calc Struct Reference

Calculation class for use when parsing fixed format input files.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/nosh.h>
```

Data Fields

- [MGparm](#) * [mgparm](#)
- [FEMparm](#) * [femparm](#)
- [BEMparm](#) * [bemparm](#)
- [GEOFLOWparm](#) * [geoflowparm](#)
- [PBAMparm](#) * [pbamparm](#)
- [PBSAMparm](#) * [pbsamparm](#)
- [PBEparm](#) * [pbeparm](#)
- [APOLparm](#) * [apolparm](#)
- [NOsh_CalcType](#) [calctype](#)

8.8.1 Detailed Description

Calculation class for use when parsing fixed format input files.

Author

Nathan Baker

Definition at line 172 of file [nosh.h](#).

8.8.2 Field Documentation

8.8.2.1 apolparm

`APOLparm*` apolparm

Non-polar parameters

Definition at line 180 of file [nosh.h](#).

8.8.2.2 bemparm

`BEMparm*` bemparm

boundary element (tabi) parameters

Definition at line 175 of file [nosh.h](#).

8.8.2.3 calctype

`NOsh_CalcType` calctype

Calculation type

Definition at line 181 of file [nosh.h](#).

8.8.2.4 femparm

`FEMparm*` femparm

Finite element parameters

Definition at line 174 of file [nosh.h](#).

8.8.2.5 geoflowparm

`GEOFLOWparm*` geoflowparm

Geometric Flow Solver

Definition at line 176 of file [nosh.h](#).

8.8.2.6 mgparm

`MGparm*` mgparm

Multigrid parameters

Definition at line 173 of file [nosh.h](#).

8.8.2.7 pbamparm

`PBAMparm*` pbamparm

Analytical Poisson-Boltzmann Solver

Definition at line 177 of file [nosh.h](#).

8.8.2.8 pbeparm

PBEparm* pbeparm

Generic PBE parameters

Definition at line 179 of file [nosh.h](#).

8.8.2.9 pbsamparm

PBSAMParm* pbsamparm

Semi-Analytical Poisson-Boltzmann Solver

Definition at line 178 of file [nosh.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/nosh.h](#)

8.9 sPBAMparm Struct Reference

Parameter structure for PBAM-specific variables from input files.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/pbamparm.h>
```

Data Fields

- [PBAMparm_CalcType](#) type
- int [parsed](#)
- double [salt](#)
- int [setsalt](#)
- char [runtype](#) [CHR_MAXLEN]
- int [setruntype](#)
- char [runname](#) [CHR_MAXLEN]
- int [setrunname](#)
- int [setrandorient](#)
- double [pbcboxlen](#)
- int [setpbcs](#)
- char [units](#) [CHR_MAXLEN]
- int [setunits](#)
- int [gridpt](#)
- int [setgridpt](#)
- char [map3dname](#) [CHR_MAXLEN]
- int [set3dmap](#)
- char [grid2Dname](#) [PBAMPARM_MAXWRITE][CHR_MAXLEN]
- char [grid2Dax](#) [PBAMPARM_MAXWRITE][CHR_MAXLEN]
- double [grid2Dloc](#) [PBAMPARM_MAXWRITE]
- int [grid2Dct](#)
- int [setgrid2Dname](#)
- char [dxname](#) [CHR_MAXLEN]
- int [setdxname](#)
- int [ntraj](#)
- int [setntraj](#)
- char [termcombine](#) [CHR_MAXLEN]
- int [settermcombine](#)
- int [diffct](#)

- char `moveType` [PBAMPARM_MAXMOL][[CHR_MAXLEN](#)]
- double `transDiff` [PBAMPARM_MAXMOL]
- double `rotDiff` [PBAMPARM_MAXMOL]
- int `termct`
- int `setterm`
- char `termnam` [PBAMPARM_MAXWRITE][[CHR_MAXLEN](#)]
- int `termnu` [PBAMPARM_MAXWRITE][1]
- double `termVal` [PBAMPARM_MAXWRITE]
- char `confil` [PBAMPARM_MAXWRITE][[CHR_MAXLEN](#)]
- double `conpad` [PBAMPARM_MAXWRITE]
- int `confilct`
- int `setxyz`
- int `xyzct` [PBAMPARM_MAXMOL]
- char `xyzfil` [PBAMPARM_MAXMOL][PBAMPARM_MAXWRITE][[CHR_MAXLEN](#)]

8.9.1 Detailed Description

Parameter structure for PBAM-specific variables from input files.

Author

Andrew Stevens, Kyle Monson

Note

If you add/delete/change something in this class, the member functions – especially `PBAMparm_copy` – must be modified accordingly

Definition at line [105](#) of file [pbamparm.h](#).

8.9.2 Field Documentation

8.9.2.1 `confil`

```
char confil[PBAMPARM_MAXWRITE][CHR\_MAXLEN]
```

Definition at line [175](#) of file [pbamparm.h](#).

8.9.2.2 `confilct`

```
int confilct
```

Definition at line [177](#) of file [pbamparm.h](#).

8.9.2.3 `conpad`

```
double conpad[PBAMPARM_MAXWRITE]
```

Definition at line [176](#) of file [pbamparm.h](#).

8.9.2.4 `diffct`

```
int diffct
```

Definition at line [164](#) of file [pbamparm.h](#).

8.9.2.5 dxname

```
char dxname[CHR_MAXLEN]
```

Definition at line 152 of file [pbamparm.h](#).

8.9.2.6 grid2Dax

```
char grid2Dax[PBAMPARM_MAXWRITE][CHR_MAXLEN]
```

Definition at line 146 of file [pbamparm.h](#).

8.9.2.7 grid2Dct

```
int grid2Dct
```

Definition at line 148 of file [pbamparm.h](#).

8.9.2.8 grid2Dloc

```
double grid2Dloc[PBAMPARM_MAXWRITE]
```

Definition at line 147 of file [pbamparm.h](#).

8.9.2.9 grid2Dname

```
char grid2Dname[PBAMPARM_MAXWRITE][CHR_MAXLEN]
```

Definition at line 145 of file [pbamparm.h](#).

8.9.2.10 gridpt

```
int gridpt
```

Definition at line 137 of file [pbamparm.h](#).

8.9.2.11 map3dname

```
char map3dname[CHR_MAXLEN]
```

Definition at line 141 of file [pbamparm.h](#).

8.9.2.12 moveType

```
char moveType[PBAMPARM_MAXMOL][CHR_MAXLEN]
```

Definition at line 165 of file [pbamparm.h](#).

8.9.2.13 ntraj

```
int ntraj
```

Definition at line 158 of file [pbamparm.h](#).

8.9.2.14 parsed

```
int parsed
```

Has this structure been filled? (0 = no, 1 = yes)

Definition at line 108 of file [pbamparm.h](#).

8.9.2.15 pbcboxlen

```
double pbcboxlen
```

Definition at line 126 of file [pbamparm.h](#).

8.9.2.16 rotDiff

```
double rotDiff[PBAMPARM_MAXMOL]
```

Definition at line 167 of file [pbamparm.h](#).

8.9.2.17 runname

```
char runname[CHR_MAXLEN]
```

Definition at line 119 of file [pbamparm.h](#).

8.9.2.18 runtype

```
char runtype[CHR_MAXLEN]
```

Definition at line 115 of file [pbamparm.h](#).

8.9.2.19 salt

```
double salt
```

Definition at line 111 of file [pbamparm.h](#).

8.9.2.20 set3dmap

```
int set3dmap
```

Definition at line 142 of file [pbamparm.h](#).

8.9.2.21 setdxname

```
int setdxname
```

Definition at line 153 of file [pbamparm.h](#).

8.9.2.22 setgrid2Dname

```
int setgrid2Dname
```

Definition at line 149 of file [pbamparm.h](#).

8.9.2.23 setgridpt

```
int setgridpt
```

Definition at line 138 of file [pbamparm.h](#).

8.9.2.24 setntraj

```
int setntraj
```

Definition at line 159 of file [pbamparm.h](#).

8.9.2.25 setpbcs

```
int setpbcs
```

Definition at line 127 of file [pbamparm.h](#).

8.9.2.26 setrandorient

```
int setrandorient
```

Definition at line 123 of file [pbamparm.h](#).

8.9.2.27 setrunname

```
int setrunname
```

Definition at line 120 of file [pbamparm.h](#).

8.9.2.28 setruntype

```
int setruntype
```

Definition at line 116 of file [pbamparm.h](#).

8.9.2.29 setsalt

```
int setsalt
```

Definition at line 112 of file [pbamparm.h](#).

8.9.2.30 setterm

```
int setterm
```

Definition at line 170 of file [pbamparm.h](#).

8.9.2.31 settermcombine

```
int settermcombine
```

Definition at line 162 of file [pbamparm.h](#).

8.9.2.32 setunits

```
int setunits
```

Definition at line 131 of file [pbamparm.h](#).

8.9.2.33 setxyz

```
int setxyz
```

Definition at line 179 of file [pbamparm.h](#).

8.9.2.34 termcombine

```
char termcombine[CHR_MAXLEN]
```

Definition at line 161 of file [pbamparm.h](#).

8.9.2.35 termct

```
int termct
```

Definition at line 169 of file [pbamparm.h](#).

8.9.2.36 termnam

```
char termnam[PBAMPARM_MAXWRITE][CHR_MAXLEN]
```

Definition at line 172 of file [pbamparm.h](#).

8.9.2.37 termnu

```
int termnu[PBAMPARM_MAXWRITE][1]
```

Definition at line 173 of file [pbamparm.h](#).

8.9.2.38 termVal

```
double termVal[PBAMPARM_MAXWRITE]
```

Definition at line 174 of file [pbamparm.h](#).

8.9.2.39 transDiff

```
double transDiff[PBAMPARM_MAXMOL]
```

Definition at line 166 of file [pbamparm.h](#).

8.9.2.40 type

[PBAMparm_CalcType](#) type

What type of PBAM calculation?

Definition at line 107 of file [pbamparm.h](#).

8.9.2.41 units

```
char units[CHR_MAXLEN]
```

Definition at line 130 of file [pbamparm.h](#).

8.9.2.42 xyzct

```
int xyzct[PBAMPARM_MAXMOL]
```

Definition at line 180 of file [pbamparm.h](#).

8.9.2.43 xyzfil

```
char xyzfil[PBAMPARM_MAXMOL][PBAMPARM_MAXWRITE][CHR_MAXLEN]
```

Definition at line 181 of file [pbamparm.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/pbamparm.h](#)

8.10 sPBEParm Struct Reference

Parameter structure for PBE variables from input files.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/pbeparm.h>
```

Data Fields

- int [molid](#)
- int [setmolid](#)
- int [useDielMap](#)
- int [dielMapID](#)
- int [useKappaMap](#)
- int [kappaMapID](#)
- int [usePotMap](#)
- int [potMapID](#)
- int [useChargeMap](#)
- int [chargeMapID](#)
- [Vhal_PBEType](#) [pbetype](#)
- int [setpbetype](#)
- [Vbcfl](#) [bcfl](#)
- int [setbcfl](#)
- int [nion](#)
- int [setnion](#)
- double [ionq](#) [[MAXION](#)]
- double [ionc](#) [[MAXION](#)]
- double [ionr](#) [[MAXION](#)]
- int [setion](#) [[MAXION](#)]
- double [pdie](#)
- int [setpdie](#)
- double [sdens](#)
- int [setsdens](#)
- double [sdie](#)
- int [setsdie](#)

- [Vsurf_Meth srfm](#)
- int [setsrfm](#)
- double [srad](#)
- int [setsrad](#)
- double [swin](#)
- int [setswin](#)
- double [temp](#)
- int [settemp](#)
- double [smsize](#)
- int [setsmsize](#)
- double [smvolume](#)
- int [setsmvolume](#)
- [PBEparm_calcEnergy calcenergy](#)
- int [setcalcenergy](#)
- [PBEparm_calcForce calcforce](#)
- int [setcalcforce](#)
- double [zmem](#)
- int [setzmem](#)
- double [Lmem](#)
- int [setLmem](#)
- double [mdie](#)
- int [setmdie](#)
- double [memv](#)
- int [setmemv](#)
- int [numwrite](#)
- char [writestem](#) [PBEPARM_MAXWRITE][VMAX_ARGLEN]
- [Vdata_Type writetype](#) [PBEPARM_MAXWRITE]
- [Vdata_Format writefmt](#) [PBEPARM_MAXWRITE]
- int [writemat](#)
- int [setwritemat](#)
- char [writematstem](#) [VMAX_ARGLEN]
- int [writematflag](#)
- char [pbam_3dmapstem](#) [VMAX_ARGLEN]
- int [pbam_3dmapflag](#)
- int [parsed](#)

8.10.1 Detailed Description

Parameter structure for PBE variables from input files.

Author

Nathan Baker

Note

If you add/delete/change something in this class, the member functions – especially `PBEparm_copy` – must be modified accordingly

Definition at line 117 of file [pbeparm.h](#).

8.10.2 Field Documentation

8.10.2.1 bcf1

`Vbcf1 bcf1`

Boundary condition method

Definition at line 136 of file [pbeparm.h](#).

8.10.2.2 calcenergy

`PBEparm_calcEnergy calcenergy`

Energy calculation flag

Definition at line 165 of file [pbeparm.h](#).

8.10.2.3 calcforce

`PBEparm_calcForce calcforce`

Atomic forces calculation

Definition at line 167 of file [pbeparm.h](#).

8.10.2.4 chargeMapID

`int chargeMapID`

Charge distribution map ID (if used)

Definition at line 133 of file [pbeparm.h](#).

8.10.2.5 dielMapID

`int dielMapID`

Dielectric map ID (if used)

Definition at line 123 of file [pbeparm.h](#).

8.10.2.6 ionc

`double ionc[MAXION]`

Counterion concentrations (in M)

Definition at line 141 of file [pbeparm.h](#).

8.10.2.7 ionq

`double ionq[MAXION]`

Counterion charges (in e)

Definition at line 140 of file [pbeparm.h](#).

8.10.2.8 ionr

`double ionr[MAXION]`

Counterion radii (in Å)

Definition at line 142 of file [pbeparm.h](#).

8.10.2.9 kappaMapID

`int kappaMapID`

Kappa map ID (if used)

Definition at line 126 of file [pbeparm.h](#).

8.10.2.10 Lmem

`double Lmem`

membrane width

Definition at line 176 of file [pbeparm.h](#).

8.10.2.11 mdie

`double mdie`

membrane dielectric constant

Definition at line 178 of file [pbeparm.h](#).

8.10.2.12 memv

`double memv`

Membrane potential

Definition at line 180 of file [pbeparm.h](#).

8.10.2.13 molid

`int molid`

Molecule ID to perform calculation on

Definition at line 119 of file [pbeparm.h](#).

8.10.2.14 nion

`int nion`

Number of counterion species

Definition at line 138 of file [pbeparm.h](#).

8.10.2.15 numwrite

`int numwrite`

Number of write statements encountered

Definition at line 185 of file [pbeparm.h](#).

8.10.2.16 parsed

`int parsed`

Has this been filled with anything other than the default values?

Definition at line 205 of file [pbeparm.h](#).

8.10.2.17 pbam_3dmapflag

```
int pbam_3dmapflag
```

Definition at line 203 of file [pbeparm.h](#).

8.10.2.18 pbam_3dmapstem

```
char pbam_3dmapstem[VMAX_ARGLEN]
```

Definition at line 202 of file [pbeparm.h](#).

8.10.2.19 pbetype

```
Vhal_PBEType pbetype
```

Which version of the PBE are we solving?

Definition at line 134 of file [pbeparm.h](#).

8.10.2.20 pdie

```
double pdie
```

Solute dielectric

Definition at line 144 of file [pbeparm.h](#).

8.10.2.21 potMapID

```
int potMapID
```

Kappa map ID (if used)

Definition at line 129 of file [pbeparm.h](#).

8.10.2.22 sdens

```
double sdens
```

Vacc sphere density

Definition at line 146 of file [pbeparm.h](#).

8.10.2.23 sdie

```
double sdie
```

Solvent dielectric

Definition at line 148 of file [pbeparm.h](#).

8.10.2.24 setbcfl

```
int setbcfl
```

Flag,

See also

[bcfl](#)

Definition at line 137 of file [pbeparm.h](#).

8.10.2.25 setcalcenergy

```
int setcalcenergy
```

Flag,

See also

[calcenergy](#)

Definition at line 166 of file [pbeparm.h](#).

8.10.2.26 setcalcforce

```
int setcalcforce
```

Flag,

See also

[calcforce](#)

Definition at line 168 of file [pbeparm.h](#).

8.10.2.27 setion

```
int setion[MAXION]
```

Flag,

See also

[ionq](#)

Definition at line 143 of file [pbeparm.h](#).

8.10.2.28 setLmem

```
int setLmem
```

Flag

Definition at line 177 of file [pbeparm.h](#).

8.10.2.29 setmdie

```
int setmdie
```

Flag

Definition at line 179 of file [pbeparm.h](#).

8.10.2.30 setmemv

```
int setmemv
```

Flag

Definition at line 181 of file [pbeparm.h](#).

8.10.2.31 setmolid

```
int setmolid
```

Flag,

See also

[molid](#)

Definition at line 120 of file [pbeparm.h](#).

8.10.2.32 setnion

```
int setnion
```

Flag,

See also

[nion](#)

Definition at line 139 of file [pbeparm.h](#).

8.10.2.33 setpbetype

```
int setpbetype
```

Flag,

See also

[pbetype](#)

Definition at line 135 of file [pbeparm.h](#).

8.10.2.34 setpdie

```
int setpdie
```

Flag,

See also

[pdie](#)

Definition at line 145 of file [pbeparm.h](#).

8.10.2.35 setsdens

```
int setsdens
```

Flag,

See also

[sdens](#)

Definition at line 147 of file [pbeparm.h](#).

8.10.2.36 setsdie

```
int setsdie
Flag,
```

See also

[sdie](#)

Definition at line 149 of file [pbeparm.h](#).

8.10.2.37 setssize

```
int setssize
Flag,
```

See also

[temp](#)

Definition at line 160 of file [pbeparm.h](#).

8.10.2.38 setsmvolume

```
int setsmvolume
Flag,
```

See also

[temp](#)

Definition at line 163 of file [pbeparm.h](#).

8.10.2.39 setsrad

```
int setsrad
Flag,
```

See also

[srad](#)

Definition at line 153 of file [pbeparm.h](#).

8.10.2.40 setsrfm

```
int setsrfm
Flag,
```

See also

[srfm](#)

Definition at line 151 of file [pbeparm.h](#).

8.10.2.41 setswin

```
int setswin
```

Flag,

See also

[swin](#)

Definition at line 155 of file [pbeparm.h](#).

8.10.2.42 settemp

```
int settemp
```

Flag,

See also

[temp](#)

Definition at line 157 of file [pbeparm.h](#).

8.10.2.43 setwritemat

```
int setwritemat
```

Flag,

See also

[writemat](#)

Definition at line 194 of file [pbeparm.h](#).

8.10.2.44 setzmem

```
int setzmem
```

Flag

Definition at line 175 of file [pbeparm.h](#).

8.10.2.45 smsize

```
double smsize
```

SMPBE size

Definition at line 159 of file [pbeparm.h](#).

8.10.2.46 smvolume

```
double smvolume
```

SMPBE size

Definition at line 162 of file [pbeparm.h](#).

8.10.2.47 srad

`double srad`

Solvent radius

Definition at line 152 of file [pbeparm.h](#).

8.10.2.48 srfm

`Vsurf_Meth srfm`

Surface calculation method

Definition at line 150 of file [pbeparm.h](#).

8.10.2.49 swin

`double swin`

Cubic spline window

Definition at line 154 of file [pbeparm.h](#).

8.10.2.50 temp

`double temp`

Temperature (in K)

Definition at line 156 of file [pbeparm.h](#).

8.10.2.51 useChargeMap

`int useChargeMap`

Indicates whether we use an external charge distribution map

Definition at line 131 of file [pbeparm.h](#).

8.10.2.52 useDielMap

`int useDielMap`

Indicates whether we use external dielectric maps (note plural)

Definition at line 121 of file [pbeparm.h](#).

8.10.2.53 useKappaMap

`int useKappaMap`

Indicates whether we use an external kappa map

Definition at line 124 of file [pbeparm.h](#).

8.10.2.54 usePotMap

`int usePotMap`

Indicates whether we use an external kappa map

Definition at line 127 of file [pbeparm.h](#).

8.10.2.55 writelfmt

`Vdata_Format writelfmt[PBE Parm_MAXWRITE]`

File format to write data in

Definition at line 189 of file [pbeparm.h](#).

8.10.2.56 writemat

`int writemat`

Write out the operator matrix?

- 0 => no
- 1 => yes

Definition at line 191 of file [pbeparm.h](#).

8.10.2.57 writematflag

`int writematflag`

What matrix should we write:

- 0 => Poisson (differential operator)
- 1 => Poisson-Boltzmann operator linearized around solution (if applicable)

Definition at line 196 of file [pbeparm.h](#).

8.10.2.58 writematstem

`char writematstem[VMAX_ARGLEN]`

File stem to write mat

Definition at line 195 of file [pbeparm.h](#).

8.10.2.59 writestem

`char writestem[PBE Parm_MAXWRITE][VMAX_ARGLEN]`

File stem to write data to

Definition at line 186 of file [pbeparm.h](#).

8.10.2.60 writetype

`Vdata_Type writetype[PBE Parm_MAXWRITE]`

What data to write

Definition at line 188 of file [pbeparm.h](#).

8.10.2.61 zmem

`double zmem`

z value of membrane bottom

Definition at line 174 of file [pbeparm.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/pbeparm.h](#)

8.11 sPBSAMparm Struct Reference

Parameter structure for PBSAM-specific variables from input files.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/pbsamparm.h>
```

Data Fields

- [PBSAMparm_CalcType](#) type
- int [parsed](#)
- int [settolsp](#)
- double [tolsp](#)
- int [setmsms](#)
- double [probe_radius](#)
- double [density](#)
- int [setsurf](#)
- int [surfct](#)
- char [surffil](#) [PBSAMPARM_MAXMOL][[CHR_MAXLEN](#)]
- int [setimat](#)
- int [imatct](#)
- char [imatfil](#) [PBSAMPARM_MAXMOL][[CHR_MAXLEN](#)]
- int [setexp](#)
- int [expct](#)
- char [expfil](#) [PBSAMPARM_MAXMOL][[CHR_MAXLEN](#)]

8.11.1 Detailed Description

Parameter structure for PBSAM-specific variables from input files.

Author

Lisa Felberg

Note

If you add/delete/change something in this class, the member functions – especially `PBSAMparm_copy` – must be modified accordingly

Definition at line [105](#) of file [pbsamparm.h](#).

8.11.2 Field Documentation

8.11.2.1 density

```
double density
```

Definition at line [117](#) of file [pbsamparm.h](#).

8.11.2.2 expct

```
int expct
```

Definition at line [128](#) of file [pbsamparm.h](#).

8.11.2.3 expfil

```
char expfil[PBSAMPARM_MAXMOL][CHR_MAXLEN]
```

Definition at line 129 of file [pbsamparm.h](#).

8.11.2.4 imatct

```
int imatct
```

Definition at line 124 of file [pbsamparm.h](#).

8.11.2.5 imatfil

```
char imatfil[PBSAMPARM_MAXMOL][CHR_MAXLEN]
```

Definition at line 125 of file [pbsamparm.h](#).

8.11.2.6 parsed

```
int parsed
```

Has this structure been filled? (0 = no, 1 = yes)

Definition at line 108 of file [pbsamparm.h](#).

8.11.2.7 probe_radius

```
double probe_radius
```

Definition at line 116 of file [pbsamparm.h](#).

8.11.2.8 setexp

```
int setexp
```

Definition at line 127 of file [pbsamparm.h](#).

8.11.2.9 setimat

```
int setimat
```

Definition at line 123 of file [pbsamparm.h](#).

8.11.2.10 setmsms

```
int setmsms
```

Definition at line 115 of file [pbsamparm.h](#).

8.11.2.11 setsurf

```
int setsurf
```

Definition at line 119 of file [pbsamparm.h](#).

8.11.2.12 settolsp

```
int settolsp
```

Definition at line 112 of file [pbsamparm.h](#).

8.11.2.13 surfct

```
int surfct
```

Definition at line 120 of file [pbsamparm.h](#).

8.11.2.14 surffil

```
char surffil[PBSAMPARM_MAXMOL][CHR_MAXLEN]
```

Definition at line 121 of file [pbsamparm.h](#).

8.11.2.15 tolspace

```
double tolspace
```

Definition at line 113 of file [pbsamparm.h](#).

8.11.2.16 type

```
PBSAMParm_CalcType type
```

What type of PBSAM calculation?

Definition at line 107 of file [pbsamparm.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/pbsamparm.h](#)

8.12 sVacc Struct Reference

Oracle for solvent- and ion-accessibility around a biomolecule.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/vacc.h>
```

Data Fields

- Vmem * [mem](#)
- Valist * [alist](#)
- Vclist * [clist](#)
- int * [atomFlags](#)
- VaccSurf * [refSphere](#)
- VaccSurf ** [surf](#)
- Vset [acc](#)
- double [surf_density](#)

8.12.1 Detailed Description

Oracle for solvent- and ion-accessibility around a biomolecule.

Author

Nathan Baker

Definition at line 108 of file [vacc.h](#).

8.12.2 Field Documentation**8.12.2.1 acc**

```
Vset acc
```

An integer array (to be treated as bitfields) of Vset type with length equal to the number of vertices in the mesh

Definition at line 120 of file [vacc.h](#).

8.12.2.2 alist

```
Valist* alist
```

Valist structure for list of atoms

Definition at line 111 of file [vacc.h](#).

8.12.2.3 atomFlags

```
int* atomFlags
```

Array of boolean flags of length `Valist_getNumberAtoms(thee->alist)` to prevent double-counting atoms during calculations

Definition at line 113 of file [vacc.h](#).

8.12.2.4 clist

```
Vclist* clist
```

Vclist structure for atom cell list

Definition at line 112 of file [vacc.h](#).

8.12.2.5 mem

```
Vmem* mem
```

Memory management object for this class

Definition at line 110 of file [vacc.h](#).

8.12.2.6 refSphere

```
VaccSurf* refSphere
```

Reference sphere for SASA calculations

Definition at line 116 of file [vacc.h](#).

8.12.2.7 surf

`VaccSurf** surf`

Array of surface points for each atom; is not initialized until needed (test against VNULL to determine initialization state)
Definition at line 117 of file [vacc.h](#).

8.12.2.8 surf_density

`double surf_density`

Minimum solvent accessible surface point density (in pts/A²)

Definition at line 122 of file [vacc.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/vacc.h](#)

8.13 sVaccSurf Struct Reference

Surface object list of per-atom surface points.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/vacc.h>
```

Data Fields

- `Vmem * mem`
- `double * xpts`
- `double * ypts`
- `double * zpts`
- `char * bpts`
- `double area`
- `int npts`
- `double probe_radius`

8.13.1 Detailed Description

Surface object list of per-atom surface points.

Author

Nathan Baker

Definition at line 84 of file [vacc.h](#).

8.13.2 Field Documentation

8.13.2.1 area

`double area`

Area spanned by these points

Definition at line 91 of file [vacc.h](#).

8.13.2.2 bpts

`char* bpts`

Array of booleans indicating whether a point is (1) or is not (0) part of the surface

Definition at line 89 of file [vacc.h](#).

8.13.2.3 mem

`Vmem* mem`

Memory object

Definition at line 85 of file [vacc.h](#).

8.13.2.4 npts

`int npts`

Length of the->xpts, ypts, zpts arrays

Definition at line 92 of file [vacc.h](#).

8.13.2.5 probe_radius

`double probe_radius`

Probe radius (A) with which this surface was constructed

Definition at line 93 of file [vacc.h](#).

8.13.2.6 xpts

`double* xpts`

Array of point x-locations

Definition at line 86 of file [vacc.h](#).

8.13.2.7 ypts

`double* ypts`

Array of point y-locations

Definition at line 87 of file [vacc.h](#).

8.13.2.8 zpts

`double* zpts`

Array of point z-locations

Definition at line 88 of file [vacc.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/vacc.h](#)

8.14 sValist Struct Reference

Container class for list of atom objects.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/valist.h>
```

Data Fields

- int [number](#)
- double [center](#) [3]
- double [mincrd](#) [3]
- double [maxcrd](#) [3]
- double [maxrad](#)
- double [charge](#)
- [Vatom](#) * [atoms](#)
- Vmem * [vmem](#)

8.14.1 Detailed Description

Container class for list of atom objects.

Author

Nathan Baker

Definition at line [78](#) of file [valist.h](#).

8.14.2 Field Documentation

8.14.2.1 atoms

[Vatom](#)* [atoms](#)

Atom list

Definition at line [86](#) of file [valist.h](#).

8.14.2.2 center

double [center](#)[3]

Molecule center (xmin - xmax)/2, etc.

Definition at line [81](#) of file [valist.h](#).

8.14.2.3 charge

double [charge](#)

Net charge

Definition at line [85](#) of file [valist.h](#).

8.14.2.4 maxcrd

double [maxcrd](#)[3]

Maximum coordinates

Definition at line [83](#) of file [valist.h](#).

8.14.2.5 maxrad

double maxrad

Maximum radius

Definition at line 84 of file [valist.h](#).

8.14.2.6 mincrd

double mincrd[3]

Minimum coordinates

Definition at line 82 of file [valist.h](#).

8.14.2.7 number

int number

Number of atoms in list

Definition at line 80 of file [valist.h](#).

8.14.2.8 vmem

Vmem* vmem

Memory management object

Definition at line 87 of file [valist.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/valist.h](#)

8.15 sVatom Struct Reference

Contains public data members for Vatom class/module.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/vatom.h>
```

Data Fields

- double [position](#) [3]
- double [radius](#)
- double [charge](#)
- double [partID](#)
- double [epsilon](#)
- int [id](#)
- char [resName](#) [VMAX_RECLEN]
- char [atomName](#) [VMAX_RECLEN]

8.15.1 Detailed Description

Contains public data members for Vatom class/module.

Author

Nathan Baker, David Gohara, Mike Schneiders

Definition at line 84 of file [vatom.h](#).

8.15.2 Field Documentation

8.15.2.1 atomName

```
char atomName[VMAX_RECLEN]
```

Atom name from PDB/PDR file

Definition at line 98 of file [vatom.h](#).

8.15.2.2 charge

```
double charge
```

Atomic charge

Definition at line 88 of file [vatom.h](#).

8.15.2.3 epsilon

```
double epsilon
```

Epsilon value for WCA calculations

Definition at line 91 of file [vatom.h](#).

8.15.2.4 id

```
int id
```

Atomic ID; this should be a unique non-negative integer assigned based on the index of the atom in a Valist atom array

Definition at line 93 of file [vatom.h](#).

8.15.2.5 partID

```
double partID
```

Partition value for assigning atoms to particular processors and/or partitions

Definition at line 89 of file [vatom.h](#).

8.15.2.6 position

```
double position[3]
```

Atomic position

Definition at line 86 of file [vatom.h](#).

8.15.2.7 radius

```
double radius
```

Atomic radius

Definition at line 87 of file [vatom.h](#).

8.15.2.8 resName

```
char resName[VMAX_RECLEN]
```

Residue name from PDB/PQR file

Definition at line 97 of file [vatom.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/vatom.h](#)

8.16 sVclist Struct Reference

Atom cell list.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/vclist.h>
```

Data Fields

- Vmem * [vmem](#)
- Valist * [alist](#)
- Vclist_DomainMode [mode](#)
- int [npts](#) [VAPBS_DIM]
- int [n](#)
- double [max_radius](#)
- VclistCell * [cells](#)
- double [lower_corner](#) [VAPBS_DIM]
- double [upper_corner](#) [VAPBS_DIM]
- double [spacs](#) [VAPBS_DIM]

8.16.1 Detailed Description

Atom cell list.

Author

Nathan Baker

Definition at line 117 of file [vclist.h](#).

8.16.2 Field Documentation

8.16.2.1 alist

```
Valist* alist
```

Original Valist structure for list of atoms

Definition at line 120 of file [vclist.h](#).

8.16.2.2 cells

```
VclistCell* cells
```

Cell array of length thee->n

Definition at line 125 of file [vclist.h](#).

8.16.2.3 lower_corner

```
double lower_corner[VAPBS_DIM]
```

Hash table grid corner

Definition at line 126 of file [vclist.h](#).

8.16.2.4 max_radius

```
double max_radius
```

Maximum probe radius

Definition at line 124 of file [vclist.h](#).

8.16.2.5 mode

```
Vclist_DomainMode mode
```

How the cell list was constructed

Definition at line 121 of file [vclist.h](#).

8.16.2.6 n

```
int n
```

```
n = nx*nz*ny
```

Definition at line 123 of file [vclist.h](#).

8.16.2.7 npts

```
int npts[VAPBS_DIM]
```

Hash table grid dimensions

Definition at line 122 of file [vclist.h](#).

8.16.2.8 spacs

```
double spacs[VAPBS_DIM]
```

Hash table grid spacings

Definition at line 128 of file [vclist.h](#).

8.16.2.9 upper_corner

```
double upper_corner[VAPBS_DIM]
```

Hash table grid corner

Definition at line 127 of file [vclist.h](#).

8.16.2.10 vmem

```
Vmem* vmem
```

Memory management object for this class

Definition at line 119 of file [vclist.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/vclist.h](#)

8.17 sVclistCell Struct Reference

Atom cell list cell.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/vclist.h>
```

Data Fields

- [Vatom](#) ** [atoms](#)
- int [natoms](#)

8.17.1 Detailed Description

Atom cell list cell.

Author

Nathan Baker

Definition at line 101 of file [vclist.h](#).

8.17.2 Field Documentation

8.17.2.1 atoms

[Vatom](#)** [atoms](#)

Array of atom objects associated with this cell

Definition at line 102 of file [vclist.h](#).

8.17.2.2 natoms

int [natoms](#)

Length of thee->atoms array

Definition at line 103 of file [vclist.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/vclist.h](#)

8.18 sVcsm Struct Reference

Charge-simplex map class.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/fem/vcsm.h>
```

Data Fields

- [Valist](#) * [alist](#)
- int [natom](#)
- Gem * [gm](#)
- int ** [sqm](#)
- int * [nsqm](#)
- int [nsimp](#)
- int [msimp](#)
- int ** [qsm](#)

- int * [nqsm](#)
- int [initFlag](#)
- Vmem * [vmem](#)

8.18.1 Detailed Description

Charge-simplex map class.

Author

Nathan Baker

Definition at line [89](#) of file [vcsn.h](#).

8.18.2 Field Documentation

8.18.2.1 alist

[Valist](#)* [alist](#)

Atom (charge) list

Definition at line [91](#) of file [vcsn.h](#).

8.18.2.2 gm

[Gem](#)* [gm](#)

Grid manager (container class for master vertex and simplex lists as well as prolongation operator for updating after refinement)

Definition at line [94](#) of file [vcsn.h](#).

8.18.2.3 initFlag

int [initFlag](#)

Indicates whether the maps have been initialized yet

Definition at line [112](#) of file [vcsn.h](#).

8.18.2.4 msimp

int [msimp](#)

The maximum number of entries that can be accomodated by sqm or nsqm – saves on realloc's

Definition at line [107](#) of file [vcsn.h](#).

8.18.2.5 natom

int [natom](#)

Size of thee->alist; redundant, but useful for convenience

Definition at line [92](#) of file [vcsn.h](#).

8.18.2.6 nqsm

```
int* nqsm
```

The length of the simplex lists in `thee->qsm`

Definition at line 111 of file [vcsn.h](#).

8.18.2.7 nsimp

```
int nsimp
```

The `_currently` used) length of `sqm`, `nsqm` – may not always be up-to-date with `Gem`

Definition at line 105 of file [vcsn.h](#).

8.18.2.8 nsqm

```
int* nsqm
```

The length of the charge lists in `thee->sqm`

Definition at line 104 of file [vcsn.h](#).

8.18.2.9 qsm

```
int** qsm
```

The inverse of `sqm`; the list of simplices associated with a given charge

Definition at line 109 of file [vcsn.h](#).

8.18.2.10 sqm

```
int** sqm
```

The map which gives the list charges associated with each simplex in `gm->simplices`. The indices of the first dimension are associated with the simplex ID's in `Vgm`. Each charge list (second dimension) contains entries corresponding to indices in `thee->alist` with lengths given in `thee->nsqm`

Definition at line 97 of file [vcsn.h](#).

8.18.2.11 vmem

```
Vmem* vmem
```

Memory management object

Definition at line 114 of file [vcsn.h](#).

The documentation for this struct was generated from the following file:

- `src/fem/vcsn.h`

8.19 sVfetk Struct Reference

Contains public data members for `Vfetk` class/module.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/fem/vfetk.h>
```

Data Fields

- `Vmem` * [vmem](#)
- `Gem` * [gm](#)

- AM * [am](#)
- Aprx * [aprx](#)
- PDE * [pde](#)
- Vpbe * [pbe](#)
- Vcsm * [csm](#)
- Vfetk_LsolvType lkey
- int lmax
- double ltol
- Vfetk_NsolvType nkey
- int nmax
- double ntol
- Vfetk_GuessType gues
- Vfetk_PrecType lprec
- int pjac
- PBEparm * [pbeparm](#)
- FEMparm * [feparm](#)
- Vhal_PBEType type
- int level

8.19.1 Detailed Description

Contains public data members for Vfetk class/module.

Author

Nathan Baker

Many of the routines and macros are borrowed from the [main.c](#) driver (written by Mike Holst) provided with the PMG code.

Definition at line [176](#) of file [vfetk.h](#).

8.19.2 Field Documentation

8.19.2.1 am

AM* [am](#)

Multilevel algebra manager.

Definition at line [182](#) of file [vfetk.h](#).

8.19.2.2 aprx

Aprx* [aprx](#)

Approximation manager.

Definition at line [183](#) of file [vfetk.h](#).

8.19.2.3 csm

Vcsm* [csm](#)

Charge-simplex map

Definition at line [186](#) of file [vfetk.h](#).

8.19.2.4 feparm

`FEMparm*` feparm

FEM-specific parameters

Definition at line 198 of file [vfetk.h](#).

8.19.2.5 gm

`Gem*` gm

Grid manager (container class for master vertex and simplex lists as well as prolongation operator for updating after refinement).

Definition at line 179 of file [vfetk.h](#).

8.19.2.6 gues

`Vfetk_GuessType` gues

Initial guess method

Definition at line 193 of file [vfetk.h](#).

8.19.2.7 level

`int` level

Refinement level (starts at 0)

Definition at line 200 of file [vfetk.h](#).

8.19.2.8 lkey

`Vfetk_LsolvType` lkey

Linear solver method

Definition at line 187 of file [vfetk.h](#).

8.19.2.9 lmax

`int` lmax

Maximum number of linear solver iterations

Definition at line 188 of file [vfetk.h](#).

8.19.2.10 lprec

`Vfetk_PrecType` lprec

Linear preconditioner

Definition at line 194 of file [vfetk.h](#).

8.19.2.11 ltol

`double` ltol

Residual tolerance for linear solver

Definition at line 189 of file [vfetk.h](#).

8.19.2.12 nkey

[Vfetk_NsolvType](#) nkey

Nonlinear solver method

Definition at line 190 of file [vfetk.h](#).

8.19.2.13 nmax

int nmax

Maximum number of nonlinear solver iterations

Definition at line 191 of file [vfetk.h](#).

8.19.2.14 ntol

double ntol

Residual tolerance for nonlinear solver

Definition at line 192 of file [vfetk.h](#).

8.19.2.15 pbe

[Vpbe*](#) pbe

Poisson-Boltzmann object

Definition at line 185 of file [vfetk.h](#).

8.19.2.16 pbeparm

[PBEparm*](#) pbeparm

Generic PB parameters

Definition at line 197 of file [vfetk.h](#).

8.19.2.17 pde

[PDE*](#) pde

FEtk PDE object

Definition at line 184 of file [vfetk.h](#).

8.19.2.18 pjac

int pjac

Flag to print the jacobians (usually set this to -1, please)

Definition at line 195 of file [vfetk.h](#).

8.19.2.19 type

[Vhal_PBEType](#) type

Version of PBE to solve

Definition at line 199 of file [vfetk.h](#).

8.19.2.20 vmem

Vmem* vmem

Memory management object

Definition at line 178 of file [vfetk.h](#).

The documentation for this struct was generated from the following file:

- [src/fem/vfetk.h](#)

8.20 sVfetk_LocalVar Struct Reference

Vfetk LocalVar subclass.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/fem/vfetk.h>
```

Data Fields

- double [nvec](#) [[VAPBS_DIM](#)]
- double [vx](#) [4][[VAPBS_DIM](#)]
- double [xq](#) [[VAPBS_DIM](#)]
- double [U](#) [[MAXV](#)]
- double [dU](#) [[MAXV](#)][[VAPBS_DIM](#)]
- double [W](#)
- double [dW](#) [[VAPBS_DIM](#)]
- double [d2W](#)
- int [sType](#)
- int [fType](#)
- double [A](#)
- double [F](#)
- double [B](#)
- double [DB](#)
- double [jumpDiel](#)
- [Vfetk](#) * [fetk](#)
- [Vgreen](#) * [green](#)
- int [initGreen](#)
- [SS](#) * [simp](#)
- [VV](#) * [verts](#) [4]
- int [nverts](#)
- double [ionConc](#) [[MAXION](#)]
- double [ionQ](#) [[MAXION](#)]
- double [ionRadii](#) [[MAXION](#)]
- double [zkappa2](#)
- double [zks2](#)
- double [ionstr](#)
- int [nion](#)
- double [Fu_v](#)
- double [DFu_wv](#)
- double [delta](#)
- double [u_D](#)
- double [u_T](#)

8.20.1 Detailed Description

Vfetk LocalVar subclass.

Author

Nathan Baker

Contains variables used when solving the PDE with FEtk
Definition at line 215 of file [vfetk.h](#).

8.20.2 Field Documentation

8.20.2.1 A

double A
Second-order differential term
Definition at line 228 of file [vfetk.h](#).

8.20.2.2 B

double B
Entire ionic strength term
Definition at line 230 of file [vfetk.h](#).

8.20.2.3 d2W

double d2W
Coulomb regularization term Laplacia
Definition at line 223 of file [vfetk.h](#).

8.20.2.4 DB

double DB
Entire ionic strength term derivative
Definition at line 231 of file [vfetk.h](#).

8.20.2.5 delta

double delta
Store delta value
Definition at line 250 of file [vfetk.h](#).

8.20.2.6 DFu_wv

double DFu_wv
Store DFu_wv value
Definition at line 249 of file [vfetk.h](#).

8.20.2.7 dU

```
double dU[MAXV][VAPBS_DIM]
```

Solution gradient

Definition at line 220 of file [vfetk.h](#).

8.20.2.8 dW

```
double dW[VAPBS_DIM]
```

Coulomb regularization term gradient

Definition at line 222 of file [vfetk.h](#).

8.20.2.9 F

```
double F
```

RHS characteristic function value

Definition at line 229 of file [vfetk.h](#).

8.20.2.10 fetk

```
Vfetk* fetk
```

Pointer to the VFETK object

Definition at line 233 of file [vfetk.h](#).

8.20.2.11 fType

```
int fType
```

Face type

Definition at line 225 of file [vfetk.h](#).

8.20.2.12 Fu_v

```
double Fu_v
```

Store Fu_v value

Definition at line 248 of file [vfetk.h](#).

8.20.2.13 green

```
Vgreen* green
```

Pointer to a Green's function object

Definition at line 234 of file [vfetk.h](#).

8.20.2.14 initGreen

```
int initGreen
```

Boolean to designate whether Green's function has been initialized

Definition at line 235 of file [vfetk.h](#).

8.20.2.15 ionConc

```
double ionConc[MAXION]
```

Counterion species' concentrations

Definition at line 241 of file [vfetk.h](#).

8.20.2.16 ionQ

```
double ionQ[MAXION]
```

Counterion species' valencies

Definition at line 242 of file [vfetk.h](#).

8.20.2.17 ionRadii

```
double ionRadii[MAXION]
```

Counterion species' radii

Definition at line 243 of file [vfetk.h](#).

8.20.2.18 ionstr

```
double ionstr
```

Ionic strength parameters (M)

Definition at line 246 of file [vfetk.h](#).

8.20.2.19 jumpDiel

```
double jumpDiel
```

Dielectric value on one side of a simplex face

Definition at line 232 of file [vfetk.h](#).

8.20.2.20 nion

```
int nion
```

Number of ion species

Definition at line 247 of file [vfetk.h](#).

8.20.2.21 nvec

```
double nvec[VAPBS_DIM]
```

Normal vector for a simplex face

Definition at line 216 of file [vfetk.h](#).

8.20.2.22 nverts

```
int nverts
```

number of vertices in the simplex

Definition at line 240 of file [vfetk.h](#).

8.20.2.23 simp

SS* simp

Pointer to the latest simplex object; set in `initElement()` and `delta()`

Definition at line 237 of file [vfetk.h](#).

8.20.2.24 sType

int sType

Simplex type

Definition at line 224 of file [vfetk.h](#).

8.20.2.25 U

double U[MAXV]

Solution value

Definition at line 219 of file [vfetk.h](#).

8.20.2.26 u_D

double u_D

Store Dirichlet value

Definition at line 251 of file [vfetk.h](#).

8.20.2.27 u_T

double u_T

Store true value

Definition at line 252 of file [vfetk.h](#).

8.20.2.28 verts

VV* verts[4]

Pointer to the latest vertices; set in `initElement`

Definition at line 239 of file [vfetk.h](#).

8.20.2.29 vx

double vx[4][VAPBS_DIM]

Vertex coordinates

Definition at line 217 of file [vfetk.h](#).

8.20.2.30 W

double W

Coulomb regularization term scalar value

Definition at line 221 of file [vfetk.h](#).

8.20.2.31 xq

double xq[VAPBS_DIM]

Quadrature pt

Definition at line 218 of file [vfetk.h](#).

8.20.2.32 zkappa2

double zkappa2

Ionic strength parameters

Definition at line 244 of file [vfetk.h](#).

8.20.2.33 zks2

double zks2

Ionic strength parameters

Definition at line 245 of file [vfetk.h](#).

The documentation for this struct was generated from the following file:

- [src/fem/vfetk.h](#)

8.21 sVgreen Struct Reference

Contains public data members for Vgreen class/module.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/vgreen.h>
```

Data Fields

- [Valist](#) * [alist](#)
- [Vmem](#) * [vmem](#)
- double * [xp](#)
- double * [yp](#)
- double * [zp](#)
- double * [qp](#)
- int [np](#)

8.21.1 Detailed Description

Contains public data members for Vgreen class/module.

Author

Nathan Baker

Definition at line 82 of file [vgreen.h](#).

8.21.2 Field Documentation

8.21.2.1 alist

`Valist* alist`

Atom (charge) list for Green's function

Definition at line 84 of file [vgreen.h](#).

8.21.2.2 np

`int np`

Set to size of above arrays

Definition at line 94 of file [vgreen.h](#).

8.21.2.3 qp

`double* qp`

Array of particle charges for use with treecode routines

Definition at line 92 of file [vgreen.h](#).

8.21.2.4 vmem

`Vmem* vmem`

Memory management object

Definition at line 85 of file [vgreen.h](#).

8.21.2.5 xp

`double* xp`

Array of particle x-coordinates for use with treecode routines

Definition at line 86 of file [vgreen.h](#).

8.21.2.6 yp

`double* yp`

Array of particle y-coordinates for use with treecode routines

Definition at line 88 of file [vgreen.h](#).

8.21.2.7 zp

`double* zp`

Array of particle z-coordinates for use with treecode routines

Definition at line 90 of file [vgreen.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/vgreen.h](#)

8.22 sVgrid Struct Reference

Electrostatic potential oracle for Cartesian mesh data.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/mg/vgrid.h>
```

Data Fields

- int [nx](#)
- int [ny](#)
- int [nz](#)
- double [hx](#)
- double [hy](#)
- double [hzed](#)
- double [xmin](#)
- double [ymin](#)
- double [zmin](#)
- double [xmax](#)
- double [ymax](#)
- double [zmax](#)
- double * [data](#)
- int [readdata](#)
- int [ctordata](#)
- Vmem * [mem](#)

8.22.1 Detailed Description

Electrostatic potential oracle for Cartesian mesh data.

Author

Nathan Baker

Definition at line [81](#) of file [vgrid.h](#).

8.22.2 Field Documentation

8.22.2.1 ctordata

```
int ctordata
```

flag indicating whether data was included at construction

Definition at line [97](#) of file [vgrid.h](#).

8.22.2.2 data

```
double* data
```

$nx \times ny \times nz$ array of data

Definition at line [95](#) of file [vgrid.h](#).

8.22.2.3 hx

```
double hx
```

Grid spacing in x direction

Definition at line [86](#) of file [vgrid.h](#).

8.22.2.4 hy

`double hy`

Grid spacing in y direction

Definition at line 87 of file [vgrid.h](#).

8.22.2.5 hzed

`double hzed`

Grid spacing in z direction

Definition at line 88 of file [vgrid.h](#).

8.22.2.6 mem

`Vmem* mem`

Memory manager object

Definition at line 99 of file [vgrid.h](#).

8.22.2.7 nx

`int nx`

Number grid points in x direction

Definition at line 83 of file [vgrid.h](#).

8.22.2.8 ny

`int ny`

Number grid points in y direction

Definition at line 84 of file [vgrid.h](#).

8.22.2.9 nz

`int nz`

Number grid points in z direction

Definition at line 85 of file [vgrid.h](#).

8.22.2.10 readdata

`int readdata`

flag indicating whether data was read from file

Definition at line 96 of file [vgrid.h](#).

8.22.2.11 xmax

`double xmax`

x coordinate of upper grid corner

Definition at line 92 of file [vgrid.h](#).

8.22.2.12 xmin

double xmin
x coordinate of lower grid corner
Definition at line 89 of file [vgrid.h](#).

8.22.2.13 ymax

double ymax
y coordinate of upper grid corner
Definition at line 93 of file [vgrid.h](#).

8.22.2.14 ymin

double ymin
y coordinate of lower grid corner
Definition at line 90 of file [vgrid.h](#).

8.22.2.15 zmax

double zmax
z coordinate of upper grid corner
Definition at line 94 of file [vgrid.h](#).

8.22.2.16 zmin

double zmin
z coordinate of lower grid corner
Definition at line 91 of file [vgrid.h](#).
The documentation for this struct was generated from the following file:

- [src/mg/vgrid.h](#)

8.23 sVmgrid Struct Reference

Multiresolution oracle for Cartesian mesh data.
`#include </builddir/build/BUILD/apbs-3.0.0/src/mg/vmgrid.h>`

Data Fields

- int [n grids](#)
- [Vgrid](#) * [grids](#) [[VMGRIDMAX](#)]

8.23.1 Detailed Description

Multiresolution oracle for Cartesian mesh data.

Author

Nathan Baker

Definition at line 84 of file [vmgrid.h](#).

8.23.2 Field Documentation

8.23.2.1 grids

`Vgrid* grids[VMGRIDMAX]`

Grids in hierarchy. Our convention will be to have the finest grid first, however, this will not be enforced as it may be useful to search multiple grids for parallel datasets, etc.

Definition at line 87 of file [vmgrid.h](#).

8.23.2.2 ngrids

`int ngrids`

Number of grids in hierarchy

Definition at line 86 of file [vmgrid.h](#).

The documentation for this struct was generated from the following file:

- [src/mg/vmgrid.h](#)

8.24 sVopot Struct Reference

Electrostatic potential oracle for Cartesian mesh data.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/mg/vopot.h>
```

Data Fields

- `Vmgrid * mgrid`
- `Vpbe * pbe`
- `Vbcfl bcfl`

8.24.1 Detailed Description

Electrostatic potential oracle for Cartesian mesh data.

Author

Nathan Baker

Definition at line 83 of file [vopot.h](#).

8.24.2 Field Documentation

8.24.2.1 bcfl

`Vbcfl bcfl`

Boundary condition flag for returning potential values at points off the grid.

Definition at line 88 of file [vopot.h](#).

8.24.2.2 mgrid

`Vmgrid*` mgrid

Multiple grid object containing potential data (in units kT/e)

Definition at line 85 of file [vopot.h](#).

8.24.2.3 pbe

`Vpbe*` pbe

Pointer to PBE object

Definition at line 87 of file [vopot.h](#).

The documentation for this struct was generated from the following file:

- [src/mg/vopot.h](#)

8.25 sVparam_AtomData Struct Reference

AtomData sub-class; stores atom data.

`#include </builddir/build/BUILD/apbs-3.0.0/src/generic/vparam.h>`

Data Fields

- char [atomName](#) [VMAX_ARGLEN]
- char [resName](#) [VMAX_ARGLEN]
- double [charge](#)
- double [radius](#)
- double [epsilon](#)

8.25.1 Detailed Description

AtomData sub-class; stores atom data.

Author

Nathan Baker

Note

The epsilon and radius members of this class refer use the following formula for calculating the van der Waals energy of atom i interacting with atom j :

$$V_{ij}(r_{ij}) = \epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - 2 \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right]$$

where $\epsilon_{ij} = \sqrt{\epsilon_i \epsilon_j}$ is the well-depth (in the desired energy units), r_{ij} is the distance between atoms i and j , and $\sigma_{ij} = \sigma_i + \sigma_j$ is the sum of the van der Waals radii.

Definition at line 92 of file [vparam.h](#).

8.25.2 Field Documentation

8.25.2.1 atomName

```
char atomName[VMAX_ARGLEN]
```

Atom name

Definition at line 93 of file [vparam.h](#).

8.25.2.2 charge

```
double charge
```

Atom charge (in e)

Definition at line 95 of file [vparam.h](#).

8.25.2.3 epsilon

```
double epsilon
```

Atom VdW well depth (ϵ_i above; in kJ/mol)

Definition at line 97 of file [vparam.h](#).

8.25.2.4 radius

```
double radius
```

Atom VdW radius (σ_i above; in Å)

Definition at line 96 of file [vparam.h](#).

8.25.2.5 resName

```
char resName[VMAX_ARGLEN]
```

Residue name

Definition at line 94 of file [vparam.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/vparam.h](#)

8.26 sVpbe Struct Reference

Contains public data members for Vpbe class/module.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/vpbe.h>
```

Data Fields

- Vmem * [vmem](#)
- Valist * [alist](#)
- Vclist * [clist](#)
- Vacc * [acc](#)
- double [T](#)
- double [soluteDiel](#)
- double [solventDiel](#)
- double [solventRadius](#)
- double [bulkIonicStrength](#)
- double [maxIonRadius](#)

- int `numlon`
- double `ionConc` [`MAXION`]
- double `ionRadii` [`MAXION`]
- double `ionQ` [`MAXION`]
- double `xkappa`
- double `deblen`
- double `zkappa2`
- double `zmagic`
- double `soluteCenter` [3]
- double `soluteRadius`
- double `soluteXlen`
- double `soluteYlen`
- double `soluteZlen`
- double `soluteCharge`
- double `smvolume`
- double `smsize`
- int `ipkey`
- int `paramFlag`
- double `z_mem`
- double `L`
- double `membraneDiel`
- double `V`
- int `param2Flag`

8.26.1 Detailed Description

Contains public data members for Vpbe class/module.

Author

Nathan Baker

Definition at line 84 of file `vpbe.h`.

8.26.2 Field Documentation

8.26.2.1 `acc`

`Vacc*` `acc`

Accessibility object

Definition at line 90 of file `vpbe.h`.

8.26.2.2 `alist`

`Valist*` `alist`

Atom (charge) list

Definition at line 88 of file `vpbe.h`.

8.26.2.3 bulkIonicStrength

double bulkIonicStrength
Bulk ionic strength (M)
Definition at line 99 of file [vpbe.h](#).

8.26.2.4 clist

Vclist* clist
Atom location cell list
Definition at line 89 of file [vpbe.h](#).

8.26.2.5 deblen

double deblen
Debye length (bulk)
Definition at line 109 of file [vpbe.h](#).

8.26.2.6 ionConc

double ionConc[MAXION]
Concentration (M) of each species
Definition at line 104 of file [vpbe.h](#).

8.26.2.7 ionQ

double ionQ[MAXION]
Charge (e) of each species
Definition at line 106 of file [vpbe.h](#).

8.26.2.8 ionRadii

double ionRadii[MAXION]
Ionic radius (A) of each species
Definition at line 105 of file [vpbe.h](#).

8.26.2.9 ipkey

int ipkey
PBE calculation type (this is a cached copy it should not be used directly in code)
Definition at line 122 of file [vpbe.h](#).

8.26.2.10 L

double L
Length of the membrane (A)
Definition at line 132 of file [vpbe.h](#).

8.26.2.11 maxIonRadius

`double maxIonRadius`

Max ion radius (A; used for calculating accessibility and defining volumes for ionic strength coefficients)

Definition at line 100 of file [vpbe.h](#).

8.26.2.12 membraneDiel

`double membraneDiel`

Membrane dielectric constant

Definition at line 133 of file [vpbe.h](#).

8.26.2.13 numIon

`int numIon`

Total number of ion species

Definition at line 103 of file [vpbe.h](#).

8.26.2.14 param2Flag

`int param2Flag`

Check to see if bcfl=3 parms have been set

Definition at line 135 of file [vpbe.h](#).

8.26.2.15 paramFlag

`int paramFlag`

Check to see if the parameters have been set

Definition at line 125 of file [vpbe.h](#).

8.26.2.16 smsize

`double smsize`

Size-Modified PBE size

Definition at line 121 of file [vpbe.h](#).

8.26.2.17 smvolume

`double smvolume`

Size-Modified PBE relative volume

Definition at line 120 of file [vpbe.h](#).

8.26.2.18 soluteCenter

`double soluteCenter[3]`

Center of solute molecule (A)

Definition at line 113 of file [vpbe.h](#).

8.26.2.19 soluteCharge

```
double soluteCharge
```

Charge of solute molecule (e)

Definition at line 118 of file [vpbe.h](#).

8.26.2.20 soluteDiel

```
double soluteDiel
```

Solute dielectric constant (unitless)

Definition at line 93 of file [vpbe.h](#).

8.26.2.21 soluteRadius

```
double soluteRadius
```

Radius of solute molecule (A)

Definition at line 114 of file [vpbe.h](#).

8.26.2.22 soluteXlen

```
double soluteXlen
```

Solute length in x-direction

Definition at line 115 of file [vpbe.h](#).

8.26.2.23 soluteYlen

```
double soluteYlen
```

Solute length in y-direction

Definition at line 116 of file [vpbe.h](#).

8.26.2.24 soluteZlen

```
double soluteZlen
```

Solute length in z-direction

Definition at line 117 of file [vpbe.h](#).

8.26.2.25 solventDiel

```
double solventDiel
```

Solvent dielectric constant (unitless)

Definition at line 94 of file [vpbe.h](#).

8.26.2.26 solventRadius

```
double solventRadius
```

Solvent probe radius (angstroms) for accessibility; determining defining volumes for the dielectric coefficient

Definition at line 95 of file [vpbe.h](#).

8.26.2.27 T

double T

Temperature (K)

Definition at line 92 of file [vpbe.h](#).

8.26.2.28 V

double V

Membrane potential

Definition at line 134 of file [vpbe.h](#).

8.26.2.29 vmem

Vmem* vmem

Memory management object

Definition at line 86 of file [vpbe.h](#).

8.26.2.30 xkappa

double xkappa

Debye-Huckel parameter (bulk)

Definition at line 108 of file [vpbe.h](#).

8.26.2.31 z_mem

double z_mem

Z value of the bottom of the membrane (A)

Definition at line 131 of file [vpbe.h](#).

8.26.2.32 zkappa2

double zkappa2

Square of modified Debye-Huckel parameter (bulk)

Definition at line 110 of file [vpbe.h](#).

8.26.2.33 zmagic

double zmagic

Delta function scaling parameter

Definition at line 111 of file [vpbe.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/vpbe.h](#)

8.27 sVpee Struct Reference

Contains public data members for Vpee class/module.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/fem/vpee.h>
```

Data Fields

- Gem * [gm](#)
- int [localPartID](#)
- double [localPartCenter](#) [3]
- double [localPartRadius](#)
- int [killFlag](#)
- double [killParam](#)
- Vmem * [mem](#)

8.27.1 Detailed Description

Contains public data members for Vpee class/module.

Author

Nathan Baker

Definition at line 89 of file [vpee.h](#).

8.27.2 Field Documentation

8.27.2.1 gm

Gem* gm

Grid manager

Definition at line 91 of file [vpee.h](#).

8.27.2.2 killFlag

int killFlag

A flag indicating the method we're using to artificially decrease the error estimate outside the local partition

Definition at line 99 of file [vpee.h](#).

8.27.2.3 killParam

double killParam

A parameter for the error estimate attenuation method

Definition at line 102 of file [vpee.h](#).

8.27.2.4 localPartCenter

double localPartCenter[3]

The coordinates of the center of the local partition

Definition at line 95 of file [vpee.h](#).

8.27.2.5 localPartID

int localPartID

The local partition ID: i.e. the partition whose boundary simplices we're keeping track of

Definition at line 92 of file [vpee.h](#).

8.27.2.6 localPartRadius

`double localPartRadius`

The radius of the circle/sphere which circumscribes the local partition

Definition at line 97 of file [vpee.h](#).

8.27.2.7 mem

`Vmem* mem`

Memory manager

Definition at line 104 of file [vpee.h](#).

The documentation for this struct was generated from the following file:

- [src/fem/vpee.h](#)

8.28 sVpmg Struct Reference

Contains public data members for Vpmg class/module.

`#include </builddir/build/BUILD/apbs-3.0.0/src/mg/vpmg.h>`

Data Fields

- `Vmem * vmem`
- `Vpmgp * pmgp`
- `Vpbe * pbe`
- `double * epsx`
- `double * epsy`
- `double * epsz`
- `double * kappa`
- `double * pot`
- `double * charge`
- `int * iparm`
- `double * rparm`
- `int * iwork`
- `double * rwork`
- `double * a1cf`
- `double * a2cf`
- `double * a3cf`
- `double * ccf`
- `double * fcf`
- `double * tcf`
- `double * u`
- `double * xf`
- `double * yf`
- `double * zf`
- `double * gxcf`
- `double * gycf`
- `double * gzcf`
- `double * pvec`
- `double extDiEnergy`
- `double extQmEnergy`

- double [extQfEnergy](#)
- double [extNpEnergy](#)
- [Vsurf_Meth](#) surfMeth
- double [splineWin](#)
- [Vchrg_Meth](#) chargeMeth
- [Vchrg_Src](#) chargeSrc
- int [filled](#)
- int [useDielXMap](#)
- [Vgrid](#) * [dielXMap](#)
- int [useDielYMap](#)
- [Vgrid](#) * [dielYMap](#)
- int [useDielZMap](#)
- [Vgrid](#) * [dielZMap](#)
- int [useKappaMap](#)
- [Vgrid](#) * [kappaMap](#)
- int [usePotMap](#)
- [Vgrid](#) * [potMap](#)
- int [useChargeMap](#)
- [Vgrid](#) * [chargeMap](#)

8.28.1 Detailed Description

Contains public data members for Vpmpg class/module.

Author

Nathan Baker

Many of the routines and macros are borrowed from the [main.c](#) driver (written by Mike Holst) provided with the PMG code.

Definition at line 116 of file [vpmpg.h](#).

8.28.2 Field Documentation

8.28.2.1 a1cf

double* [a1cf](#)

Operator coefficient values (a11) – this array can be overwritten

Definition at line 138 of file [vpmpg.h](#).

8.28.2.2 a2cf

double* [a2cf](#)

Operator coefficient values (a22) – this array can be overwritten

Definition at line 140 of file [vpmpg.h](#).

8.28.2.3 a3cf

double* [a3cf](#)

Operator coefficient values (a33) – this array can be overwritten

Definition at line 142 of file [vpmpg.h](#).

8.28.2.4 ccf

`double* ccf`

Helmholtz term – this array can be overwritten

Definition at line 144 of file [vpmg.h](#).

8.28.2.5 charge

`double* charge`

Charge map

Definition at line 132 of file [vpmg.h](#).

8.28.2.6 chargeMap

`Vgrid* chargeMap`

External charge distribution map

Definition at line 188 of file [vpmg.h](#).

8.28.2.7 chargeMeth

`Vchrg_Meth chargeMeth`

Charge discretization method

Definition at line 165 of file [vpmg.h](#).

8.28.2.8 chargeSrc

`Vchrg_Src chargeSrc`

Charge source

Definition at line 166 of file [vpmg.h](#).

8.28.2.9 dielXMap

`Vgrid* dielXMap`

External x-shifted dielectric map

Definition at line 172 of file [vpmg.h](#).

8.28.2.10 dielYMap

`Vgrid* dielYMap`

External y-shifted dielectric map

Definition at line 175 of file [vpmg.h](#).

8.28.2.11 dielZMap

`Vgrid* dielZMap`

External z-shifted dielectric map

Definition at line 178 of file [vpmg.h](#).

8.28.2.12 epsx

double* epsx

X-shifted dielectric map

Definition at line 127 of file [vpmg.h](#).

8.28.2.13 epsy

double* epsy

Y-shifted dielectric map

Definition at line 128 of file [vpmg.h](#).

8.28.2.14 epsz

double* epsz

Y-shifted dielectric map

Definition at line 129 of file [vpmg.h](#).

8.28.2.15 extDiEnergy

double extDiEnergy

Stores contributions to the dielectric energy from regions outside the problem domain

Definition at line 155 of file [vpmg.h](#).

8.28.2.16 extNpEnergy

double extNpEnergy

Stores contributions to the apolar energy from regions outside the problem domain

Definition at line 161 of file [vpmg.h](#).

8.28.2.17 extQfEnergy

double extQfEnergy

Stores contributions to the fixed charge energy from regions outside the problem domain

Definition at line 159 of file [vpmg.h](#).

8.28.2.18 extQmEnergy

double extQmEnergy

Stores contributions to the mobile ion energy from regions outside the problem domain

Definition at line 157 of file [vpmg.h](#).

8.28.2.19 fcf

double* fcf

Right-hand side – this array can be overwritten

Definition at line 145 of file [vpmg.h](#).

8.28.2.20 filled

`int filled`

Indicates whether `Vpmg_fillco` has been called

Definition at line 168 of file [vpmg.h](#).

8.28.2.21 gxcf

`double* gxcf`

Boundary conditions for x faces

Definition at line 151 of file [vpmg.h](#).

8.28.2.22 gycf

`double* gycf`

Boundary conditions for y faces

Definition at line 152 of file [vpmg.h](#).

8.28.2.23 gzcf

`double* gzcf`

Boundary conditions for z faces

Definition at line 153 of file [vpmg.h](#).

8.28.2.24 iparm

`int* iparm`

Passing int parameters to FORTRAN

Definition at line 134 of file [vpmg.h](#).

8.28.2.25 iwork

`int* iwork`

Work array

Definition at line 136 of file [vpmg.h](#).

8.28.2.26 kappa

`double* kappa`

Ion accessibility map ($0 \leq \text{kappa}(x) \leq 1$)

Definition at line 130 of file [vpmg.h](#).

8.28.2.27 kappaMap

`Vgrid* kappaMap`

External kappa map

Definition at line 181 of file [vpmg.h](#).

8.28.2.28 pbe

`Vpbe*` pbe

Information about the PBE system

Definition at line 120 of file [vpmg.h](#).

8.28.2.29 pmgp

`Vpmgp*` pmgp

Parameters

Definition at line 119 of file [vpmg.h](#).

8.28.2.30 pot

`double*` pot

Potential map

Definition at line 131 of file [vpmg.h](#).

8.28.2.31 potMap

`Vgrid*` potMap

External potential map

Definition at line 184 of file [vpmg.h](#).

8.28.2.32 pvec

`double*` pvec

Partition mask array

Definition at line 154 of file [vpmg.h](#).

8.28.2.33 rparm

`double*` rparm

Passing real parameters to FORTRAN

Definition at line 135 of file [vpmg.h](#).

8.28.2.34 rwork

`double*` rwork

Work array

Definition at line 137 of file [vpmg.h](#).

8.28.2.35 splineWin

`double` splineWin

Spline window parm for surf defs

Definition at line 164 of file [vpmg.h](#).

8.28.2.36 surfMeth

`Vsurf_Meth` surfMeth

Surface definition method

Definition at line 163 of file [vpmg.h](#).

8.28.2.37 tcf

`double*` tcf

True solution

Definition at line 146 of file [vpmg.h](#).

8.28.2.38 u

`double*` u

Solution

Definition at line 147 of file [vpmg.h](#).

8.28.2.39 useChargeMap

`int` useChargeMap

Indicates whether Vpmg_fillco was called with an external charge distribution map

Definition at line 186 of file [vpmg.h](#).

8.28.2.40 useDielXMap

`int` useDielXMap

Indicates whether Vpmg_fillco was called with an external x-shifted dielectric map

Definition at line 170 of file [vpmg.h](#).

8.28.2.41 useDielYMap

`int` useDielYMap

Indicates whether Vpmg_fillco was called with an external y-shifted dielectric map

Definition at line 173 of file [vpmg.h](#).

8.28.2.42 useDielZMap

`int` useDielZMap

Indicates whether Vpmg_fillco was called with an external z-shifted dielectric map

Definition at line 176 of file [vpmg.h](#).

8.28.2.43 useKappaMap

`int` useKappaMap

Indicates whether Vpmg_fillco was called with an external kappa map

Definition at line 179 of file [vpmg.h](#).

8.28.2.44 usePotMap

```
int usePotMap
```

Indicates whether Vpmg_fillco was called with an external potential map

Definition at line 182 of file [vpmg.h](#).

8.28.2.45 vmem

```
Vmem* vmem
```

Memory management object for this class

Definition at line 118 of file [vpmg.h](#).

8.28.2.46 xf

```
double* xf
```

Mesh point x coordinates

Definition at line 148 of file [vpmg.h](#).

8.28.2.47 yf

```
double* yf
```

Mesh point y coordinates

Definition at line 149 of file [vpmg.h](#).

8.28.2.48 zf

```
double* zf
```

Mesh point z coordinates

Definition at line 150 of file [vpmg.h](#).

The documentation for this struct was generated from the following file:

- [src/mg/vpmg.h](#)

8.29 sVpmgp Struct Reference

Contains public data members for Vpmgp class/module.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/mg/vpmgp.h>
```

Data Fields

- int [nx](#)
- int [ny](#)
- int [nz](#)
- int [nlev](#)
- double [hx](#)
- double [hy](#)
- double [hz](#)
- int [nonlin](#)
- int [nxc](#)
- int [nyc](#)

- int [nzc](#)
- int [nf](#)
- int [nc](#)
- int [narrc](#)
- int [n_rpc](#)
- int [n_iz](#)
- int [n_ipc](#)
- size_t [nrwk](#)
- int [niwk](#)
- int [narr](#)
- int [ipkey](#)
- double [xcent](#)
- double [ycent](#)
- double [zcent](#)
- double [errtol](#)
- int [itmax](#)
- int [istop](#)
- int [iinfo](#)
- [Vbcfl](#) [bcfl](#)
- int [key](#)
- int [iperf](#)
- int [meth](#)
- int [mgkey](#)
- int [nu1](#)
- int [nu2](#)
- int [mgsmoo](#)
- int [mgprol](#)
- int [mgcoar](#)
- int [mgsolv](#)
- int [mgdisc](#)
- double [omegal](#)
- double [omegan](#)
- int [irite](#)
- int [ipcon](#)
- double [xlen](#)
- double [ylen](#)
- double [zlen](#)
- double [xmin](#)
- double [ymin](#)
- double [zmin](#)
- double [xmax](#)
- double [ymax](#)
- double [zmax](#)

8.29.1 Detailed Description

Contains public data members for Vpmgp class/module.

Author

Nathan Baker

Bug Value ipcon does not currently allow for preconditioning in PMG

Definition at line 80 of file [vpmgp.h](#).

8.29.2 Field Documentation

8.29.2.1 bcfl

`Vbcfl bcfl`

Boundary condition method [default = BCFL_SDH]

Definition at line 135 of file [vpmgp.h](#).

8.29.2.2 errtol

`double errtol`

Desired error tolerance [default = 1e-9]

Definition at line 121 of file [vpmgp.h](#).

8.29.2.3 hx

`double hx`

Grid x spacings [no default]

Definition at line 87 of file [vpmgp.h](#).

8.29.2.4 hy

`double hy`

Grid y spacings [no default]

Definition at line 88 of file [vpmgp.h](#).

8.29.2.5 hzed

`double hzed`

Grid z spacings [no default]

Definition at line 89 of file [vpmgp.h](#).

8.29.2.6 iinfo

`int iinfo`

Runtime status messages [default = 1]

- 0: none
- 1: some
- 2: lots
- 3: more

Definition at line 130 of file [vpmgp.h](#).

8.29.2.7 ipcon

`int ipcon`

Preconditioning method [default = 3]

- 0: diagonal
- 1: ICCG
- 2: ICCGDW
- 3: MICCGDW
- 4: none

Definition at line 183 of file [vpmgp.h](#).

8.29.2.8 iperf

`int iperf`

Analysis of the operator [default = 0]

- 0: no
- 1: condition number
- 2: spectral radius
- 3: cond. number & spectral radius

Definition at line 139 of file [vpmgp.h](#).

8.29.2.9 ipkey

`int ipkey`

Toggles nonlinearity (set by `nonlin`)

- -2: Size-Modified PBE
- -1: Linearized PBE
- 0: Nonlinear PBE with capped sinh term [default]
- >1: Polynomial approximation to sinh, note that `ipkey` must be odd

Definition at line 109 of file [vpmgp.h](#).

8.29.2.10 irite

`int irite`

FORTTRAN output unit [default = 8]

Definition at line 182 of file [vpmgp.h](#).

8.29.2.11 istop

`int istop`

Stopping criterion [default = 1]

- 0: residual
- 1: relative residual
- 2: diff
- 3: errc
- 4: errd
- 5: aerrd

Definition at line 123 of file [vpmgp.h](#).

8.29.2.12 itmax

`int itmax`

Maximum number of iters [default = 100]

Definition at line 122 of file [vpmgp.h](#).

8.29.2.13 key

`int key`

Print solution to file [default = 0]

- 0: no
- 1: yes

Definition at line 136 of file [vpmgp.h](#).

8.29.2.14 meth

`int meth`

Solution method [default = 2]

- 0: conjugate gradient multigrid
- 1: newton
- 2: multigrid
- 3: conjugate gradient
- 4: successive overrelaxation
- 5: red-black gauss-seidel
- 6: weighted jacobi
- 7: richardson
- 8: conjugate gradient multigrid aqua
- 9: newton aqua

Definition at line 144 of file [vpmgp.h](#).

8.29.2.15 mgcoar

`int mgcoar`

Coarsening method [default = 2]

- 0: standard
- 1: harmonic
- 2: galerkin

Definition at line 170 of file [vpmgp.h](#).

8.29.2.16 mgdisc

`int mgdisc`

Discretization method [default = 0]

- 0: finite volume
- 1: finite element

Definition at line 177 of file [vpmgp.h](#).

8.29.2.17 mgkey

`int mgkey`

Multigrid method [default = 0]

- 0: variable v-cycle
- 1: nested iteration

Definition at line 155 of file [vpmgp.h](#).

8.29.2.18 mgprol

`int mgprol`

Prolongation method [default = 0]

- 0: trilinear
- 1: operator-based
- 2: mod. operator-based

Definition at line 166 of file [vpmgp.h](#).

8.29.2.19 mgsmoo

`int mgsmoo`

Smoothing method [default = 1]

- 0: weighted jacobi
- 1: gauss-seidel

- 2: SOR
- 3: richardson
- 4: cghs

Definition at line 160 of file [vpmgp.h](#).

8.29.2.20 mgsolv

`int mgsolv`

Coarse equation solve method [default = 1]

- 0: cghs
- 1: banded linpack

Definition at line 174 of file [vpmgp.h](#).

8.29.2.21 n_ipc

`int n_ipc`

Integer info work array required storage

Definition at line 104 of file [vpmgp.h](#).

8.29.2.22 n_iz

`int n_iz`

Integer storage parameter (index max)

Definition at line 103 of file [vpmgp.h](#).

8.29.2.23 n_rpc

`int n_rpc`

Real info work array required storage

Definition at line 102 of file [vpmgp.h](#).

8.29.2.24 narr

`int narr`

Array work storage

Definition at line 108 of file [vpmgp.h](#).

8.29.2.25 narrc

`int narrc`

Size of vector on coarse level

Definition at line 101 of file [vpmgp.h](#).

8.29.2.26 nc

```
int nc
```

Number of coarse grid unknowns

Definition at line 100 of file [vpmgp.h](#).

8.29.2.27 nf

```
int nf
```

Number of fine grid unknowns

Definition at line 99 of file [vpmgp.h](#).

8.29.2.28 niwk

```
int niwk
```

Integer work storage

Definition at line 107 of file [vpmgp.h](#).

8.29.2.29 nlev

```
int nlev
```

Number of mesh levels [no default]

Definition at line 86 of file [vpmgp.h](#).

8.29.2.30 nonlin

```
int nonlin
```

Problem type [no default]

- 0: linear
- 1: nonlinear
- 2: linear then nonlinear

Definition at line 90 of file [vpmgp.h](#).

8.29.2.31 nrw

```
size_t nrw
```

Real work storage

Definition at line 106 of file [vpmgp.h](#).

8.29.2.32 nu1

```
int nul
```

Number of pre-smoothings [default = 2]

Definition at line 158 of file [vpmgp.h](#).

8.29.2.33 nu2

```
int nu2
```

Number of post-smoothings [default = 2]

Definition at line 159 of file [vpmgp.h](#).

8.29.2.34 nx

```
int nx
```

Grid x dimensions [no default]

Definition at line 83 of file [vpmgp.h](#).

8.29.2.35 nxc

```
int nxc
```

Coarse level grid x dimensions

Definition at line 96 of file [vpmgp.h](#).

8.29.2.36 ny

```
int ny
```

Grid y dimensions [no default]

Definition at line 84 of file [vpmgp.h](#).

8.29.2.37 nyc

```
int nyc
```

Coarse level grid y dimensions

Definition at line 97 of file [vpmgp.h](#).

8.29.2.38 nz

```
int nz
```

Grid z dimensions [no default]

Definition at line 85 of file [vpmgp.h](#).

8.29.2.39 nzc

```
int nzc
```

Coarse level grid z dimensions

Definition at line 98 of file [vpmgp.h](#).

8.29.2.40 omegal

```
double omegal
```

Linear relax parameter [default = 8e-1]

Definition at line 180 of file [vpmgp.h](#).

8.29.2.41 omegan

`double omegan`

Nonlin relax parameter [default = 9e-1]

Definition at line 181 of file [vpmgp.h](#).

8.29.2.42 xcent

`double xcent`

Grid x center [0]

Definition at line 118 of file [vpmgp.h](#).

8.29.2.43 xlen

`double xlen`

Domain x length

Definition at line 189 of file [vpmgp.h](#).

8.29.2.44 xmax

`double xmax`

Domain upper x corner

Definition at line 195 of file [vpmgp.h](#).

8.29.2.45 xmin

`double xmin`

Domain lower x corner

Definition at line 192 of file [vpmgp.h](#).

8.29.2.46 ycent

`double ycent`

Grid y center [0]

Definition at line 119 of file [vpmgp.h](#).

8.29.2.47 ylen

`double ylen`

Domain y length

Definition at line 190 of file [vpmgp.h](#).

8.29.2.48 ymax

double ymax

Domain upper y corner

Definition at line 196 of file [vpmgp.h](#).

8.29.2.49 ymin

double ymin

Domain lower y corner

Definition at line 193 of file [vpmgp.h](#).

8.29.2.50 zcent

double zcent

Grid z center [0]

Definition at line 120 of file [vpmgp.h](#).

8.29.2.51 zlen

double zlen

Domain z length

Definition at line 191 of file [vpmgp.h](#).

8.29.2.52 zmax

double zmax

Domain upper z corner

Definition at line 197 of file [vpmgp.h](#).

8.29.2.53 zmin

double zmin

Domain lower z corner

Definition at line 194 of file [vpmgp.h](#).

The documentation for this struct was generated from the following file:

- [src/mg/vpmgp.h](#)

8.30 Vparam Struct Reference

Reads and assigns charge/radii parameters.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/vparam.h>
```

Data Fields

- Vmem * [vmem](#)
- int [nResData](#)
- [Vparam_ResData](#) * [resData](#)

8.30.1 Detailed Description

Reads and assigns charge/radii parameters.

Author

Nathan Baker

Definition at line 135 of file [vparam.h](#).

8.30.2 Field Documentation

8.30.2.1 nResData

```
int nResData
```

Number of [Vparam_ResData](#) objects associated with this object

Definition at line 138 of file [vparam.h](#).

8.30.2.2 resData

```
Vparam_ResData* resData
```

Array of nResData [Vparam_ResData](#) objects

Definition at line 140 of file [vparam.h](#).

8.30.2.3 vmem

```
Vmem* vmem
```

Memory management object for this class

Definition at line 137 of file [vparam.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/vparam.h](#)

8.31 Vparam_ResData Struct Reference

ResData sub-class; stores residue data.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/vparam.h>
```

Data Fields

- Vmem * [vmem](#)
- char [name](#) [VMAX_ARGLEN]
- int [nAtomData](#)
- [Vparam_AtomData](#) * [atomData](#)

8.31.1 Detailed Description

ResData sub-class; stores residue data.

Author

Nathan Baker

Definition at line 114 of file [vparam.h](#).

8.31.2 Field Documentation

8.31.2.1 atomData

`Vparam_AtomData* atomData`

Array of Vparam_AtomData natom objects

Definition at line 119 of file [vparam.h](#).

8.31.2.2 name

`char name[VMAX_ARGLEN]`

Residue name

Definition at line 116 of file [vparam.h](#).

8.31.2.3 nAtomData

`int nAtomData`

Number of Vparam_AtomData objects associated with this object

Definition at line 117 of file [vparam.h](#).

8.31.2.4 vmem

`Vmem* vmem`

Pointer to memory manager from [Vparam](#) master class

Definition at line 115 of file [vparam.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/vparam.h](#)

Chapter 9

File Documentation

9.1 mainpage.h

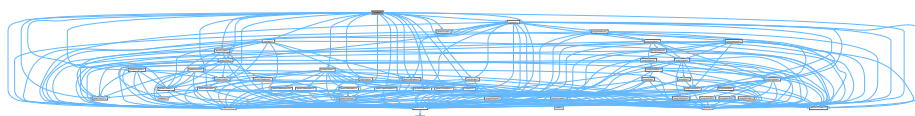
00001

9.2 src/apbs.h File Reference

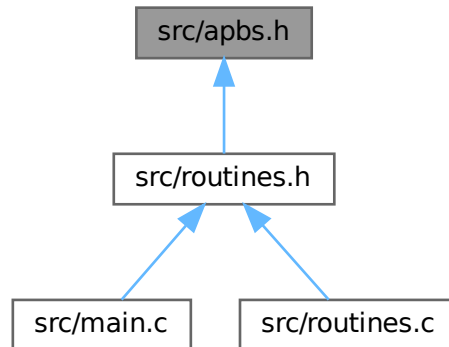
Header file for header dependencies.

```
#include "apbscfg.h"
#include "malloc/malloc.h"
#include "generic/nosh.h"
#include "generic/mgparm.h"
#include "generic/pbeparm.h"
#include "generic/femparm.h"
#include "generic/bemparm.h"
#include "generic/geoflowparm.h"
#include "generic/vacc.h"
#include "generic/valist.h"
#include "generic/vatom.h"
#include "generic/vcap.h"
#include "generic/vhal.h"
#include "generic/vpbe.h"
#include "generic/vstring.h"
#include "generic/vunit.h"
#include "generic/vparam.h"
#include "generic/vgreen.h"
#include "mg/vgrid.h"
#include "mg/vmgrid.h"
#include "mg/vopot.h"
#include "mg/vpmg.h"
#include "mg/vpmgp.h"
```

Include dependency graph for apbs.h:



This graph shows which files directly or indirectly include this file:



9.2.1 Detailed Description

Header file for header dependencies.

Author

Nathan Baker

Version

\$Id\$

Attention

```

*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
*
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* Portions Copyright (c) 1999-2002, The Regents of the University of
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* Portions Copyright (c) 1995, Michael Holst.
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```

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```

Definition in file [apbs.h](#).

9.3 apbs.h

[Go to the documentation of this file.](#)

```

00001
00061 #ifndef _APBSHEADERS_H_
00062 #define _APBSHEADERS_H_
00063
00064 #include "apbscfg.h"
00065
00066 /* MALLOC headers */
00067 #include "malloc/malloc.h"
00068
00069 /* Generic headers */
00070 #include "generic/nosh.h"
00071 #include "generic/mgparm.h"
00072 #include "generic/pbeparm.h"
00073 #include "generic/femparm.h"
00074 #include "generic/bemparm.h"
00075 #include "generic/geoflowparm.h"
00076 #include "generic/vacc.h"
00077 #include "generic/valist.h"
00078 #include "generic/vatom.h"
00079 #include "generic/vcap.h"
00080 #include "generic/vhal.h"
00081 #include "generic/vpbe.h"
00082 #include "generic/vstring.h"
00083 #include "generic/vunit.h"
00084 #include "generic/vparam.h"
00085 #include "generic/vgreen.h"
00086
00087 // #include "geoflow/cpbconcz2.h"
00088
00089 /* MG headers */
00090 #include "mg/vgrid.h"
00091 #include "mg/vmgrid.h"
00092 #include "mg/vopot.h"
00093 #include "mg/vpmg.h"
00094 #include "mg/vpmgp.h"
00095
00096 /* FEM headers */
00097 #if defined(FETK_ENABLED)
00098     #include "fem/vfetc.h"
00099     #include "fem/vpee.h"
00100 #endif
00101
00102 #endif /* _APBSHEADERS_H_ */

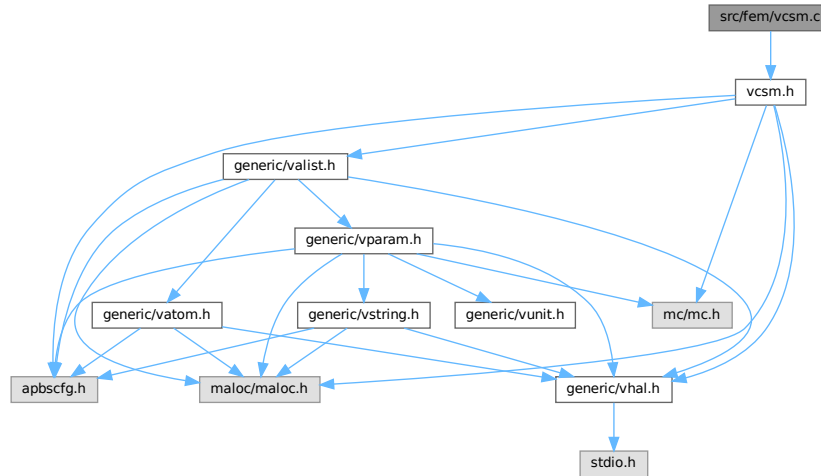
```

9.4 src/fem/vcsm.c File Reference

Class Vcsm methods.

```
#include "vcsm.h"
```

Include dependency graph for vcsm.c:



Functions

- VPUBLIC Valist * Vcsm_getValist (Vcsm *thee)
Get atom list.
- VPUBLIC int Vcsm_getNumberAtoms (Vcsm *thee, int isimp)
Get number of atoms associated with a simplex.
- VPUBLIC Vatom * Vcsm_getAtom (Vcsm *thee, int iatom, int isimp)
Get particular atom associated with a simplex.
- VPUBLIC int Vcsm_getAtomIndex (Vcsm *thee, int iatom, int isimp)
Get ID of particular atom in a simplex.
- VPUBLIC int Vcsm_getNumberSimplexes (Vcsm *thee, int iatom)
Get number of simplexes associated with an atom.
- VPUBLIC SS * Vcsm_getSimplex (Vcsm *thee, int isimp, int iatom)
Get particular simplex associated with an atom.
- VPUBLIC int Vcsm_getSimplexIndex (Vcsm *thee, int isimp, int iatom)
Get index particular simplex associated with an atom.
- VPUBLIC unsigned long int Vcsm_memChk (Vcsm *thee)
Return the memory used by this structure (and its contents) in bytes.
- VPUBLIC Vcsm * Vcsm_ctor (Valist *alist, Gem *gm)
Construct Vcsm object.
- VPUBLIC int Vcsm_ctor2 (Vcsm *thee, Valist *alist, Gem *gm)
FORTTRAN stub to construct Vcsm object.
- VPUBLIC void Vcsm_init (Vcsm *thee)
Initialize charge-simplex map with mesh and atom data.
- VPUBLIC void Vcsm_dtor (Vcsm **thee)

Destroy Vcsm object.

- VPUBLIC void [Vcsm_dtor2](#) ([Vcsm](#) *three)

FORTTRAN stub to destroy Vcsm object.

- VPUBLIC int [Vcsm_update](#) ([Vcsm](#) *three, SS **simps, int num)

Update the charge-simplex and simplex-charge maps after refinement.

9.4.1 Detailed Description

Class Vcsm methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
*
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*
*
```

Definition in file [vcsn.c](#).

9.5 vcsn.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "vcsn.h"
00058
00059 /* Inlineable methods */
00060 #if !defined(VINLINE_VCSN)
00061
00062 VPUBLIC Valist* Vcsn_getValist(Vcsn *thee) {
00063
00064     VASSERT(thee != VNULL);
00065     return thee->alist;
00066 }
00067
00068
00069 VPUBLIC int Vcsn_getNumberAtoms(Vcsn *thee, int isimp) {
00070
00071     VASSERT(thee != VNULL);
00072     VASSERT(thee->initFlag);
00073     return thee->nsqm[isimp];
00074 }
00075
00076
00077 VPUBLIC Vatom* Vcsn_getAtom(Vcsn *thee, int iatom, int isimp) {
00078
00079     VASSERT(thee != VNULL);
00080     VASSERT(thee->initFlag);
00081
00082     VASSERT(iatom < (thee->nsqm)[isimp]);
00083     return Valist_getAtom(thee->alist, (thee->sqm)[isimp][iatom]);
00084 }
00085
00086
00087 VPUBLIC int Vcsn_getAtomIndex(Vcsn *thee, int iatom, int isimp) {
00088
00089     VASSERT(thee != VNULL);
00090     VASSERT(thee->initFlag);
00091
00092     VASSERT(iatom < (thee->nsqm)[isimp]);
00093     return (thee->sqm)[isimp][iatom];
00094 }
00095
00096
00097
00098
00099 VPUBLIC int Vcsn_getNumberSimplices(Vcsn *thee, int iatom) {
00100
00101     VASSERT(thee != VNULL);
00102     VASSERT(thee->initFlag);
00103
00104     return (thee->nqsm)[iatom];
00105 }
00106
00107
00108
00109 VPUBLIC SS* Vcsn_getSimplex(Vcsn *thee, int isimp, int iatom) {
00110
00111     VASSERT(thee != VNULL);
00112     VASSERT(thee->initFlag);
00113
00114     return Gem_SS(thee->gm, (thee->qsm)[iatom][isimp]);
00115 }
00116
00117
00118
00119 VPUBLIC int Vcsn_getSimplexIndex(Vcsn *thee, int isimp, int iatom) {
00120
00121     VASSERT(thee != VNULL);
00122     VASSERT(thee->initFlag);
00123
00124     return (thee->qsm)[iatom][isimp];
00125 }
00126
00127
00128

```

```

00129 VPUBLIC unsigned long int Vcsn_memChk(Vcsn *thee) {
00130     if (thee == VNULL) return 0;
00131     return Vmem_bytes(thee->vmem);
00132 }
00133
00134 #endif /* if !defined(VINLINE_VCSN) */
00135
00136 VPUBLIC Vcsn* Vcsn_ctor(Valist *alist, Gem *gm) {
00137
00138     /* Set up the structure */
00139     Vcsn *thee = VNULL;
00140     thee = (Vcsn*)Vmem_malloc(VNULL, 1, sizeof(Vcsn) );
00141     VASSERT( thee != VNULL);
00142     VASSERT( Vcsn_ctor2(thee, alist, gm));
00143
00144     return thee;
00145 }
00146
00147 VPUBLIC int Vcsn_ctor2(Vcsn *thee, Valist *alist, Gem *gm) {
00148
00149     VASSERT( thee != VNULL );
00150
00151     /* Memory management object */
00152     thee->vmem = Vmem_ctor("APBS:VCSN");
00153
00154     /* Set up the atom list and grid manager */
00155     if( alist == VNULL) {
00156         Vnm_print(2, "Vcsn_ctor2: got null pointer to Valist object!\n");
00157         return 0;
00158     }
00159     thee->alist = alist;
00160     if( gm == VNULL) {
00161         Vnm_print(2, "Vcsn_ctor2: got a null pointer to the Gem object!\n");
00162         return 0;
00163     }
00164     thee->gm = gm;
00165
00166     thee->initFlag = 0;
00167     return 1;
00168 }
00169
00170 VPUBLIC void Vcsn_init(Vcsn *thee) {
00171
00172     /* Counters */
00173     int iatom,
00174         jatom,
00175         isimp,
00176         jsimp,
00177         gotSimp;
00178
00179     /* Atomic information */
00180     Vatom *atom;
00181     double *position;
00182
00183     /* Simplex/Vertex information */
00184     SS *simplex;
00185     /* Basis function values */
00186
00187     if (thee == VNULL) {
00188         Vnm_print(2, "Vcsn_init: Error! Got NULL thee!\n");
00189         VASSERT(0);
00190     }
00191     if (thee->gm == VNULL) {
00192         Vnm_print(2, "Vcsn_init: Error! Got NULL thee->gm!\n");
00193         VASSERT(0);
00194     }
00195     thee->nsimp = Gem_numSS(thee->gm);
00196     if (thee->nsimp <= 0) {
00197         Vnm_print(2, "Vcsn_init: Error! Got %d simplices!\n", thee->nsimp);
00198         VASSERT(0);
00199     }
00200     thee->natom = Valist_getNumberAtoms(thee->alist);
00201
00202     /* Allocate and initialize space for the first dimensions of the
00203      * simplex-charge map, the simplex array, and the counters */
00204     thee->sqm = (int**)Vmem_malloc(thee->vmem, thee->nsimp, sizeof(int *));
00205     VASSERT(thee->sqm != VNULL);
00206     thee->nsqm = (int*)Vmem_malloc(thee->vmem, thee->nsimp, sizeof(int));
00207     VASSERT(thee->nsqm != VNULL);
00208     for (isimp=0; isimp<thee->nsimp; isimp++) (thee->nsqm)[isimp] = 0;
00209
00210     /* Count the number of charges per simplex. */
00211     for (iatom=0; iatom<thee->natom; iatom++) {

```

```

00210     atom = Valist_getAtom(thee->alist, iatom);
00211     position = Vatom_getPosition(atom);
00212     gotSimp = 0;
00213     for (isimp=0; isimp<thee->nsimp; isimp++) {
00214         simplex = Gem_SS(thee->gm, isimp);
00215         if (Gem_pointInSimplex(thee->gm, simplex, position)) {
00216             (thee->nsqm)[isimp]++;
00217             gotSimp = 1;
00218         }
00219     }
00220 }
00221
00222 /* @todo Combine the following two loops? - PCE */
00223 /* Allocate the space for the simplex-charge map */
00224 for (isimp=0; isimp<thee->nsimp; isimp++) {
00225     if ((thee->nsqm)[isimp] > 0) {
00226         thee->sqm[isimp] = (int*)Vmem_malloc(thee->vmem, (thee->nsqm)[isimp],
00227             sizeof(int));
00228         VASSERT(thee->sqm[isimp] != VNULL);
00229     }
00230 }
00231
00232 /* Finally, set up the map */
00233 for (isimp=0; isimp<thee->nsimp; isimp++) {
00234     jsimp = 0;
00235     simplex = Gem_SS(thee->gm, isimp);
00236     for (iatom=0; iatom<thee->natom; iatom++) {
00237         atom = Valist_getAtom(thee->alist, iatom);
00238         position = Vatom_getPosition(atom);
00239         /* Check to see if the atom's in this simplex */
00240         if (Gem_pointInSimplex(thee->gm, simplex, position)) {
00241             /* Assign the entries in the next vacant spot */
00242             (thee->sqm)[isimp][jsimp] = iatom;
00243             jsimp++;
00244         }
00245     }
00246 }
00247
00248 thee->msimp = thee->nsimp;
00249
00250 /* Allocate space for the charge-simplex map */
00251 thee->qsm = (int**)Vmem_malloc(thee->vmem, thee->natom, sizeof(int *));
00252 VASSERT(thee->qsm != VNULL);
00253 thee->nqsm = (int*)Vmem_malloc(thee->vmem, thee->natom, sizeof(int));
00254 VASSERT(thee->nqsm != VNULL);
00255 for (iatom=0; iatom<thee->natom; iatom++) (thee->nqsm)[iatom] = 0;
00256 /* Loop through the list of simplices and count the number of times
00257  * each atom appears */
00258 for (isimp=0; isimp<thee->nsimp; isimp++) {
00259     for (iatom=0; iatom<thee->nsqm[isimp]; iatom++) {
00260         jatom = thee->sqm[isimp][iatom];
00261         thee->nqsm[jatom]++;
00262     }
00263 }
00264 /* Do a TIME-CONSUMING SANITY CHECK to make sure that each atom was
00265  * placed in at simplex */
00266 for (iatom=0; iatom<thee->natom; iatom++) {
00267     if (thee->nqsm[iatom] == 0) {
00268         Vnm_print(2, "Vcsm_init: Atom %d not placed in simplex!\n", iatom);
00269         VASSERT(0);
00270     }
00271 }
00272 /* Allocate the appropriate amount of space for each entry in the
00273  * charge-simplex map and clear the counter for re-use in assignment */
00274 for (iatom=0; iatom<thee->natom; iatom++) {
00275     thee->qsm[iatom] = (int*)Vmem_malloc(thee->vmem, (thee->nqsm)[iatom],
00276         sizeof(int));
00277     VASSERT(thee->qsm[iatom] != VNULL);
00278     thee->nqsm[iatom] = 0;
00279 }
00280 /* Assign the simplices to atoms */
00281 for (isimp=0; isimp<thee->nsimp; isimp++) {
00282     for (iatom=0; iatom<thee->nsqm[isimp]; iatom++) {
00283         jatom = thee->sqm[isimp][iatom];
00284         thee->qsm[jatom][thee->nqsm[jatom]] = isimp;
00285         thee->nqsm[jatom]++;
00286     }
00287 }
00288
00289 thee->initFlag = 1;
00290 }

```



```

00291
00292 VPUBLIC void Vcsn_dtor(Vcsn **thee) {
00293     if ((*thee) != VNULL) {
00294         Vcsn_dtor2(*thee);
00295         Vmem_free(VNULL, 1, sizeof(Vcsn), (void **)thee);
00296         (*thee) = VNULL;
00297     }
00298 }
00299
00300 VPUBLIC void Vcsn_dtor2(Vcsn *thee) {
00301     int i;
00302
00303     if ((thee != VNULL) && thee->initFlag) {
00304         for (i=0; i<thee->msimp; i++) {
00305             if (thee->nsqm[i] > 0) Vmem_free(thee->vmem, thee->nsqm[i],
00306                 sizeof(int), (void **)&(thee->sqm[i]));
00307         }
00308         for (i=0; i<thee->natom; i++) {
00309             if (thee->nqsm[i] > 0) Vmem_free(thee->vmem, thee->nqsm[i],
00310                 sizeof(int), (void **)&(thee->qsm[i]));
00311         }
00312         Vmem_free(thee->vmem, thee->msimp, sizeof(int *),
00313             (void **)&(thee->sqm));
00314         Vmem_free(thee->vmem, thee->msimp, sizeof(int),
00315             (void **)&(thee->nsqm));
00316         Vmem_free(thee->vmem, thee->natom, sizeof(int *),
00317             (void **)&(thee->qsm));
00318         Vmem_free(thee->vmem, thee->natom, sizeof(int),
00319             (void **)&(thee->nqsm));
00320     }
00321     Vmem_dtor(&(thee->vmem));
00322 }
00323
00324 }
00325
00326 VPUBLIC int Vcsn_update(Vcsn *thee, SS **simps, int num) {
00327     /* Counters */
00328     int isimp, jsimp, iatom, jatom, atomID, simpID;
00329     int nsimps, gotMem;
00330     /* Object info */
00331     Vatom *atom;
00332     SS *simplex;
00333     double *position;
00334     /* Lists */
00335     int *qParent, nqParent;
00336     int **sqmNew, *nsqmNew;
00337     int *affAtoms, nAffAtoms;
00338     int *dnqsm, *nqsmNew, **qsmNew;
00339
00340     VASSERT(thee != VNULL);
00341     VASSERT(thee->initFlag);
00342
00343     /* If we don't have enough memory to accommodate the new entries,
00344      * add more by doubling the existing amount */
00345     isimp = thee->nsimp + num - 1;
00346     gotMem = 0;
00347     while (!gotMem) {
00348         if (isimp > thee->msimp) {
00349             isimp = 2 * isimp;
00350             thee->nsqm = (int*)Vmem_realloc(thee->vmem, thee->msimp, sizeof(int),
00351                 (void **)&(thee->nsqm), isimp);
00352             VASSERT(thee->nsqm != VNULL);
00353             thee->sqm = (int**)Vmem_realloc(thee->vmem, thee->msimp, sizeof(int *),
00354                 (void **)&(thee->sqm), isimp);
00355             VASSERT(thee->sqm != VNULL);
00356             thee->msimp = isimp;
00357         } else gotMem = 1;
00358     }
00359     /* Initialize the nsqm entires we just allocated */
00360     for (isimp = thee->nsimp; isimp<thee->nsimp+num-1; isimp++) {
00361         thee->nsqm[isimp] = 0;
00362     }
00363
00364     thee->nsimp = thee->nsimp + num - 1;
00365
00366     /* There's a simple case to deal with: if simps[0] didn't have a
00367      * charge in the first place */
00368     isimp = SS_id(simps[0]);
00369     if (thee->nsqm[isimp] == 0) {
00370         for (isimp=1; isimp<num; isimp++) {

```

```

00372         thee->nsqm[SS_id(simps[isimp])] = 0;
00373     }
00374     return 1;
00375 }
00376
00377 /* The more complicated case has occurred; the parent simplex had one or
00378  * more charges. First, generate the list of affected charges. */
00379 isimp = SS_id(simps[0]);
00380 nqParent = thee->nsqm[isimp];
00381 qParent = thee->sqm[isimp];
00382
00383 sqmNew = (int**)Vmem_malloc(thee->vmem, num, sizeof(int *));
00384 VASSERT(sqmNew != VNULL);
00385 nsqmNew = (int*)Vmem_malloc(thee->vmem, num, sizeof(int));
00386 VASSERT(nsqmNew != VNULL);
00387 for (isimp=0; isimp<num; isimp++) nsqmNew[isimp] = 0;
00388
00389 /* Loop throught the affected atoms to determine how many atoms each
00390  * simplex will get. */
00391 for (iatom=0; iatom<nqParent; iatom++) {
00392
00393     atomID = qParent[iatom];
00394     atom = Valist_getAtom(thee->alist, atomID);
00395     position = Vatom_getPosition(atom);
00396     nsimps = 0;
00397
00398     jsimp = 0;
00399
00400     for (isimp=0; isimp<num; isimp++) {
00401         simplex = simps[isimp];
00402         if (Gem_pointInSimplex(thee->gm, simplex, position)) {
00403             nsqmNew[isimp]++;
00404             jsimp = 1;
00405         }
00406     }
00407
00408     VASSERT(jsimp != 0);
00409 }
00410
00411 /* Sanity check that we didn't lose any atoms... */
00412 iatom = 0;
00413 for (isimp=0; isimp<num; isimp++) iatom += nsqmNew[isimp];
00414 if (iatom < nqParent) {
00415     Vnm_print(2,"Vcsm_update: Lost %d (of %d) atoms!\n",
00416              nqParent - iatom, nqParent);
00417     VASSERT(0);
00418 }
00419
00420 /* Allocate the storage */
00421 for (isimp=0; isimp<num; isimp++) {
00422     if (nsqmNew[isimp] > 0) {
00423         sqmNew[isimp] = (int*)Vmem_malloc(thee->vmem, nsqmNew[isimp],
00424                                           sizeof(int));
00425         VASSERT(sqmNew[isimp] != VNULL);
00426     }
00427 }
00428
00429 /* Assign charges to simplices */
00430 for (isimp=0; isimp<num; isimp++) {
00431
00432     jsimp = 0;
00433     simplex = simps[isimp];
00434
00435     /* Loop over the atoms associated with the parent simplex */
00436     for (iatom=0; iatom<nqParent; iatom++) {
00437
00438         atomID = qParent[iatom];
00439         atom = Valist_getAtom(thee->alist, atomID);
00440         position = Vatom_getPosition(atom);
00441         if (Gem_pointInSimplex(thee->gm, simplex, position)) {
00442             sqmNew[isimp][jsimp] = atomID;
00443             jsimp++;
00444         }
00445     }
00446 }
00447
00448 /* Update the QSM map using the old and new SQM lists */
00449 /* The affected atoms are those contained in the parent simplex; i.e.
00450  * thee->sqm[SS_id(simps[0])] */
00451 affAtoms = thee->sqm[SS_id(simps[0])];
00452 nAffAtoms = thee->nsqm[SS_id(simps[0])];

```

```

00453     /* Each of these atoms will go somewhere else; i.e., the entries in
00454     * thee->qsm are never destroyed and thee->nqsm never decreases.
00455     * However, it is possible that a subdivision could cause an atom to be
00456     * shared by two child simplices. Here we record the change, if any,
00457     * in the number of simplices associated with each atom. */
00458     dnqsm = (int*)Vmem_malloc(thee->vmem, nAffAtoms, sizeof(int));
00459     VASSERT(dnqsm != VNULL);
00460     nqsmNew = (int*)Vmem_malloc(thee->vmem, nAffAtoms, sizeof(int));
00461     VASSERT(nqsmNew != VNULL);
00462     qsmNew = (int**)Vmem_malloc(thee->vmem, nAffAtoms, sizeof(int*));
00463     VASSERT(qsmNew != VNULL);
00464     for (iatom=0; iatom<nAffAtoms; iatom++) {
00465         dnqsm[iatom] = -1;
00466         atomID = affAtoms[iatom];
00467         for (isimp=0; isimp<num; isimp++) {
00468             for (jatom=0; jatom<nqsmNew[isimp]; jatom++) {
00469                 if (sqmNew[isimp][jatom] == atomID) dnqsm[iatom]++;
00470             }
00471         }
00472         VASSERT(dnqsm[iatom] > -1);
00473     }
00474     /* Setup the new entries in the array */
00475     for (iatom=0; iatom<nAffAtoms; iatom++) {
00476         atomID = affAtoms[iatom];
00477         qsmNew[iatom] = (int*)Vmem_malloc(thee->vmem,
00478             (dnqsm[iatom] + thee->nqsm[atomID]),
00479             sizeof(int));
00480         nqsmNew[iatom] = 0;
00481         VASSERT(qsmNew[iatom] != VNULL);
00482     }
00483     /* Fill the new entries in the array */
00484     /* First, do the modified entries */
00485     for (isimp=0; isimp<num; isimp++) {
00486         simpID = SS_id(simps[isimp]);
00487         for (iatom=0; iatom<nqsmNew[isimp]; iatom++) {
00488             atomID = sqmNew[isimp][iatom];
00489             for (jatom=0; jatom<nAffAtoms; jatom++) {
00490                 if (atomID == affAtoms[jatom]) break;
00491             }
00492             if (jatom < nAffAtoms) {
00493                 qsmNew[jatom][nqsmNew[jatom]] = simpID;
00494                 nqsmNew[jatom]++;
00495             }
00496         }
00497     }
00498     /* Now do the unmodified entries */
00499     for (iatom=0; iatom<nAffAtoms; iatom++) {
00500         atomID = affAtoms[iatom];
00501         for (isimp=0; isimp<thee->nqsm[atomID]; isimp++) {
00502             for (jsimp=0; jsimp<num; jsimp++) {
00503                 simpID = SS_id(simps[jsimp]);
00504                 if (thee->qsm[atomID][isimp] == simpID) break;
00505             }
00506             if (jsimp == num) {
00507                 qsmNew[iatom][nqsmNew[iatom]] = thee->qsm[atomID][isimp];
00508                 nqsmNew[iatom]++;
00509             }
00510         }
00511     }
00512
00513     /* Replace the existing entries in the table. Do the QSM entires
00514     * first, since they require affAtoms = thee->sqm[simps[0]] */
00515     for (iatom=0; iatom<nAffAtoms; iatom++) {
00516         atomID = affAtoms[iatom];
00517         Vmem_free(thee->vmem, thee->nqsm[atomID], sizeof(int),
00518             (void *)&(thee->qsm[atomID]));
00519         thee->qsm[atomID] = qsmNew[iatom];
00520         thee->nqsm[atomID] = nqsmNew[iatom];
00521     }
00522     for (isimp=0; isimp<num; isimp++) {
00523         simpID = SS_id(simps[isimp]);
00524         if (thee->nqsm[simpID] > 0) Vmem_free(thee->vmem, thee->nqsm[simpID],
00525             sizeof(int), (void *)&(thee->sqm[simpID]));
00526         thee->sqm[simpID] = sqmNew[isimp];
00527         thee->nqsm[simpID] = nqsmNew[isimp];
00528     }
00529
00530     Vmem_free(thee->vmem, num, sizeof(int *), (void *)&sqmNew);
00531     Vmem_free(thee->vmem, num, sizeof(int), (void *)&nqsmNew);
00532     Vmem_free(thee->vmem, nAffAtoms, sizeof(int *), (void *)&qsmNew);
00533     Vmem_free(thee->vmem, nAffAtoms, sizeof(int), (void *)&nqsmNew);

```

```

00534     Vmem_free(thee->vmem, nAffAtoms, sizeof(int), (void **)&dnqsm);
00535
00536
00537     return 1;
00538
00539
00540 }
```

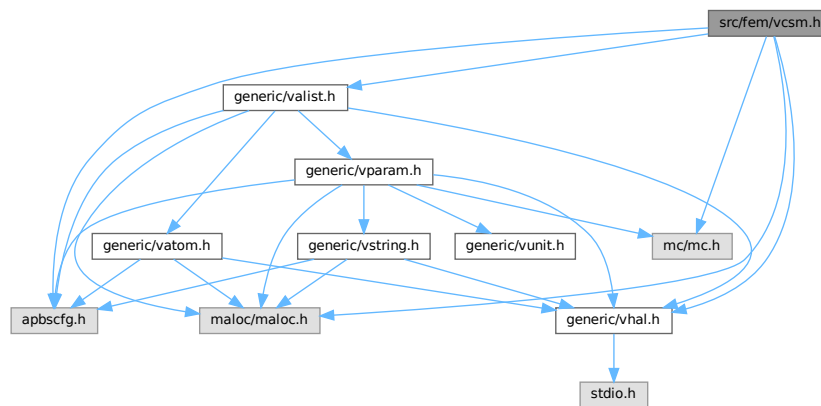
9.6 src/fem/vcsm.h File Reference

Contains declarations for the Vcsm class.

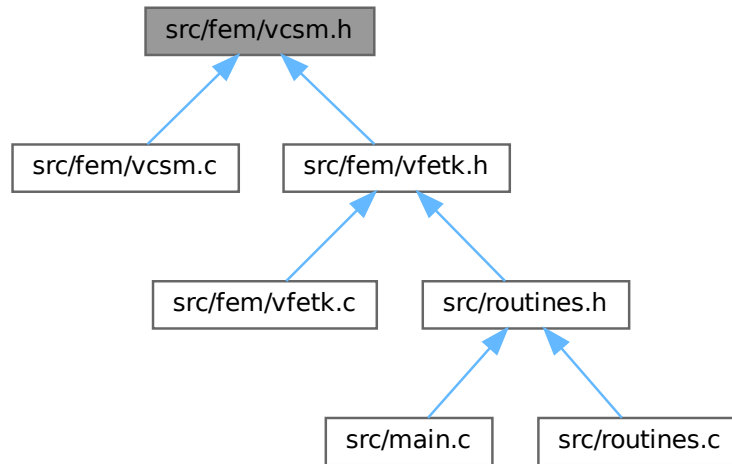
```

#include "apbscfg.h"
#include "maloc/maloc.h"
#include "mc/mc.h"
#include "generic/vhal.h"
#include "generic/valist.h"
```

Include dependency graph for vcsm.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVcsm](#)
Charge-simplex map class.

Typedefs

- typedef struct [sVcsm](#) [Vcsm](#)
Declaration of the Vcsm class as the Vcsm structure.

Functions

- VEXTERNC void [Gem_setExternalUpdateFunction](#) ([Gem](#) *thee, void(*externalUpdate)(SS **simps, int num))
External function for FEtk Gem class to use during mesh refinement.
- VEXTERNC [Valist](#) * [Vcsm_getValist](#) ([Vcsm](#) *thee)
Get atom list.
- VEXTERNC int [Vcsm_getNumberAtoms](#) ([Vcsm](#) *thee, int isimp)
Get number of atoms associated with a simplex.
- VEXTERNC [Vatom](#) * [Vcsm_getAtom](#) ([Vcsm](#) *thee, int iatom, int isimp)
Get particular atom associated with a simplex.
- VEXTERNC int [Vcsm_getAtomIndex](#) ([Vcsm](#) *thee, int iatom, int isimp)
Get ID of particular atom in a simplex.
- VEXTERNC int [Vcsm_getNumberSimplexes](#) ([Vcsm](#) *thee, int iatom)
Get number of simplexes associated with an atom.
- VEXTERNC SS * [Vcsm_getSimplex](#) ([Vcsm](#) *thee, int isimp, int iatom)
Get particular simplex associated with an atom.
- VEXTERNC int [Vcsm_getSimplexIndex](#) ([Vcsm](#) *thee, int isimp, int iatom)

Get index particular simplex associated with an atom.

- VEXTERNC unsigned long int `Vcsm_memChk` (`Vcsm *thee`)

Return the memory used by this structure (and its contents) in bytes.

- VEXTERNC `Vcsm * Vcsm_ctor` (`Valist *alist`, `Gem *gm`)

Construct Vcsm object.

- VEXTERNC int `Vcsm_ctor2` (`Vcsm *thee`, `Valist *alist`, `Gem *gm`)

FORTTRAN stub to construct Vcsm object.

- VEXTERNC void `Vcsm_dtor` (`Vcsm **thee`)

Destroy Vcsm object.

- VEXTERNC void `Vcsm_dtor2` (`Vcsm *thee`)

FORTTRAN stub to destroy Vcsm object.

- VEXTERNC void `Vcsm_init` (`Vcsm *thee`)

Initialize charge-simplex map with mesh and atom data.

- VEXTERNC int `Vcsm_update` (`Vcsm *thee`, `SS **simps`, int num)

Update the charge-simplex and simplex-charge maps after refinement.

9.6.1 Detailed Description

Contains declarations for the Vcsm class.

Version

\$Id\$

Author

Nathan A. Baker

Attention

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*
*

```

Definition in file [vcsn.h](#).

9.7 vcsn.h

[Go to the documentation of this file.](#)

```

00001
00063 #ifndef _VCSN_H_
00064 #define _VCSN_H_
00065
00066 #include "apbsofg.h"
00067
00068 #include "malloc/malloc.h"
00069 #include "mc/mc.h"
00070
00071 #include "generic/vhal.h"
00072 #include "generic/valist.h"
00073
00078 VEXTERNC void Gem_setExternalUpdateFunction(
00079     Gem *thee,
00080     void (*externalUpdate)(SS **simps, int num)
00083     );
00084
00089 struct sVcsn {
00090
00091     Valist *alist;
00092     int natom;
00094     Gem *gm;
00097     int **sqm;
00104     int *nsqm;
00105     int nsimp;
00107     int msimp;
00109     int **qsm;
00111     int *nqsm;
00112     int initFlag;
00114     Vmem *vmem;
00116 };
00117
00122 typedef struct sVcsn Vcsn;
00123
00124 /* ////////////////////////////////////////
00125 // Class Vcsn: Inlineable methods (vcsn.c)
00127
00128 #if !defined(VINLINE_VCSN)
00129
00135     VEXTERNC Valist* Vcsn_getValist(
00136         Vcsn *thee /**< The Vcsn object */
00137     );
00138
00144     VEXTERNC int Vcsn_getNumberAtoms(
00145         Vcsn *thee,
00146         int isimp
00147     );
00148
00154     VEXTERNC Vatom* Vcsn_getAtom(
00155         Vcsn *thee,
00156         int iatom,
00157         int isimp
00158     );

```

```

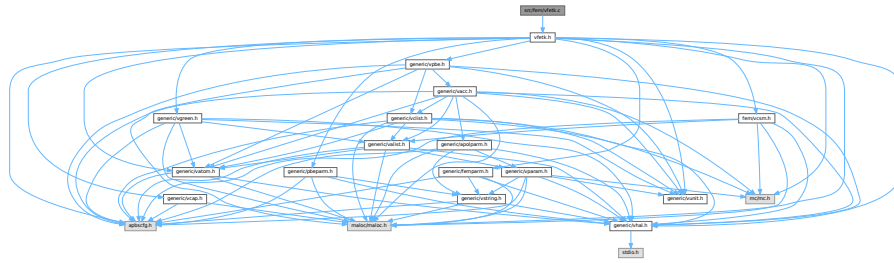
00159
00165     VEXTERNC int Vcsm_getAtomIndex(
00166         Vcsm *thee,
00167         int iatom,
00168         int isimp
00169     );
00170
00176     VEXTERNC int Vcsm_getNumberSimplices(
00177         Vcsm *thee,
00178         int iatom
00179     );
00180
00186     VEXTERNC SS* Vcsm_getSimplex(
00187         Vcsm *thee,
00188         int isimp,
00189         int iatom
00190     );
00191
00197     VEXTERNC int Vcsm_getSimplexIndex(
00198         Vcsm *thee,
00199         int isimp,
00200         int iatom
00201     );
00202
00209     VEXTERNC unsigned long int Vcsm_memChk(
00210         Vcsm *thee
00211     );
00212
00213 #else /* if defined(VINLINE_VCSM) */
00214 #   define Vcsm_getValist(thee) ((thee)->alist)
00215 #   define Vcsm_getNumberAtoms(thee, isimp) ((thee)->nsgm[isimp])
00216 #   define Vcsm_getAtom(thee, iatom, isimp) (Valist_getAtom((thee)->alist, ((thee)->sgm[isimp][iatom]))
00217 #   define Vcsm_getAtomIndex(thee, iatom, isimp) (((thee)->sgm[isimp][iatom])
00218 #   define Vcsm_getNumberSimplices(thee, iatom) (((thee)->nqsm[iatom])
00219 #   define Vcsm_getSimplex(thee, isimp, iatom) (Gem_SS((thee)->gm, ((thee)->qsm[iatom][isimp]))
00220 #   define Vcsm_getSimplexIndex(thee, isimp, iatom) (((thee)->qsm[iatom][isimp])
00221 #   define Vcsm_memChk(thee) (Vmem_bytes((thee)->vmem))
00222 #endif /* if !defined(VINLINE_VCSM) */
00223
00224 /* ////////////////////////////////////////
00225 // Class Vcsm: Non-Inlineable methods (vcsm.c)
00226
00227
00236 VEXTERNC Vcsm* Vcsm_ctor(
00237     Valist *alist, /**< List of atoms */
00238     Gem *gm
00239 );
00240
00249 VEXTERNC int Vcsm_ctor2(
00250     Vcsm *thee,
00251     Valist *alist,
00252     Gem *gm
00253 );
00254
00259 VEXTERNC void Vcsm_dtor(
00260     Vcsm **thee
00261 );
00262
00267 VEXTERNC void Vcsm_dtor2(
00268     Vcsm *thee
00269 );
00270
00277 VEXTERNC void Vcsm_init(
00278     Vcsm *thee
00279 );
00280
00287 VEXTERNC int Vcsm_update(
00288     Vcsm *thee,
00289     SS **simps,
00294     int num
00295 );
00296
00297 #endif /* ifndef _VCSM_H_ */

```

9.8 src/fem/vfetc.c File Reference

Class Vfetc methods.

Include dependency graph for vftk.c:



- Get the "fixed charge" contribution to the electrostatic energy.*

 - VPUBLIC double [Vfetk_dqmEnergy](#) ([Vfetk](#) *thee, int color)
- Get the "mobile charge" and "polarization" contributions to the electrostatic energy.*

 - VPUBLIC void [Vfetk_setAtomColors](#) ([Vfetk](#) *thee)
- Transfer color (partition ID) information from a partitioned mesh to the atoms.*

 - VPUBLIC unsigned long int [Vfetk_memChk](#) ([Vfetk](#) *thee)
- Return the memory used by this structure (and its contents) in bytes.*

 - VPUBLIC Vrc_Codes [Vfetk_genCube](#) ([Vfetk](#) *thee, double center[3], double length[3], [Vfetk_MeshLoad](#) mesh↔Type)
- Construct a rectangular mesh (in the current Vfetk object)*

 - VPUBLIC Vrc_Codes [Vfetk_loadMesh](#) ([Vfetk](#) *thee, double center[3], double length[3], [Vfetk_MeshLoad](#) mesh↔Type, Vio *sock)
- Loads a mesh into the Vfetk (and associated) object(s).*

 - VPUBLIC void [Bmat_printHB](#) (Bmat *thee, char *fname)
- Writes a Bmat to disk in Harwell-Boeing sparse matrix format.*

 - VPUBLIC PDE * [Vfetk_PDE_ctor](#) ([Vfetk](#) *fetk)
- Constructs the FEtk PDE object.*

 - VPUBLIC int [Vfetk_PDE_ctor2](#) (PDE *thee, [Vfetk](#) *fetk)
- Initializes the FEtk PDE object.*

 - VPUBLIC void [Vfetk_PDE_dtor](#) (PDE **thee)
- Destroys FEtk PDE object.*

 - VPUBLIC void [Vfetk_PDE_dtor2](#) (PDE *thee)
- FORTTRAN stub: destroys FEtk PDE object.*

 - VPUBLIC void [Vfetk_PDE_initAssemble](#) (PDE *thee, int ip[], double rp[])
- Do once-per-assembly initialization.*

 - VPUBLIC void [Vfetk_PDE_initElement](#) (PDE *thee, int elementType, int chart, double txx[][3], void *data)
 - VPUBLIC void [Vfetk_PDE_initFace](#) (PDE *thee, int faceType, int chart, double tnvex[])
- Do once-per-face initialization.*

 - VPUBLIC void [Vfetk_PDE_initPoint](#) (PDE *thee, int pointType, int chart, double txq[], double tU[], double tdU[][3])
 - VPUBLIC void [Vfetk_PDE_Fu](#) (PDE *thee, int key, double F[])
- Evaluate strong form of PBE. For interior points, this is:*

 - VPUBLIC double [Vfetk_PDE_Fu_v](#) (PDE *thee, int key, double V[], double dV[][[VAPBS_DIM](#)])
- This is the weak form of the PBE; i.e. the strong form integrated with a test function to give:*

 - VPUBLIC double [Vfetk_PDE_DFu_wv](#) (PDE *thee, int key, double W[], double dW[][[VAPBS_DIM](#)], double V[], double dV[][3])
 - VPUBLIC void [Vfetk_PDE_delta](#) (PDE *thee, int type, int chart, double txq[], void *user, double F[])
- Evaluate a (discretized) delta function source term at the given point.*

 - VPUBLIC void [Vfetk_PDE_u_D](#) (PDE *thee, int type, int chart, double txq[], double F[])
- Evaluate the Dirichlet boundary condition at the given point.*

 - VPUBLIC void [Vfetk_PDE_u_T](#) (PDE *thee, int type, int chart, double txq[], double F[])
- Evaluate the "true solution" at the given point for comparison with the numerical solution.*

 - VPUBLIC void [Vfetk_PDE_bisectEdge](#) (int dim, int dimII, int edgeType, int chart[], double vx[][3])
 - VPUBLIC void [Vfetk_PDE_mapBoundary](#) (int dim, int dimII, int vertexType, int chart, double vx[3])
 - VPUBLIC int [Vfetk_PDE_markSimplex](#) (int dim, int dimII, int simplexType, int faceType[[VAPBS_NVS](#)], int vertex↔Type[[VAPBS_NVS](#)], int chart[], double vx[][3], void *simplex)
 - VPUBLIC void [Vfetk_PDE_oneChart](#) (int dim, int dimII, int objType, int chart[], double vx[][3], int dimV)
 - VPUBLIC double [Vfetk_PDE_Ju](#) (PDE *thee, int key)
- Energy functional. This returns the energy (less delta function terms) in the form:*

- VPUBLIC void [Vfetk_externalUpdateFunction](#) (SS **simps, int num)
External hook to simplex subdivision routines in Gem. Called each time a simplex is subdivided (we use it to update the charge-simplex map)
- VPUBLIC int [Vfetk_PDE_simplexBasisInit](#) (int key, int dim, int comp, int *ndof, int dof[])
Initialize the bases for the trial or the test space, for a particular component of the system, at all quadrature points on the master simplex element.
- VPUBLIC void [Vfetk_PDE_simplexBasisForm](#) (int key, int dim, int comp, int pdkey, double xq[], double basis[])
Evaluate the bases for the trial or test space, for a particular component of the system, at all quadrature points on the master simplex element.
- VPUBLIC void [Vfetk_dumpLocalVar](#) ()
Debugging routine to print out local variables used by PDE object.
- VPUBLIC int [Vfetk_fillArray](#) ([Vfetk](#) *thee, Bvec *vec, [Vdata_Type](#) type)
Fill an array with the specified data.
- VPUBLIC int [Vfetk_write](#) ([Vfetk](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, Bvec *vec, [Vdata_Format](#) format)
Write out data.

Variables

- VPRIVATE [Vfetk_LocalVar](#) var
- VPRIVATE char * [diriCubeString](#)
- VPRIVATE char * [neumCubeString](#)
- VPRIVATE int [dim_2DP1](#) = 3
- VPRIVATE int [lgr_2DP1](#) [3][VMAXP]
- VPRIVATE int [lgr_2DP1x](#) [3][VMAXP]
- VPRIVATE int [lgr_2DP1y](#) [3][VMAXP]
- VPRIVATE int [lgr_2DP1z](#) [3][VMAXP]
- VPRIVATE int [dim_3DP1](#) = [VAPBS_NVS](#)
- VPRIVATE int [lgr_3DP1](#) [[VAPBS_NVS](#)][VMAXP]
- VPRIVATE int [lgr_3DP1x](#) [[VAPBS_NVS](#)][VMAXP]
- VPRIVATE int [lgr_3DP1y](#) [[VAPBS_NVS](#)][VMAXP]
- VPRIVATE int [lgr_3DP1z](#) [[VAPBS_NVS](#)][VMAXP]
- VPRIVATE const int [P_DEG](#) =1
- VPRIVATE int [numP](#)
- VPRIVATE double [c](#) [VMAXP][VMAXP]
- VPRIVATE double [cx](#) [VMAXP][VMAXP]
- VPRIVATE double [cy](#) [VMAXP][VMAXP]
- VPRIVATE double [cz](#) [VMAXP][VMAXP]

9.8.1 Detailed Description

Class Vfetk methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```

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*
*

```

Definition in file [vfetk.c](#).

9.8.2 Function Documentation**9.8.2.1 polyEval()**

```

VPRIVATE void polyEval (
    int numP,
    double p[],
    double c[][VMAXP],
    double xv[] )

```

Definition at line [2095](#) of file [vfetk.c](#).

9.8.2.2 Vfetc_PDE_bisectEdge()

```
VPUBLIC void Vfetc_PDE_bisectEdge (
    int dim,
    int dimII,
    int edgeType,
    int chart[],
    double vx[][3] )
```

Definition at line 1902 of file [vfetc.c](#).

9.8.2.3 Vfetc_PDE_DFu_wv()

```
VPUBLIC double Vfetc_PDE_DFu_wv (
    PDE * thee,
    int key,
    double W[],
    double dW[][VAPBS_DIM],
    double V[],
    double dV[][3] )
```

Definition at line 1741 of file [vfetc.c](#).

9.8.2.4 Vfetc_PDE_initElement()

```
VPUBLIC void Vfetc_PDE_initElement (
    PDE * thee,
    int elementType,
    int chart,
    double tvx[][3],
    void * data )
```

Definition at line 1528 of file [vfetc.c](#).

9.8.2.5 Vfetc_PDE_initPoint()

```
VPUBLIC void Vfetc_PDE_initPoint (
    PDE * thee,
    int pointType,
    int chart,
    double txq[],
    double tU[],
    double tdU[][3] )
```

Definition at line 1571 of file [vfetc.c](#).

9.8.2.6 Vfetc_PDE_mapBoundary()

```
VPUBLIC void Vfetc_PDE_mapBoundary (
    int dim,
    int dimII,
    int vertexType,
    int chart,
    double vx[3] )
```

Definition at line 1912 of file [vfetc.c](#).

9.8.2.7 Vfetk_PDE_markSimplex()

```
VPUBLIC int Vfetk_PDE_markSimplex (
    int dim,
    int dimII,
    int simplexType,
    int faceType[VAPBS_NVS],
    int vertexType[VAPBS_NVS],
    int chart[],
    double vx[][3],
    void * simplex )
```

Definition at line 1917 of file [vfetk.c](#).

9.8.2.8 Vfetk_PDE_oneChart()

```
VPUBLIC void Vfetk_PDE_oneChart (
    int dim,
    int dimII,
    int objType,
    int chart[],
    double vx[][3],
    int dimV )
```

Definition at line 1998 of file [vfetk.c](#).

9.8.3 Variable Documentation

9.8.3.1 c

```
VPRIVATE double c[VMAXP][VMAXP]
```

Definition at line 483 of file [vfetk.c](#).

9.8.3.2 cx

```
VPRIVATE double cx[VMAXP][VMAXP]
```

Definition at line 484 of file [vfetk.c](#).

9.8.3.3 cy

```
VPRIVATE double cy[VMAXP][VMAXP]
```

Definition at line 485 of file [vfetk.c](#).

9.8.3.4 cz

```
VPRIVATE double cz[VMAXP][VMAXP]
```

Definition at line 486 of file [vfetk.c](#).

9.8.3.5 dim_2DP1

```
VPRIVATE int dim_2DP1 = 3
```

Definition at line 366 of file [vfetk.c](#).

9.8.3.6 dim_3DP1

```
VPRIVATE int dim_3DP1 = VAPBS_NVS
```

Definition at line 437 of file [vfetk.c](#).

9.8.3.7 diriCubeString

```
VPRIVATE char* diriCubeString
```

Definition at line 93 of file [vfetk.c](#).

9.8.3.8 lgr_2DP1

```
VPRIVATE int lgr_2DP1[3][VMAXP]
```

Initial value:

```
= {
{ 2, -2, -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
}
```

Definition at line 386 of file [vfetk.c](#).

9.8.3.9 lgr_2DP1x

```
VPRIVATE int lgr_2DP1x[3][VMAXP]
```

Initial value:

```
= {
{ -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
}
```

Definition at line 395 of file [vfetk.c](#).

9.8.3.10 lgr_2DP1y

```
VPRIVATE int lgr_2DP1y[3][VMAXP]
```

Initial value:

```
= {
{ -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
}
```

Definition at line 402 of file [vfetk.c](#).

9.8.3.11 lgr_2DP1z

```
VPRIVATE int lgr_2DP1z[3][VMAXP]
```

Initial value:

```
= {
{ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
}
```

```
}
```

Definition at line 409 of file [vfetk.c](#).

9.8.3.12 lgr_3DP1

```
VPRIVATE int lgr_3DP1[VAPBS_NVS][VMAXP]
```

Initial value:

```
= {
{ 2, -2, -2, -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
}
```

Definition at line 438 of file [vfetk.c](#).

9.8.3.13 lgr_3DP1x

```
VPRIVATE int lgr_3DP1x[VAPBS_NVS][VMAXP]
```

Initial value:

```
= {
{ -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
}
```

Definition at line 446 of file [vfetk.c](#).

9.8.3.14 lgr_3DP1y

```
VPRIVATE int lgr_3DP1y[VAPBS_NVS][VMAXP]
```

Initial value:

```
= {
{ -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
}
```

Definition at line 454 of file [vfetk.c](#).

9.8.3.15 lgr_3DP1z

```
VPRIVATE int lgr_3DP1z[VAPBS_NVS][VMAXP]
```

Initial value:

```
= {
{ -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
}
```

Definition at line 462 of file [vfetk.c](#).

9.8.3.16 neumCubeString

```
VPRIVATE char* neumCubeString
```

Definition at line 130 of file [vfetk.c](#).

9.8.3.17 numP

VPRIVATE int numP

Definition at line 482 of file [vfetk.c](#).

9.8.3.18 P_DEG

VPRIVATE const int P_DEG =1

Definition at line 476 of file [vfetk.c](#).

9.8.3.19 var

VPRIVATE Vfetk_LocalVar var

Definition at line 86 of file [vfetk.c](#).

9.9 vfetk.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "vfetk.h"
00058
00059 /* Define the macro DONEUMANN to run with all-Neumann boundary conditions.
00060  * Set this macro at your own risk! */
00061 /* #define DONEUMANN 1 */
00062
00063 /*
00064  * @brief Calculate the contribution to the charge-potential energy from one
00065  * atom
00066  * @ingroup Vfetk
00067  * @author Nathan Baker
00068  * @param thee current Vfetk object
00069  * @param iatom current atom index
00070  * @param color simplex subset (partition) under consideration
00071  * @param sol current solution
00072  * @returns Per-atom energy
00073  */
00074 VPRIVATE double Vfetk_qfEnergyAtom(
00075     Vfetk *thee,
00076     int iatom,
00077     int color,
00078     double *sol
00079 );
00080
00081 /*
00082  * @brief Container for local variables
00083  * @ingroup Vfetk
00084  * @bug Not thread-safe
00085  */
00086 VPRIVATE Vfetk_LocalVar var;
00087
00088 /*
00089  * @brief MCSF-format cube mesh (all Dirichlet)
00090  * @ingroup Vfetk
00091  * @author Based on mesh by Mike Holst
00092  */
00093 VPRIVATE char *diriCubeString =
00094 "mcsf_begin=1;\n\
00095 \n\
00096 dim=3;\n\
00097 dimii=3;\n\
00098 vertices=8;\n\
00099 simplices=6;\n\
00100 \n\
00101 vert=[\n\
00102 0 0 -0.5 -0.5 -0.5\n\
00103 1 0 0.5 -0.5 -0.5\n\
00104 2 0 -0.5 0.5 -0.5\n\
00105 3 0 0.5 0.5 -0.5\n\
00106 4 0 -0.5 -0.5 0.5\n\

```

```

00107 5 0 0.5 -0.5 0.5\n\
00108 6 0 -0.5 0.5 0.5\n\
00109 7 0 0.5 0.5 0.5\n\
00110 ];\n\
00111 \n\
00112 simp=[\n\
00113 0 0 0 0 1 0 1 0 5 1 2\n\
00114 1 0 0 0 1 1 0 0 5 2 4\n\
00115 2 0 0 0 1 0 1 1 5 3 2\n\
00116 3 0 0 0 1 0 1 3 5 7 2\n\
00117 4 0 0 1 1 0 0 2 5 7 6\n\
00118 5 0 0 1 1 0 0 2 5 6 4\n\
00119 ];\n\
00120 \n\
00121 mcsf_end=1;\n\
00122 \n\
00123 ";
00124
00125 /*
00126 * @brief MCSF-format cube mesh (all Neumann)
00127 * @ingroup Vfetk
00128 * @author Based on mesh by Mike Holst
00129 */
00130 VPRIVATE char *neumCubeString =
00131 "mcsf_begin=1;\n\
00132 \n\
00133 dim=3;\n\
00134 dimii=3;\n\
00135 vertices=8;\n\
00136 simplices=6;\n\
00137 \n\
00138 vert=[\n\
00139 0 0 -0.5 -0.5 -0.5\n\
00140 1 0 0.5 -0.5 -0.5\n\
00141 2 0 -0.5 0.5 -0.5\n\
00142 3 0 0.5 0.5 -0.5\n\
00143 4 0 -0.5 -0.5 0.5\n\
00144 5 0 0.5 -0.5 0.5\n\
00145 6 0 -0.5 0.5 0.5\n\
00146 7 0 0.5 0.5 0.5\n\
00147 ];\n\
00148 \n\
00149 simp=[\n\
00150 0 0 0 0 2 0 2 0 5 1 2\n\
00151 1 0 0 0 2 2 0 0 5 2 4\n\
00152 2 0 0 0 2 0 2 1 5 3 2\n\
00153 3 0 0 0 2 0 2 3 5 7 2\n\
00154 4 0 0 2 2 0 0 2 5 7 6\n\
00155 5 0 0 2 2 0 0 2 5 6 4\n\
00156 ];\n\
00157 \n\
00158 mcsf_end=1;\n\
00159 \n\
00160 ";
00161
00162 /*
00163 * @brief Return the smoothed value of the dielectric coefficient at the
00164 * current point using a fast, chart-based method
00165 * @ingroup Vfetk
00166 * @author Nathan Baker
00167 * @returns Value of dielectric coefficient
00168 * @bug Not thread-safe
00169 */
00170 VPRIVATE double diel();
00171
00172 /*
00173 * @brief Return the smoothed value of the ion accessibility at the
00174 * current point using a fast, chart-based method
00175 * @ingroup Vfetk
00176 * @author Nathan Baker
00177 * @returns Value of mobile ion coefficient
00178 * @bug Not thread-safe
00179 */
00180 VPRIVATE double ionacc();
00181
00182 /*
00183 * @brief Smooths a mesh-based coefficient with a simple harmonic function
00184 * @ingroup Vfetk
00185 * @author Nathan Baker
00186 * @param meth Method for smoothing
00187 * \li 0 ==> arithmetic mean (gives bad results)

```

```

00188 * \li 1 ==> geometric mean
00189 * @param nverts Number of vertices
00190 * @param dist distance from point to each vertex
00191 * @param coeff coefficient value at each vertex
00192 * @note Thread-safe
00193 * @return smoothed value of coefficient at point of interest */
00194 VPRIVATE double smooth(
00195     int nverts,
00196     double dist[VAPBS_NVS],
00197     double coeff[VAPBS_NVS],
00198     int meth
00199 );
00200
00201
00202 /*
00203 * @brief Return the analytical multi-sphere Debye-Huckel approximation (in
00204 * kT/e) at the specified point
00205 * @ingroup Vfetk
00206 * @author Nathan Baker
00207 * @param pbe Vpbe object
00208 * @param d Dimension of x
00209 * @param x Coordinates of point of interest (in &Aring;)
00210 * @note Thread-safe
00211 * @returns Multi-sphere Debye-Huckel potential in kT/e
00212 */
00213 VPRIVATE double debye_U(
00214     Vpbe *pbe,
00215     int d,
00216     double x[]
00217 );
00218
00219 /*
00220 * @brief Return the difference between the analytical multi-sphere
00221 * Debye-Huckel approximation and Coulomb's law (in kT/e) at the specified
00222 * point
00223 * @ingroup Vfetk
00224 * @author Nathan Baker
00225 * @param pbe Vpbe object
00226 * @param d Dimension of x
00227 * @param x Coordinates of point of interest (in &Aring;)
00228 * @note Thread-safe
00229 * @returns Multi-sphere Debye-Huckel potential in kT/e */
00230 VPRIVATE double debye_Udiff(
00231     Vpbe *pbe,
00232     int d,
00233     double x[]
00234 );
00235
00236 /*
00237 * @brief Calculate the Coulomb's
00238 * Debye-Huckel approximation and Coulomb's law (in kT/e) at the specified
00239 * point
00240 * @ingroup Vfetk
00241 * @author Nathan Baker
00242 * @param pbe Vpbe object
00243 * @param d Dimension of x
00244 * @param x Coordinates of point of interest (in &Aring;)
00245 * @param eps Dielectric constant
00246 * @param U Set to potential (in kT/e)
00247 * @param dU Set to potential gradient (in kT/e/&Aring;)
00248 * @param d2U Set to Laplacian of potential (in  $f kT e^{-1} \AA^{-2} f$ )
00249 * @returns Multi-sphere Debye-Huckel potential in kT/e */
00250 VPRIVATE void coulomb(
00251     Vpbe *pbe,
00252     int d,
00253     double x[],
00254     double eps,
00255     double *U,
00256     double dU[],
00257     double *d2U
00258 );
00259
00260 /*
00261 * @brief 2D linear master simplex information generator
00262 * @ingroup Vfetk
00263 * @author Mike Holst
00264 * @param dimIS dunno
00265 * @param ndof dunno
00266 * @param dof dunno
00267 * @param c dunno
00268 * @param cx dunno

```

```

00269  * @note Trust in Mike */
00270 VPRIVATE void init_2DP1(
00271     int dimIS[],
00272     int *ndof,
00273     int dof[],
00274     double c[][VMAXP],
00275     double cx[][VMAXP],
00276     double cy[][VMAXP],
00277     double cz[][VMAXP]
00278 );
00279
00280 /*
00281  * @brief 3D linear master simplex information generator
00282  * @ingroup Vfetk
00283  * @author Mike Holst
00284  * @param dimIS dunno
00285  * @param ndof dunno
00286  * @param dof dunno
00287  * @param c dunno
00288  * @param cx dunno
00289  * @param cy dunno
00290  * @param cz dunno
00291  * @note Trust in Mike */
00292 VPRIVATE void init_3DP1(
00293     int dimIS[],
00294     int *ndof,
00295     int dof[],
00296     double c[][VMAXP],
00297     double cx[][VMAXP],
00298     double cy[][VMAXP],
00299     double cz[][VMAXP]
00300 );
00301
00302 /*
00303  * @brief Setup coefficients of polynomials from integer table data
00304  * @ingroup Vfetk
00305  * @author Mike Holst
00306  * @param numP dunno
00307  * @param c dunno
00308  * @param cx dunno
00309  * @param cy dunno
00310  * @param cz dunno
00311  * @param ic dunno
00312  * @param icx dunno
00313  * @param icy dunno
00314  * @param icz dunno
00315  * @note Trust in Mike */
00316 VPRIVATE void setCoef(
00317     int numP,
00318     double c[][VMAXP],
00319     double cx[][VMAXP],
00320     double cy[][VMAXP],
00321     double cz[][VMAXP],
00322     int ic[][VMAXP],
00323     int icx[][VMAXP],
00324     int icy[][VMAXP],
00325     int icz[][VMAXP]
00326 );
00327
00328 /*
00329  * @brief Evaluate a collection of at most cubic polynomials at a
00330  * specified point in at most R^3.
00331  * @ingroup Vfetk
00332  * @author Mike Holst
00333  * @param numP the number of polynomials to evaluate
00334  * @param p the results of the evaluation
00335  * @param c the coefficients of each polynomial
00336  * @param xv the point (x,y,z) to evaluate the polynomials.
00337  * @note Mike says:
00338  * <pre>
00339  * Note that "VMAXP" must be >= 19 for cubic polynomials.
00340  * The polynomials are build from the coefficients c[][] as
00341  * follows. To build polynomial "k", fix k and set:
00342  *
00343  * c0=c[k][0], c1=c[k][1], ... , cp=c[k][p]
00344  *
00345  * Then evaluate as:
00346  *
00347  * p3(x,y,z) = c0 + c1*x + c2*y + c3*z
00348  *             + c4*x*x + c5*y*y + c6*z*z + c7*x*y + c8*x*z + c9*y*z
00349  *             + c10*x*x*x + c11*y*y*y + c12*z*z*z

```

```

00350 *          + c13*x*x*y + c14*x*x*z + c15*x*y*y
00351 *          + c16*y*y*z + c17*x*z*z + c18*y*z*z
00352 * </pre>
00353 */
00354 VPRIVATE void polyEval(
00355     int numP,
00356     double p[],
00357     double c[][VMAXP],
00358     double xv[]
00359 );
00360
00361 /*
00362 * @brief I have no clue what this variable does, but we need it to initialize
00363 * the simplices
00364 * @ingroup Vfetk
00365 * @author Mike Holst */
00366 VPRIVATE int dim_2DP1 = 3;
00367
00368 /*
00369 * @brief I have no clue what these variable do, but we need it to initialize
00370 * the simplices
00371 * @ingroup Vfetk
00372 * @author Mike Holst
00373 * @note Mike says:
00374 * <pre>
00375 * 2D-P1 Basis:
00376 *
00377 * p1(x,y) = c0 + c1*x + c2*y
00378 *
00379 * Lagrange Point      Lagrange Basis Function Definition
00380 * -----
00381 * (0, 0)              p[0](x,y) = 1 - x - y
00382 * (1, 0)              p[1](x,y) = x
00383 * (0, 1)              p[2](x,y) = y
00384 * </pre>
00385 */
00386 VPRIVATE int lgr_2DP1[3][VMAXP] = {
00387     /*c0 c1 c2 c3
00388     * ----- */
00389     /* 1 x y z
00390     * ----- */
00391     { 2, -2, -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00392     { 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00393     { 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
00394 };
00395 VPRIVATE int lgr_2DP1x[3][VMAXP] = {
00396     /*c0 ----- */
00397     /* 1 ----- */
00398     { -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00399     { 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00400     { 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
00401 };
00402 VPRIVATE int lgr_2DP1y[3][VMAXP] = {
00403     /*c0 ----- */
00404     /* 1 ----- */
00405     { -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00406     { 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00407     { 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
00408 };
00409 VPRIVATE int lgr_2DP1z[3][VMAXP] = {
00410     /*c0 ----- */
00411     /* 1 ----- */
00412     { 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00413     { 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00414     { 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
00415 };
00416
00417
00418 /*
00419 * @brief I have no clue what these variable do, but we need it to initialize
00420 * the simplices
00421 * @ingroup Vfetk
00422 * @author Mike Holst
00423 * @note Mike says:
00424 * <pre>
00425 * 3D-P1 Basis:
00426 *
00427 * p1(x,y,z) = c0 + c1*x + c2*y + c3*z
00428 *
00429 * Lagrange Point      Lagrange Basis Function Definition
00430 * -----

```

```

00431 * (0, 0, 0)          p[0](x,y,z) = 1 - x - y - z
00432 * (1, 0, 0)          p[1](x,y,z) = x
00433 * (0, 1, 0)          p[2](x,y,z) = y
00434 * (0, 0, 1)          p[3](x,y,z) = z
00435 * </pre>
00436 */
00437 VPRIVATE int dim_3DP1 = VAPBS_NVS;
00438 VPRIVATE int lgr_3DP1[VAPBS_NVS][VMAXP] = {
00439 /*c0 c1 c2 c3 ----- */
00440 /* 1 x y z ----- */
00441 { 2, -2, -2, -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00442 { 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00443 { 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00444 { 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
00445 };
00446 VPRIVATE int lgr_3DP1x[VAPBS_NVS][VMAXP] = {
00447 /*c0 ----- */
00448 /* 1 ----- */
00449 { -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00450 { 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00451 { 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00452 { 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
00453 };
00454 VPRIVATE int lgr_3DP1y[VAPBS_NVS][VMAXP] = {
00455 /*c0 ----- */
00456 /* 1 ----- */
00457 { -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00458 { 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00459 { 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00460 { 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
00461 };
00462 VPRIVATE int lgr_3DP1z[VAPBS_NVS][VMAXP] = {
00463 /*c0 ----- */
00464 /* 1 ----- */
00465 { -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00466 { 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00467 { 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00468 { 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
00469 };
00470
00471 /*
00472 * @brief Another Holst variable
00473 * @ingroup Vfetk
00474 * @author Mike Holst
00475 * @note Mike says: 1 = linear, 2 = quadratic */
00476 VPRIVATE const int P_DEG=1;
00477
00478 /*
00479 * @brief Another Holst variable
00480 * @ingroup Vfetk
00481 * @author Mike Holst */
00482 VPRIVATE int numP;
00483 VPRIVATE double c[VMAXP][VMAXP];
00484 VPRIVATE double cx[VMAXP][VMAXP];
00485 VPRIVATE double cy[VMAXP][VMAXP];
00486 VPRIVATE double cz[VMAXP][VMAXP];
00487
00488 #if !defined(VINLINE_VFETK)
00489
00490 VPUBLIC Gem* Vfetk_getGem(Vfetk *thee) {
00491
00492     VASSERT(thee != VNULL);
00493     return thee->gm;
00494 }
00495
00496 VPUBLIC AM* Vfetk_getAM(Vfetk *thee) {
00497
00498     VASSERT(thee != VNULL);
00499     return thee->am;
00500 }
00501
00502 VPUBLIC Vpbe* Vfetk_getVpbe(Vfetk *thee) {
00503
00504     VASSERT(thee != VNULL);
00505     return thee->pbe;
00506 }
00507
00508
00509 VPUBLIC Vcsm* Vfetk_getVcsm(Vfetk *thee) {
00510
00511

```

```

00512     VASSERT(thee != VNULL);
00513     return thee->csm;
00514 }
00515 }
00516
00517 VPUBLIC int Vfetk_getAtomColor(Vfetk *thee,
00518                               int iatom
00519                               ) {
00520
00521     int natoms;
00522
00523     VASSERT(thee != VNULL);
00524
00525     natoms = Valist_getNumberAtoms(Vpbe_getValist(thee->pbe));
00526     VASSERT(iatom < natoms);
00527
00528     return Vatom_getPartID(Valist_getAtom(Vpbe_getValist(thee->pbe), iatom));
00529 }
00530 #endif /* if !defined(VINLINE_VFETK) */
00531
00532 VPUBLIC Vfetk* Vfetk_ctor(Vpbe *pbe,
00533                          Vhal_PBEType type
00534                          ) {
00535
00536     /* Set up the structure */
00537     Vfetk *thee = VNULL;
00538     thee = (Vfetk*)Vmem_malloc(VNULL, 1, sizeof(Vfetk) );
00539     VASSERT(thee != VNULL);
00540     VASSERT(Vfetk_ctor2(thee, pbe, type));
00541
00542     return thee;
00543 }
00544
00545 VPUBLIC int Vfetk_ctor2(Vfetk *thee,
00546                       Vpbe *pbe,
00547                       Vhal_PBEType type
00548                       ) {
00549
00550     int i;
00551     double center[VAPBS_DIM];
00552
00553     /* Make sure things have been properly initialized & store them */
00554     VASSERT(pbe != VNULL);
00555     thee->pbe = pbe;
00556     VASSERT(pbe->alist != VNULL);
00557     VASSERT(pbe->acc != VNULL);
00558
00559     /* Store PBE type */
00560     thee->type = type;
00561
00562     /* Set up memory management object */
00563     thee->vmem = Vmem_ctor("APBS:VFETK");
00564
00565     /* Set up FEtk objects */
00566     Vnm_print(0, "Vfetk_ctor2: Constructing PDE...\n");
00567     thee->pde = Vfetk_PDE_ctor(thee);
00568     Vnm_print(0, "Vfetk_ctor2: Constructing Gem...\n");
00569     thee->gm = Gem_ctor(thee->vmem, thee->pde);
00570     Vnm_print(0, "Vfetk_ctor2: Constructing Aprx...\n");
00571     thee->aprx = Aprx_ctor(thee->vmem, thee->gm, thee->pde);
00572     Vnm_print(0, "Vfetk_ctor2: Constructing Aprx...\n");
00573     thee->am = AM_ctor(thee->vmem, thee->aprx);
00574
00575     /* Reset refinement level */
00576     thee->level = 0;
00577
00578     /* Set default solver variables */
00579     thee->lkey = VLT_MG;
00580     thee->lmax = 1000000;
00581     thee->ltol = 1e-5;
00582     thee->lprec = VPT_MG;
00583     thee->nkey = VNT_NEW;
00584     thee->nmax = 1000000;
00585     thee->ntol = 1e-5;
00586     thee->gues = VGT_ZERO;
00587     thee->pjac = -1;
00588
00589     /* Store local copy of myself */
00590     var.fetk = thee;
00591     var.initGreen = 0;
00592

```

```

00593      /* Set up the external Gem subdivision hook */
00594      Gem_setExternalUpdateFunction(thee->gm, Vfetk_externalUpdateFunction);
00595
00596      /* Set up ion-related variables */
00597      var.zkappa2 = Vpbe_getZkappa2(var.fetk->pbe);
00598      var.ionstr = Vpbe_getBulkIonicStrength(var.fetk->pbe);
00599      if (var.ionstr > 0.0) var.zks2 = 0.5*var.zkappa2/var.ionstr;
00600      else var.zks2 = 0.0;
00601      Vpbe_getIons(var.fetk->pbe, &(var.nion), var.ionConc, var.ionRadii,
00602                  var.ionQ);
00603      for (i=0; i<var.nion; i++) {
00604          var.ionConc[i] = var.zks2 * var.ionConc[i] * var.ionQ[i];
00605      }
00606
00607      /* Set uninitialized objects to NULL */
00608      thee->pbeparm = VNULL;
00609      thee->feparm = VNULL;
00610      thee->csm = VNULL;
00611
00612      return 1;
00613 }
00614
00615 VPUBLIC void Vfetk_setParameters(Vfetk *thee,
00616                                PBEparm *pbeparm,
00617                                FEMparm *feparm
00618                                ) {
00619
00620     VASSERT(thee != VNULL);
00621     thee->feparm = feparm;
00622     thee->pbeparm = pbeparm;
00623 }
00624
00625 VPUBLIC void Vfetk_dtor(Vfetk **thee) {
00626     if ((*thee) != VNULL) {
00627         Vfetk_dtor2(*thee);
00628         //Vmem_free(VNULL, 1, sizeof(Vfetk), (void **)thee);
00629         (*thee) = VNULL;
00630     }
00631 }
00632
00633 VPUBLIC void Vfetk_dtor2(Vfetk *thee) {
00634     Vcsm_dtor(&(thee->csm));
00635     AM_dtor(&(thee->am));
00636     Aprx_dtor(&(thee->apr));
00637     Vfetk_PDE_dtor(&(thee->pde));
00638     Vmem_dtor(&(thee->vmem));
00639 }
00640
00641 VPUBLIC double* Vfetk_getSolution(Vfetk *thee,
00642                                  int *length
00643                                  ) {
00644
00645     int i;
00646     double *solution,
00647            *theAnswer;
00648     AM *am;
00649
00650     VASSERT(thee != VNULL);
00651
00652     /* Get the AM object */
00653     am = thee->am;
00654     /* Copy the solution into the w0 vector */
00655     Bvec_copy(am->w0, am->u);
00656     /* Add the Dirichlet conditions */
00657     Bvec_axpy(am->w0, am->ud, 1.);
00658     /* Get the data from the Bvec */
00659     solution = Bvec_addr(am->w0);
00660     /* Get the length of the data from the Bvec */
00661     *length = Bvec_numRT(am->w0);
00662     /* Make sure that we got scalar data (only one block) for the solution
00663        * to the FETK */
00664     VASSERT(1 == Bvec_numB(am->w0));
00665     /* Allocate space for the returned vector and copy the solution into it */
00666     theAnswer = VNULL;
00667     theAnswer = (double*)Vmem_malloc(VNULL, *length, sizeof(double));
00668     VASSERT(theAnswer != VNULL);
00669     for (i=0; i<(*length); i++) theAnswer[i] = solution[i];
00670
00671     return theAnswer;
00672 }
00673

```



```

00674
00693 VPUBLIC double Vfetk_energy(Vfetk *thee,
00694                             int color,
00698                             int nonlin
00700                             ) {
00701
00702     double totEnergy = 0.0,
00703           qfEnergy = 0.0,
00704           dqmEnergy = 0.0;
00706     VASSERT(thee != VNULL);
00707
00708     if (nonlin && (Vpbe_getBulkIonicStrength(thee->pbe) > 0.)) {
00709         Vnm_print(0, "Vfetk_energy: calculating full PBE energy\n");
00710         Vnm_print(0, "Vfetk_energy: bulk ionic strength = %g M\n",
00711                 Vpbe_getBulkIonicStrength(thee->pbe));
00712         dqmEnergy = Vfetk_dqmEnergy(thee, color);
00713         Vnm_print(0, "Vfetk_energy: dqmEnergy = %g kT\n", dqmEnergy);
00714         qfEnergy = Vfetk_qfEnergy(thee, color);
00715         Vnm_print(0, "Vfetk_energy: qfEnergy = %g kT\n", qfEnergy);
00716
00717         totEnergy = qfEnergy - dqmEnergy;
00718     } else {
00719         Vnm_print(0, "Vfetk_energy: calculating only q-phi energy\n");
00720         dqmEnergy = Vfetk_dqmEnergy(thee, color);
00721         Vnm_print(0, "Vfetk_energy: dqmEnergy = %g kT (NOT USED)\n", dqmEnergy);
00722         qfEnergy = Vfetk_qfEnergy(thee, color);
00723         Vnm_print(0, "Vfetk_energy: qfEnergy = %g kT\n", qfEnergy);
00724         totEnergy = 0.5*qfEnergy;
00725     }
00726
00727     return totEnergy;
00728 }
00729 }
00730
00731
00732 VPUBLIC double Vfetk_qfEnergy(Vfetk *thee,
00733                             int color
00734                             ) {
00735
00736     double *sol,
00737           energy = 0.0;
00738     int nsol,
00739         iatom,
00740         natoms;
00741     AM *am;
00742
00743     VASSERT(thee != VNULL);
00744     am = thee->am;
00745
00746     /* Get the finest level solution */
00747     sol = VNULL;
00748     sol = Vfetk_getSolution(thee, &nsol);
00749     VASSERT(sol != VNULL);
00750
00751     /* Make sure the number of entries in the solution array matches the
00752      * number of vertices currently in the mesh */
00753     if (nsol != Gem_numVV(thee->gm)) {
00754         Vnm_print(2, "Vfetk_qfEnergy: Number of unknowns in solution does not match\n");
00755         Vnm_print(2, "Vfetk_qfEnergy: number of vertices in mesh!!! Bailing out!\n");
00756         VASSERT(0);
00757     }
00758
00759     /* Now we do the sum over atoms... */
00760     natoms = Valist_getNumberAtoms(thee->pbe->alist);
00761     for (iatom=0; iatom<natoms; iatom++) {
00762
00763         energy = energy + Vfetk_qfEnergyAtom(thee, iatom, color, sol);
00764
00765     } /* end for iatom */
00766
00767     /* Destroy the finest level solution */
00768     Vmem_free(VNULL, nsol, sizeof(double), (void **)&sol);
00769
00770     /* Return the energy */
00771     return energy;
00772 }
00773
00774 VPRIVATE double Vfetk_qfEnergyAtom(
00775     Vfetk *thee,
00776     int iatom,
00777     int color,

```

```

00778         double *sol) {
00779
00780     Vatom *atom;
00781     double charge,
00782            phi[VAPBS_NVS],
00783            phix[VAPBS_NVS][3],
00784            *position,
00785            uval,
00786            energy = 0.0;
00787     int isimp,
00788         nsimps,
00789         icolor,
00790         ivert,
00791         usingColor;
00792     SS *simp;
00793
00794
00795     /* Get atom information */
00796     atom = Valist_getAtom(thee->pbe->alist, iatom);
00797     icolor = Vfetc_getAtomColor(thee, iatom);
00798     charge = Vatom_getCharge(atom);
00799     position = Vatom_getPosition(atom);
00800
00801     /* Find out if we're using colors */
00802     usingColor = (color >= 0);
00803
00804     if (usingColor && (icolor<0)) {
00805         Vnm_print(2, "Vfetc_qfEnergy: Atom colors not set!\n");
00806         VASSERT(0);
00807     }
00808
00809     /* Check if this atom belongs to the specified partition */
00810     if ((icolor==color) || (!usingColor)) {
00811         /* Loop over the simps associated with this atom */
00812         nsimps = Vcsm_getNumberSimplices(thee->csm, iatom);
00813
00814         /* Get the first simp of the correct color; we can use just one
00815          * simplex for energy evaluations, but not for force
00816          * evaluations */
00817         for (isimp=0; isimp<nsimps; isimp++) {
00818
00819             simp = Vcsm_getSimplex(thee->csm, isimp, iatom);
00820
00821             /* If we've asked for a particular partition AND if the atom
00822              * is our partition, then compute the energy */
00823             if ((SS_chart(simp)==color) || (color<0)) {
00824                 /* Get the value of each basis function evaluated at this
00825                  * point */
00826                 Gem_pointInSimplexVal(thee->gm, simp, position, phi, phix);
00827                 for (ivert=0; ivert<SS_dimVV(simp); ivert++) {
00828                     uval = sol[VV_id(SS_vertex(simp,ivert))];
00829                     energy += (charge*phi[ivert]*uval);
00830                 } /* end for ivert */
00831                 /* We only use one simplex of the appropriate color for
00832                  * energy calculations, so break here */
00833                 break;
00834             } /* endif (color) */
00835         } /* end for isimp */
00836     }
00837
00838     return energy;
00839 }
00840
00841
00842 VPUBLIC double Vfetc_dqmEnergy(Vfetc *thee,
00843                               int color) {
00844
00845     return AM_evalJ(thee->am);
00846 }
00847
00848
00849 VPUBLIC void Vfetc_setAtomColors(Vfetc *thee) {
00850
00851     SS *simp;
00852     Vatom *atom;
00853     int i,
00854         natoms;
00855
00856     VASSERT(thee != VNULL);
00857
00858     natoms = Valist_getNumberAtoms(thee->pbe->alist);

```

```

00859     for (i=0; i<natoms; i++) {
00860         atom = Valist_getAtom(thee->pbe->alist, i);
00861         simp = Vcsm_getSimplex(thee->csm, 0, i);
00862         Vatom_setPartID(atom, SS_chart(simp));
00863     }
00864 }
00865 }
00866
00867 VPUBLIC unsigned long int Vfetk_memChk(Vfetk *thee) {
00868     int memUse = 0;
00869
00870     if (thee == VNULL) return 0;
00871
00872     memUse = memUse + sizeof(Vfetk);
00873     memUse = memUse + Vcsm_memChk(thee->csm);
00874
00875     return memUse;
00876 }
00877 }
00878
00885 VPUBLIC Vrc_Codes Vfetk_genCube(Vfetk *thee,
00886                                 double center[3],
00887                                 double length[3],
00888                                 Vfetk_MeshLoad meshType
00889                                 ) {
00890
00891     VASSERT(thee != VNULL);
00892
00893     AM *am = VNULL; /* @todo - no idea what this is */
00894     Gem *gm = VNULL; /* Geometry manager */
00895
00896     int skey = 0, /* Simplex format */
00897         bufsize = 0, /* Buffer size */
00898         i, /* Loop counter */
00899         j; /* Loop counter */
00900     char *key = "r", /* Read */
00901         *iodev = "BUFF", /* Buffer */
00902         *iofmt = "ASC", /* ASCII */
00903         *iohost = "localhost", /* localhost (dummy) */
00904         *iofile = "0", /*< socket 0 (dummy) */
00905         buf[VMAX_BUF_SIZE]; /* Socket buffer */
00906     Vio *sock = VNULL; /* Socket object */
00907     VV *vx = VNULL; /* @todo - no idea what this is */
00908     double x;
00909
00910     am = thee->am;
00911     VASSERT(am != VNULL);
00912     gm = thee->gm;
00913     VASSERT(gm != VNULL);
00914
00915     /* @note This code is based on Gem_makeCube by Mike Holst */
00916     /* Write mesh string to buffer and read back */
00917     switch (meshType) {
00918     case VML_DIRICUBE:
00919         /* Create a new copy of the DIRICUBE mesh (see globals higher in this file) */
00920         bufsize = strlen(diriCubeString);
00921         VASSERT( bufsize <= VMAX_BUF_SIZE );
00922         strncpy(buf, diriCubeString, VMAX_BUF_SIZE);
00923         break;
00924     case VML_NEUMCUBE:
00925         /* Create a new copy of the NEUMCUBE mesh (see globals higher in this file) */
00926         bufsize = strlen(neumCubeString);
00927         Vnm_print(2, "Vfetk_genCube: WARNING! USING EXPERIMENTAL NEUMANN BOUNDARY CONDITIONS!\n");
00928         VASSERT( bufsize <= VMAX_BUF_SIZE );
00929         strncpy(buf, neumCubeString, VMAX_BUF_SIZE);
00930         break;
00931     case VML_EXTERNAL:
00932         Vnm_print(2, "Vfetk_genCube: Got request for external mesh!\n");
00933         Vnm_print(2, "Vfetk_genCube: How did we get here?\n");
00934         return VRC_FAILURE;
00935     default:
00936         Vnm_print(2, "Vfetk_genCube: Unknown mesh type (%d)\n", meshType);
00937         return VRC_FAILURE;
00938     }
00939
00940     VASSERT( VNULL != (sock=Vio_socketOpen(key,iodev,iofmt,iohost,iofile)) ); /* Open socket */
00941     Vio_bufTake(sock, buf, bufsize); /* Initialize internal buffer for socket */
00942     AM_read(am, skey, sock); /* Take the initial mesh from the socket and load
00943                               into internal AM data structure with simplex
00944                               format */
00945     Vio_connectFree(sock); /* Purge output buffers */

```

```

00946     Vio_bufGive(sock); /* Get pointer to output buffer? No assignment of return value... */
00947     Vio_dtor(&sock); /* Destroy output buffer */
00948
00949     /* @todo - could the following be done in a single pass? - PCE */
00950     /* Scale (unit) cube - for each vertex, set the new coordinates of that
00951        vertex based on the vertex length */
00952     for (i=0; i<Gem_numVV(gm); i++) {
00953         vx = Gem_VV(gm, i);
00954         for (j=0; j<3; j++) {
00955             x = VV_coord(vx, j);
00956             x *= length[j];
00957             VV_setCoord(vx, j, x);
00958         }
00959     }
00960
00961     /* Add new center - for each vertex, set a new center for the vertex */
00962     for (i=0; i<Gem_numVV(gm); i++) {
00963         vx = Gem_VV(gm, i);
00964         for (j=0; j<3; j++) {
00965             x = VV_coord(vx, j);
00966             x += center[j];
00967             VV_setCoord(vx, j, x);
00968         }
00969     }
00970
00971     return VRC_SUCCESS;
00972 }
00973
00980 VPUBLIC Vrc_Codes Vfetc_loadMesh(Vfetc *thee, /* Vfetc object to load into */
00981                                double center[3], /* Center for mesh (if constructed) */
00982                                double length[3], /* Mesh lengths (if constructed) */
00983                                Vfetc_MeshLoad meshType, /* Type of mesh to load */
00984                                Vio *sock /* Socket for external mesh data (NULL otherwise) */
00985                                ) {
00986
00987     Vrc_Codes vrc; /* Function return codes - see vhal.h for enum */
00988     int skey = 0; /* Simplex format */
00989
00990     /* Load mesh from socket if external mesh, otherwise generate mesh */
00991     switch (meshType) {
00992     case VML_EXTERNAL:
00993         if (sock == VNULL) {
00994             Vnm_print(2, "Vfetc_loadMesh: Got NULL socket!\n");
00995             return VRC_FAILURE;
00996         }
00997         AM_read(thee->am, skey, sock);
00998         Vio_connectFree(sock);
00999         Vio_bufGive(sock);
01000         Vio_dtor(&sock);
01001         break;
01002     case VML_DIRICUBE:
01003     case VML_NEUMCUBE:
01004         /* Create new mesh and store in thee */
01005         vrc = Vfetc_genCube(thee, center, length, meshType);
01006         if (vrc == VRC_FAILURE) return VRC_FAILURE;
01007         break;
01008     default:
01009         Vnm_print(2, "Vfetc_loadMesh: unrecognized mesh type (%d)!\n",
01010                 meshType);
01011         return VRC_FAILURE;
01012     };
01013
01014     /* Setup charge-simplex map */
01015     Vnm_print(0, "Vfetc_ctor2: Constructing Vcsm...\n");
01016     thee->csm = VNULL;
01017     /* Construct a new Vcsm with the atom list and gem data */
01018     thee->csm = Vcsm_ctor(Vpbe_getValist(thee->pbe), thee->gm);
01019     VASSERT(thee->csm != VNULL);
01020     Vcsm_init(thee->csm);
01021
01022     return VRC_SUCCESS;
01023 }
01024
01025
01026 VPUBLIC void Bmat_printHB(Bmat *thee,
01027                          char *fname
01028                          ) {
01029
01030     Mat *Ablock;
01031     MATsym pqsym;
01032     int i, j, jj;

```

```

01033     int *IA, *JA;
01034     double *D, *L, *U;
01035     FILE *fp;
01036
01037     char mmtitle[72];
01038     char mmkey[] = {"8charkey"};
01039     int totc = 0, ptrc = 0, indc = 0, valc = 0;
01040     char mxtyp[] = {"RUA"}; /* Real Unsymmetric Assembled */
01041     int nrow = 0, ncol = 0, numZ = 0;
01042     int numZdigits = 0, nrowdigits = 0;
01043     int nptrline = 8, nindline = 8, nvalline = 5;
01044     char ptrfmt[] = {"(8I10)"}; /* ptrfmtstr[] = {"%10d"};
01045     char indfmt[] = {"(8I10)"}; /* indfmtstr[] = {"%10d"};
01046     char valfmt[] = {"(5E16.8)"}; /* valfmtstr[] = {"%16.8E"};
01047
01048     VASSERT( thee->numB == 1 ); /* HARDWARE FOR NOW */
01049     Ablock = thee->AD[0][0];
01050
01051     VASSERT( Mat_format( Ablock ) == DRC_FORMAT ); /* HARDWARE FOR NOW */
01052
01053     pqsym = Mat_sym( Ablock );
01054
01055     if ( pqsym == IS_SYM ) {
01056         mxtyp[1] = 'S';
01057     } else if ( pqsym == ISNOT_SYM ) {
01058         mxtyp[1] = 'U';
01059     } else {
01060         VASSERT( 0 ); /* NOT VALID */
01061     }
01062
01063     nrow = Bmat_numRT( thee ); /* Number of rows */
01064     ncol = Bmat_numCT( thee ); /* Number of cols */
01065     numZ = Bmat_numZT( thee ); /* Number of entries */
01066
01067     nrowdigits = (int) (log( nrow )/log( 10 )) + 1;
01068     numZdigits = (int) (log( numZ )/log( 10 )) + 1;
01069
01070     nptrline = (int) ( 80 / (numZdigits + 1) );
01071     nindline = (int) ( 80 / (nrowdigits + 1) );
01072
01073     sprintf(ptrfmt, "(%dI%d)", nptrline, numZdigits+1);
01074     sprintf(ptrfmtstr, "%%%dd", numZdigits+1);
01075     sprintf(indfmt, "(%dI%d)", nindline, nrowdigits+1);
01076     sprintf(indfmtstr, "%%%dd", nrowdigits+1);
01077
01078     ptrc = (int) ( ( ncol + 1 ) - 1 ) / nptrline ) + 1;
01079     indc = (int) ( ( numZ - 1 ) / nindline ) + 1;
01080     valc = (int) ( ( numZ - 1 ) / nvalline ) + 1;
01081
01082     totc = ptrc + indc + valc;
01083
01084     sprintf( mmtitle, "Sparse '%s' Matrix - Harwell-Boeing Format - '%s'",
01085             thee->name, fname );
01086
01087     /* Step 0: Open the file for writing */
01088
01089     fp = fopen( fname, "w" );
01090     if (fp == VNULL) {
01091         Vnm_print(2, "Bmat_printHB: Ouch couldn't open file <%s>\n", fname);
01092         return;
01093     }
01094
01095     /* Step 1: Print the header information */
01096
01097     fprintf( fp, "%-72s%-8s\n", mmtitle, mmkey );
01098     fprintf( fp, "%14d%14d%14d%14d\n", totc, ptrc, indc, valc, 0 );
01099     fprintf( fp, "%3s%11s%14d%14d%14d\n", mxtyp, " ", nrow, ncol, numZ );
01100     fprintf( fp, "%-16s%-16s%-20s%-20s\n", ptrfmt, indfmt, valfmt, "6E13.5" );
01101
01102     IA = Ablock->IA;
01103     JA = Ablock->JA;
01104     D = Ablock->diag;
01105     L = Ablock->offL;
01106     U = Ablock->offU;
01107
01108     if ( pqsym == IS_SYM ) {
01109
01110         /* Step 2: Print the pointer information */
01111
01112         for (i=0; i<(ncol+1); i++) {
01113             fprintf( fp, ptrfmtstr, Ablock->IA[i] + (i+1) );

```

```

01114         if ( ( i+1 ) % nptrline ) == 0 ) {
01115             fprintf( fp, "\n" );
01116         }
01117     }
01118
01119     if ( ( (ncol+1) % nptrline ) != 0 ) {
01120         fprintf( fp, "\n" );
01121     }
01122
01123     /* Step 3: Print the index information */
01124
01125     j = 0;
01126     for (i=0; i<ncol; i++) {
01127         fprintf( fp, indfmtstr, i+1); /* diagonal */
01128         if ( ( (j+1) % nindline ) == 0 ) {
01129             fprintf( fp, "\n" );
01130         }
01131         j++;
01132         for (jj=IA[i]; jj<IA[i+1]; jj++) {
01133             fprintf( fp, indfmtstr, JA[jj] + 1 ); /* lower triangle */
01134             if ( ( (j+1) % nindline ) == 0 ) {
01135                 fprintf( fp, "\n" );
01136             }
01137             j++;
01138         }
01139     }
01140
01141     if ( ( j % nindline ) != 0 ) {
01142         fprintf( fp, "\n" );
01143     }
01144
01145     /* Step 4: Print the value information */
01146
01147     j = 0;
01148     for (i=0; i<ncol; i++) {
01149         fprintf( fp, valfmtstr, D[i] );
01150         if ( ( (j+1) % nvalline ) == 0 ) {
01151             fprintf( fp, "\n" );
01152         }
01153         j++;
01154         for (jj=IA[i]; jj<IA[i+1]; jj++) {
01155             fprintf( fp, valfmtstr, L[jj] );
01156             if ( ( (j+1) % nvalline ) == 0 ) {
01157                 fprintf( fp, "\n" );
01158             }
01159             j++;
01160         }
01161     }
01162
01163     if ( ( j % nvalline ) != 0 ) {
01164         fprintf( fp, "\n" );
01165     }
01166
01167     } else { /* ISNOT_SYM */
01168
01169         VASSERT( 0 ); /* NOT CODED YET */
01170     }
01171
01172     /* Step 5: Close the file */
01173     fclose( fp );
01174 }
01175
01176 VPUBLIC PDE* Vfetk_PDE_ctor(Vfetk *fetk) {
01177
01178     PDE *thee = VNULL;
01179
01180     thee = (PDE*)Vmem_malloc(fetk->vmem, 1, sizeof(PDE));
01181     VASSERT(thee != VNULL);
01182     VASSERT(Vfetk_PDE_ctor2(thee, fetk));
01183
01184     return thee;
01185 }
01186
01187 VPUBLIC int Vfetk_PDE_ctor2(PDE *thee,
01188                             Vfetk *fetk
01189                             ) {
01190
01191     int i;
01192
01193     if (thee == VNULL) {
01194         Vnm_print(2, "Vfetk_PDE_ctor2: Got NULL thee!\n");

```

```

01195         return 0;
01196     }
01197
01198     /* Store a local copy of the Vfetk class */
01199     var.fetk = fetk;
01200
01201     /* PDE-specific parameters and function pointers */
01202     thee->initAssemble = Vfetk_PDE_initAssemble;
01203     thee->initElement = Vfetk_PDE_initElement;
01204     thee->initFace = Vfetk_PDE_initFace;
01205     thee->initPoint = Vfetk_PDE_initPoint;
01206     thee->Fu = Vfetk_PDE_Fu;
01207     thee->Fu_v = Vfetk_PDE_Fu_v;
01208     thee->DFu_wv = Vfetk_PDE_DFu_wv;
01209     thee->delta = Vfetk_PDE_delta;
01210     thee->u_D = Vfetk_PDE_u_D;
01211     thee->u_T = Vfetk_PDE_u_T;
01212     thee->Ju = Vfetk_PDE_Ju;
01213     thee->vec = 1; /* FIX! */
01214     thee->sym[0][0] = 1;
01215     thee->est[0] = 1.0;
01216     for (i=0; i<VMAX_BDTYPE; i++) thee->bmap[0][i] = i;
01217
01218     /* Manifold-specific function pointers */
01219     thee->bisectEdge = Vfetk_PDE_bisectEdge;
01220     thee->mapBoundary = Vfetk_PDE_mapBoundary;
01221     thee->markSimplex = Vfetk_PDE_markSimplex;
01222     thee->oneChart = Vfetk_PDE_oneChart;
01223
01224     /* Element-specific function pointers */
01225     thee->simplexBasisInit = Vfetk_PDE_simplexBasisInit;
01226     thee->simplexBasisForm = Vfetk_PDE_simplexBasisForm;
01227
01228     return 1;
01229 }
01230
01231 VPUBLIC void Vfetk_PDE_dtor(PDE **thee) {
01232
01233     if ((*thee) != VNULL) {
01234         Vfetk_PDE_dtor2(*thee);
01235         /* TODO: The following line is commented out because at the moment,
01236            there is a seg fault when deallocating at the end of a run. Since
01237            this routine is called only once at the very end, we'll leave it
01238            commented out. However, this could be a memory leak.
01239            */
01240         /* Vmem_free(var.fetk->vmem, 1, sizeof(PDE), (void **)thee); */
01241         (*thee) = VNULL;
01242     }
01243
01244 }
01245
01246 VPUBLIC void Vfetk_PDE_dtor2(PDE *thee) {
01247     var.fetk = VNULL;
01248 }
01249
01250 VPRIVATE double smooth(int nverts, double dist[VAPBS_NVS], double coeff[VAPBS_NVS], int meth) {
01251
01252     int i;
01253     double weight;
01254     double num = 0.0;
01255     double den = 0.0;
01256
01257     for (i=0; i<nverts; i++) {
01258         if (dist[i] < VSMALL) return coeff[i];
01259         weight = 1.0/dist[i];
01260         if (meth == 0) {
01261             num += (weight * coeff[i]);
01262             den += weight;
01263         } else if (meth == 1) {
01264             /* Small coefficients reset the average to 0; we need to break out
01265                * of the loop */
01266             if (coeff[i] < VSMALL) {
01267                 num = 0.0;
01268                 break;
01269             } else {
01270                 num += weight; den += (weight/coeff[i]);
01271             }
01272         } else VASSERT(0);
01273     }
01274
01275     return (num/den);

```

```

01276
01277 }
01278
01279 VPRIVATE double diel() {
01280
01281     int i, j;
01282     double eps, epsp, epsw, dist[5], coeff[5], srاد, swin, *vx;
01283     Vsurf_Meth srfm;
01284     Vacc *acc;
01285     PBEparm *pbeparm;
01286
01287     epsp = Vpbe_getSoluteDiel(var.fetk->pbe);
01288     epsw = Vpbe_getSolventDiel(var.fetk->pbe);
01289     VASSERT(var.fetk->pbeparm != VNULL);
01290     pbeparm = var.fetk->pbeparm;
01291     srfm = pbeparm->srfm;
01292     srاد = pbeparm->srاد;
01293     swin = pbeparm->swin;
01294     acc = var.fetk->pbe->acc;
01295
01296     eps = 0;
01297
01298     if (VABS(epsp - epsw) < VSMALL) return epsp;
01299     switch (srfm) {
01300     case VSM_MOL:
01301         eps = ((epsw-epsp)*Vacc_molAcc(acc, var.xq, srاد) + epsp);
01302         break;
01303     case VSM_MOLSMOOTH:
01304         for (i=0; i<var.nverts; i++) {
01305             dist[i] = 0;
01306             vx = var.vx[i];
01307             for (j=0; j<3; j++) {
01308                 dist[i] += VSQR(var.xq[j] - vx[j]);
01309             }
01310             dist[i] = VSQRT(dist[i]);
01311             coeff[i] = (epsw-epsp)*Vacc_molAcc(acc, var.xq, srاد) + epsp;
01312         }
01313         eps = smooth(var.nverts, dist, coeff, 1);
01314         break;
01315     case VSM_SPLINE:
01316         eps = ((epsw-epsp)*Vacc_splineAcc(acc, var.xq, swin, 0.0) + epsp);
01317         break;
01318     default:
01319         Vnm_print(2, "Undefined surface method (%d)!\n", srfm);
01320         VASSERT(0);
01321     }
01322
01323     return eps;
01324 }
01325
01326 VPRIVATE double ionacc() {
01327
01328     int i, j;
01329     double dist[5], coeff[5], irاد, swin, *vx, accval;
01330     Vsurf_Meth srfm;
01331     Vacc *acc = VNULL;
01332     PBEparm *pbeparm = VNULL;
01333
01334     VASSERT(var.fetk->pbeparm != VNULL);
01335     pbeparm = var.fetk->pbeparm;
01336     srfm = pbeparm->srfm;
01337     irاد = Vpbe_getMaxIonRadius(var.fetk->pbe);
01338     swin = pbeparm->swin;
01339     acc = var.fetk->pbe->acc;
01340
01341     if (var.zks2 < VSMALL) return 0.0;
01342     switch (srfm) {
01343     case VSM_MOL:
01344         accval = Vacc_ivdwAcc(acc, var.xq, irاد);
01345         break;
01346     case VSM_MOLSMOOTH:
01347         for (i=0; i<var.nverts; i++) {
01348             dist[i] = 0;
01349             vx = var.vx[i];
01350             for (j=0; j<3; j++) {
01351                 dist[i] += VSQR(var.xq[j] - vx[j]);
01352             }
01353             dist[i] = VSQRT(dist[i]);
01354             coeff[i] = Vacc_ivdwAcc(acc, var.xq, irاد);
01355         }
01356         accval = smooth(var.nverts, dist, coeff, 1);

```



```

01357         break;
01358     case VSM_SPLINE:
01359         accval = Vacc_splineAcc(acc, var.xq, swin, irad);
01360         break;
01361     default:
01362         Vnm_print(2, "Undefined surface method (%d)!\n", srfm);
01363         VASSERT(0);
01364     }
01365
01366     return accval;
01367 }
01368
01369 VPRIVATE double debye_U(Vpbe *pbe, int d, double x[]) {
01370
01371     double size, *position, charge, xkappa, eps_w, dist, T, pot, val;
01372     int iatom, i;
01373     Valist *alist;
01374     Vatom *atom;
01375
01376     eps_w = Vpbe_getSolventDiel(pbe);
01377     xkappa = (1.0e10)*Vpbe_getXkappa(pbe);
01378     T = Vpbe_getTemperature(pbe);
01379     alist = Vpbe_getValist(pbe);
01380     val = 0;
01381     pot = 0;
01382
01383     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
01384         atom = Valist_getAtom(alist, iatom);
01385         position = Vatom_getPosition(atom);
01386         charge = Vunit_ec*Vatom_getCharge(atom);
01387         size = (1e-10)*Vatom_getRadius(atom);
01388         dist = 0;
01389         for (i=0; i<d; i++) {
01390             dist += VSQR(position[i] - x[i]);
01391         }
01392         dist = (1.0e-10)*VSQRT(dist);
01393         val = (charge)/(4*VPI*Vunit_eps0*eps_w*dist);
01394         if (xkappa != 0.0) {
01395             val = val*(exp(-xkappa*(dist-size))/(1+xkappa*size));
01396         }
01397         pot = pot + val;
01398     }
01399     pot = pot*Vunit_ec/(Vunit_kb*T);
01400
01401     return pot;
01402 }
01403
01404 VPRIVATE double debye_Udiff(Vpbe *pbe, int d, double x[]) {
01405
01406     double size, *position, charge, eps_p, dist, T, pot, val;
01407     double Ufull;
01408     int iatom, i;
01409     Valist *alist;
01410     Vatom *atom;
01411
01412     Ufull = debye_U(pbe, d, x);
01413
01414     eps_p = Vpbe_getSoluteDiel(pbe);
01415     T = Vpbe_getTemperature(pbe);
01416     alist = Vpbe_getValist(pbe);
01417     val = 0;
01418     pot = 0;
01419
01420     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
01421         atom = Valist_getAtom(alist, iatom);
01422         position = Vatom_getPosition(atom);
01423         charge = Vunit_ec*Vatom_getCharge(atom);
01424         size = (1e-10)*Vatom_getRadius(atom);
01425         dist = 0;
01426         for (i=0; i<d; i++) {
01427             dist += VSQR(position[i] - x[i]);
01428         }
01429         dist = (1.0e-10)*VSQRT(dist);
01430         val = (charge)/(4*VPI*Vunit_eps0*eps_p*dist);
01431         pot = pot + val;
01432     }
01433     pot = pot*Vunit_ec/(Vunit_kb*T);
01434
01435     pot = Ufull - pot;
01436
01437     return pot;

```

```

01438 }
01439
01440 VPRIVATE void coulomb(Vpbe *pbe, int d, double pt[], double eps, double *U,
01441     double dU[], double *d2U) {
01442
01443     int iatom, i;
01444     double T, pot, fx, fy, fz, x, y, z, scale;
01445     double *position, charge, dist, dist2, val, vec[3], dUold[3], Uold;
01446     Valist *alist;
01447     Vatom *atom;
01448
01449     /* Initialize variables */
01450     T = Vpbe_getTemperature(pbe);
01451     alist = Vpbe_getValist(pbe);
01452     pot = 0; fx = 0; fy = 0; fz = 0;
01453     x = pt[0]; y = pt[1]; z = pt[2];
01454
01455     /* Calculate */
01456     if (!Vgreen_coulombD(var.green, 1, &x, &y, &z, &pot, &fx, &fy, &fz)) {
01457         Vnm_print(2, "Error calculating Green's function!\n");
01458         VASSERT(0);
01459     }
01460
01461
01462     /* Scale the results */
01463     scale = Vunit_ec/(eps*Vunit_kb*T);
01464     *U = pot*scale;
01465     *d2U = 0.0;
01466     dU[0] = -fx*scale;
01467     dU[1] = -fy*scale;
01468     dU[2] = -fz*scale;
01469
01470 #if 0
01471     /* Compare with old results */
01472     val = 0.0;
01473     Uold = 0.0; dUold[0] = 0.0; dUold[1] = 0.0; dUold[2] = 0.0;
01474     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
01475         atom = Valist_getAtom(alist, iatom);
01476         position = Vatom_getPosition(atom);
01477         charge = Vatom_getCharge(atom);
01478         dist2 = 0;
01479         for (i=0; i<d; i++) {
01480             vec[i] = (position[i] - pt[i]);
01481             dist2 += VSQR(vec[i]);
01482         }
01483         dist = VSQRT(dist2);
01484
01485         /* POTENTIAL */
01486         Uold = Uold + charge/dist;
01487
01488         /* GRADIENT */
01489         for (i=0; i<d; i++) dUold[i] = dUold[i] + vec[i]*charge/(dist2*dist);
01490     }
01491     Uold = Uold*VSQR(Vunit_ec)*(1.0e10)/(4*VPI*Vunit_eps0*eps*Vunit_kb*T);
01492     for (i=0; i<d; i++) {
01493         dUold[i] = dUold[i]*VSQR(Vunit_ec)*(1.0e10)/(4*VPI*Vunit_eps0*eps*Vunit_kb*T);
01494     }
01495
01496     printf("Unew - Uold = %g - %g = %g\n", *U, Uold, (*U - Uold));
01497     printf("||dUnew - dUold||^2 = %g\n", (VSQR(dU[0] - dUold[0])
01498         + VSQR(dU[1] - dUold[1]) + VSQR(dU[2] - dUold[2])));
01499     printf("dUnew[0] = %g, dUold[0] = %g\n", dU[0], dUold[0]);
01500     printf("dUnew[1] = %g, dUold[1] = %g\n", dU[1], dUold[1]);
01501     printf("dUnew[2] = %g, dUold[2] = %g\n", dU[2], dUold[2]);
01502
01503 #endif
01504
01505 }
01506
01507
01508 VPUBLIC void Vfetk_PDE_initAssemble(PDE *thee, int ip[], double rp[]) {
01509
01510 #if 1
01511     /* Re-initialize the Green's function oracle in case the atom list has
01512      * changed */
01513     if (var.initGreen) {
01514         Vgreen_dtor(&(var.green));
01515         var.initGreen = 0;
01516     }
01517     var.green = Vgreen_ctor(var.fetk->pbe->alist);
01518     var.initGreen = 1;

```

```

01519 #else
01520     if (!var.initGreen) {
01521         var.green = Vgreen_ctor(var.fetk->pbe->alist);
01522         var.initGreen = 1;
01523     }
01524 #endif
01525 }
01526 }
01527
01528 VPUBLIC void Vfetk_PDE_initElement(PDE *thee, int elementType, int chart,
01529     double tvx[][3], void *data) {
01530
01531     int i, j;
01532     double epsp, epsw;
01533
01534     /* We assume that the simplex has been passed in as the void *data *
01535      * argument. Store it */
01536     VASSERT(data != NULL);
01537     var.simp = (SS *)data;
01538
01539     /* save the element type */
01540     var.sType = elementType;
01541
01542     /* Grab the vertices from this simplex */
01543     var.nverts = thee->dim+1;
01544     for (i=0; i<thee->dim+1; i++) var.verts[i] = SS_vertex(var.simp, i);
01545
01546     /* Vertex locations of this simplex */
01547     for (i=0; i<thee->dim+1; i++) {
01548         for (j=0; j<thee->dim; j++) {
01549             var.vx[i][j] = tvx[i][j];
01550         }
01551     }
01552
01553     /* Set the dielectric constant for this element for use in the jump term *
01554      * of the residual-based error estimator. The value is set to the average
01555      * * value of the vertices */
01556     var.jumpDiel = 0; /* NOT IMPLEMENTED YET! */
01557 }
01558
01559 VPUBLIC void Vfetk_PDE_initFace(PDE *thee, int faceType, int chart,
01560     double tnvec[]) {
01561
01562     int i;
01563
01564     /* unit normal vector of this face */
01565     for (i=0; i<thee->dim; i++) var.nvec[i] = tnvec[i];
01566
01567     /* save the face type */
01568     var.fType = faceType;
01569 }
01570
01571 VPUBLIC void Vfetk_PDE_initPoint(PDE *thee, int pointType, int chart,
01572     double txq[], double tU[], double tdU[][3]) {
01573
01574     int i, j, ichop;
01575     double u2, coef2, eps_p;
01576     Vhal_PBEType pdetype;
01577     Vpbe *pbe = VNULL;
01578
01579     eps_p = Vpbe_getSoluteDiel(var.fetk->pbe);
01580     pdetype = var.fetk->type;
01581     pbe = var.fetk->pbe;
01582
01583     /* the point, the solution value and gradient, and the Coulomb value and *
01584      * gradient at the point */
01585     if ((pdetype == PBE_LRPBE) || (pdetype == PBE_NRPBE)) {
01586         coulomb(pbe, thee->dim, txq, eps_p, &(var.W), var.dW, &(var.d2W));
01587     }
01588     for (i=0; i<thee->vec; i++) {
01589         var.U[i] = tU[i];
01590         for (j=0; j<thee->dim; j++) {
01591             var.xq[j] = txq[j];
01592             var.dU[i][j] = tdU[i][j];
01593         }
01594     }
01595
01596     /* interior form case */
01597     if (pointType == 0) {
01598
01599         /* Get the dielectric values */

```

```

01600     var.diel = diel();
01601     var.ionacc = ionacc();
01602     var.A = var.diel;
01603     var.F = (var.diel - eps_p);
01604
01605     switch (pdetype) {
01606
01607         case PBE_LPBE:
01608             var.DB = var.ionacc*var.zkappa2*var.ionstr;
01609             var.B = var.DB*var.U[0];
01610             break;
01611
01612         case PBE_NPBE:
01613
01614             var.B = 0;
01615             var.DB = 0;
01616             if ((var.ionacc > VSMALL) && (var.zks2 > VSMALL)) {
01617                 for (i=0; i<var.nion; i++) {
01618                     u2 = -1.0 * var.U[0] * var.ionQ[i];
01619
01620                     /* NONLINEAR TERM */
01621                     coef2 = -1.0 * var.ionacc * var.zks2 * var.ionConc[i];
01622                     var.B += (coef2 * Vcap_exp(u2, &ichop));
01623                     /* LINEARIZED TERM */
01624                     coef2 = -1.0 * var.ionQ[i] * coef2;
01625                     var.DB += (coef2 * Vcap_exp(u2, &ichop));
01626                 }
01627             }
01628             break;
01629
01630         case PBE_LRPBE:
01631             var.DB = var.ionacc*var.zkappa2*var.ionstr;
01632             var.B = var.DB*(var.U[0]+var.W);
01633             break;
01634
01635         case PBE_NRPBE:
01636
01637             var.B = 0;
01638             var.DB = 0;
01639             if ((var.ionacc > VSMALL) && (var.zks2 > VSMALL)) {
01640                 for (i=0; i<var.nion; i++) {
01641                     u2 = -1.0 * (var.U[0] + var.W) * var.ionQ[i];
01642
01643                     /* NONLINEAR TERM */
01644                     coef2 = -1.0 * var.ionacc * var.zks2 * var.ionConc[i];
01645                     var.B += (coef2 * Vcap_exp(u2, &ichop));
01646
01647                     /* LINEARIZED TERM */
01648                     coef2 = -1.0 * var.ionQ[i] * coef2;
01649                     var.DB += (coef2 * Vcap_exp(u2, &ichop));
01650                 }
01651             }
01652             break;
01653
01654         case PBE_SMPBE: /* SMPBE Temp */
01655
01656             var.B = 0;
01657             var.DB = 0;
01658             if ((var.ionacc > VSMALL) && (var.zks2 > VSMALL)) {
01659                 for (i=0; i<var.nion; i++) {
01660                     u2 = -1.0 * var.U[0] * var.ionQ[i];
01661
01662                     /* NONLINEAR TERM */
01663                     coef2 = -1.0 * var.ionacc * var.zks2 * var.ionConc[i];
01664                     var.B += (coef2 * Vcap_exp(u2, &ichop));
01665                     /* LINEARIZED TERM */
01666                     coef2 = -1.0 * var.ionQ[i] * coef2;
01667                     var.DB += (coef2 * Vcap_exp(u2, &ichop));
01668                 }
01669             }
01670             break;
01671         default:
01672             Vnm_print(2, "Vfetk_PDE_initPoint: Unknown PBE type (%d)!\n",
01673                 pdetype);
01674             VASSERT(0);
01675             break;
01676     }
01677
01678     /* boundary form case */
01679 } else {
01680

```

```

01681 #ifdef DONEUMANN
01682     ;
01683 #else
01684     Vnm_print(2, "Vfetk: Whoa! I just got a boundary point to evaluate (%d)!\n", pointType);
01685     Vnm_print(2, "Vfetk: Did you do that on purpose?\n");
01686 #endif
01687 }
01688
01689 #if 0 /* THIS IS VERY NOISY! */
01690     Vfetk_dumpLocalVar();
01691 #endif
01692
01693 }
01694
01695 VPUBLIC void Vfetk_PDE_Fu(PDE *thee, int key, double F[]) {
01696     //Vnm_print(2, "Vfetk_PDE_Fu: Setting error to zero!\n");
01697
01698     F[0] = 0.;
01699 }
01700
01701 }
01702
01703 VPUBLIC double Vfetk_PDE_Fu_v(
01704     PDE *thee,
01705     int key,
01706     double V[],
01707     double dV[][VAPBS_DIM]
01708 ) {
01709     Vhal_PBEType type;
01710     int i;
01711     double value = 0.;
01712
01713     type = var.fetk->type;
01714
01715     /* interior form case */
01716     if (key == 0) {
01717         for (i=0; i<thee->dim; i++) value += ( var.A * var.dU[0][i] * dV[0][i] );
01718         value += var.B * V[0];
01719
01720         if ((type == PBE_LRPBE) || (type == PBE_NRPBE)) {
01721             for (i=0; i<thee->dim; i++) {
01722                 if (var.F > VSMALL) value += (var.F * var.dW[i] * dV[0][i]);
01723             }
01724         }
01725     }
01726
01727     /* boundary form case */
01728 } else {
01729     #ifdef DONEUMANN
01730         value = 0.0;
01731     #else
01732         Vnm_print(2, "Vfetk: Whoa! I was just asked to evaluate a boundary weak form for point type
01733             %d!\n", key);
01734     #endif
01735 }
01736
01737     var.Fu_v = value;
01738     return value;
01739 }
01740
01741 VPUBLIC double Vfetk_PDE_DFu_wv(
01742     PDE *thee,
01743     int key,
01744     double W[],
01745     double dW[][VAPBS_DIM],
01746     double V[],
01747     double dV[][3]
01748 ) {
01749     Vhal_PBEType type;
01750     int i;
01751     double value = 0.;
01752
01753     type = var.fetk->type;
01754
01755     /* Interior form */
01756     if (key == 0) {
01757         value += var.DB * W[0] * V[0];
01758         for (i=0; i<thee->dim; i++) value += ( var.A * dW[0][i] * dV[0][i] );
01759     }
01760

```

```

01761      /* boundary form case */
01762    } else {
01763 #ifdef DONEUMANN
01764     value = 0.0;
01765 #else
01766     Vnm_print(2, "Vfetk: Whoa! I was just asked to evaluate a boundary weak form for point type
    %d!\n", key);
01767 #endif
01768    }
01769    var.DFu_wv = value;
01771    return value;
01772 }
01773
01776 #define VRINGMAX 1000
01779 #define VATOMMAX 1000000
01780 VPUBLIC void Vfetk_PDE_delta(PDE *thee, int type, int chart, double txq[],
01781 void *user, double F[]) {
01782
01783     int iatom, jatom, natoms, atomIndex, atomList[VATOMMAX], nAtomList;
01784     int gotAtom, numString, isimp, iver, sid;
01785     double *position, charge, phi[VAPBS_NVS], phix[VAPBS_NVS][3], value;
01786     Vatom *atom;
01787     Vhal_PBEType pdetype;
01788     SS *sring[VRINGMAX];
01789     VV *vertex = (VV *)user;
01790
01791     pdetype = var.fetk->type;
01792
01793     F[0] = 0.0;
01794
01795     if ((pdetype == PBE_LPBE) || (pdetype == PBE_NPBE) || (pdetype == PBE_SMPBE) /* SMPBE Added */) {
01796         VASSERT( vertex != VNULL);
01797         numString = 0;
01798         sring[numString] = VV_firstSS(vertex);
01799         while (sring[numString] != VNULL) {
01800             numString++;
01801             sring[numString] = SS_link(sring[numString-1], vertex);
01802         }
01803         VASSERT( numString > 0 );
01804         VASSERT( numString <= VRINGMAX );
01805
01806         /* Move around the simplex ring and determine the charge locations */
01807         F[0] = 0.;
01808         charge = 0.;
01809         nAtomList = 0;
01810         for (isimp=0; isimp<numString; isimp++) {
01811             sid = SS_id(sring[isimp]);
01812             natoms = Vcsm_getNumberAtoms(Vfetk_getVcsm(var.fetk), sid);
01813             for (iatom=0; iatom<natoms; iatom++) {
01814                 /* Get the delta function information */
01815                 atomIndex = Vcsm_getAtomIndex(Vfetk_getVcsm(var.fetk),
01816 iatom, sid);
01817                 gotAtom = 0;
01818                 for (jatom=0; jatom<nAtomList; jatom++) {
01819                     if (atomList[jatom] == atomIndex) {
01820                         gotAtom = 1;
01821                         break;
01822                     }
01823                 }
01824                 if (!gotAtom) {
01825                     VASSERT(nAtomList < VATOMMAX);
01826                     atomList[nAtomList] = atomIndex;
01827                     nAtomList++;
01828
01829                     atom = Vcsm_getAtom(Vfetk_getVcsm(var.fetk), iatom, sid);
01830                     charge = Vatom_getCharge(atom);
01831                     position = Vatom_getPosition(atom);
01832
01833                     /* Get the test function value at the delta function I
01834 * used to do a VASSERT to make sure the point was in the
01835 * simplex (i.e., make sure round-off error isn't an
01836 * issue), but round off errors became an issue */
01837                     if (!Gem_pointInSimplexVal(Vfetk_getGem(var.fetk),
01838 sring[isimp], position, phi, phix)) {
01839                         if (!Gem_pointInSimplex(Vfetk_getGem(var.fetk),
01840 sring[isimp], position)) {
01841                             Vnm_print(2, "delta: Both Gem_pointInSimplexVal \
01842 and Gem_pointInSimplex detected misplaced point charge!\n");
01843                             Vnm_print(2, "delta: I think you have problems: \
01844 phi = {}");

```

```

01845                                     for (ivert=0; ivert<Gem_dimVV(Vfetk_getGem(var.fetk)); ivert++) Vnm_print(2,
01846 "%e ", phi[ivert]);
01847 Vnm_print(2, "\n");
01848     }
01849     value = 0;
01850     for (ivert=0; ivert<Gem_dimVV(Vfetk_getGem(var.fetk)); ivert++) {
01851         if (VV_id(SS_vertex(sring[isimp], ivert)) == VV_id(vertex)) value += phi[ivert];
01852     }
01853
01854     F[0] += (value * Vpbe_getZmagic(var.fetk->pbe) * charge);
01855     } /* if !gotAtom */
01856     } /* for iatom */
01857     } /* for isimp */
01858
01859     } else if ((pdetype == PBE_LRPBE) || (pdetype == PBE_NRPBE)) {
01860         F[0] = 0.0;
01861     } else { VASSERT(0); }
01862
01863     var.delta = F[0];
01864 }
01865 }
01866
01867 VPUBLIC void Vfetk_PDE_u_D(PDE *thee, int type, int chart, double txq[],
01868 double F[]) {
01869
01870     if ((var.fetk->type == PBE_LPBPE) || (var.fetk->type == PBE_NPBPE) || (var.fetk->type == PBE_SMPBE) /*
01871 SMPBE Added */) {
01872         F[0] = debye_U(var.fetk->pbe, thee->dim, txq);
01873     } else if ((var.fetk->type == PBE_LRPBE) || (var.fetk->type == PBE_NRPBE)) {
01874         F[0] = debye_Udiff(var.fetk->pbe, thee->dim, txq);
01875     } else VASSERT(0);
01876
01877     var.u_D = F[0];
01878 }
01879
01886 VPUBLIC void Vfetk_PDE_u_T(PDE *thee, int type, int chart, double txq[],
01887 double F[]) {
01888     /*VPUBLIC void Vfetk_PDE_u_T(sPDE *thee,
01889 int type,
01890 int chart,
01891 double txq[],
01892 double F[],
01893 double dF[][3]
01894 ) { */
01895
01896     F[0] = 0.0;
01897     var.u_T = F[0];
01898 }
01899 }
01900
01901
01902 VPUBLIC void Vfetk_PDE_bisectEdge(int dim, int dimII, int edgeType,
01903 int chart[], double vx[][3]) {
01904
01905     int i;
01906
01907     for (i=0; i<dimII; i++) vx[2][i] = .5 * (vx[0][i] + vx[1][i]);
01908     chart[2] = chart[0];
01909 }
01910 }
01911
01912 VPUBLIC void Vfetk_PDE_mapBoundary(int dim, int dimII, int vertexType,
01913 int chart, double vx[3]) {
01914 }
01915 }
01916
01917 VPUBLIC int Vfetk_PDE_markSimplex(int dim, int dimII, int simplexType,
01918 int faceType[VAPBS_NVS], int vertexType[VAPBS_NVS], int chart[], double vx[][3],
01919 void *simplex) {
01920
01921     double targetRes, edgeLength, srاد, swin, myAcc, refAcc;
01922     int i, natoms;
01923     Vsurf_Meth srfrm;
01924     Vhal_PBEType type;
01925     FEMparm *feparm = VNULL;
01926     PBEparm *pbeparm = VNULL;
01927     Vpbe *pbe = VNULL;
01928     Vacc *acc = VNULL;

```

```

01929     Vcsm *csm = VNULL;
01930     SS *simp = VNULL;
01931
01932     VASSERT(var.fetk->feparm != VNULL);
01933     feparm = var.fetk->feparm;
01934     VASSERT(var.fetk->pbeparm != VNULL);
01935     pbeparm = var.fetk->pbeparm;
01936     pbe = var.fetk->pbe;
01937     csm = Vfetk_getVcsm(var.fetk);
01938     acc = pbe->acc;
01939     targetRes = feparm->targetRes;
01940     srfm = pbeparm->srfm;
01941     srad = pbeparm->srad;
01942     swin = pbeparm->swin;
01943     simp = (SS *)simplex;
01944     type = var.fetk->type;
01945
01946     /* Check to see if this simplex is smaller than the target size */
01947     /* NAB WARNING: I am providing face=-1 here to conform to the new MC API; however, I'm not sure if
this is the correct behavior. */
01948     Gem_longestEdge(var.fetk->gm, simp, -1, &edgeLength);
01949     if (edgeLength < targetRes) return 0;
01950
01951     /* For non-regularized PBE, check charge-simplex map */
01952     if ((type == PBE_LPBE) || (type == PBE_NPBE) || (type == PBE_SMPBE) /* SMPBE Added */) {
01953         natoms = Vcsm_getNumberAtoms(csm, SS_id(simp));
01954         if (natoms > 0) {
01955             return 1;
01956         }
01957     }
01958
01959     /* We would like to resolve the mesh between the van der Waals surface the
* max distance from this surface where there could be coefficient
* changes */
01960     switch(srfm) {
01961     case VSM_MOL:
01962         refAcc = Vacc_molAcc(acc, vx[0], srad);
01963         for (i=1; i<(dim+1); i++) {
01964             myAcc = Vacc_molAcc(acc, vx[i], srad);
01965             if (myAcc != refAcc) {
01966                 return 1;
01967             }
01968         }
01969         break;
01970     case VSM_MOLSMOOTH:
01971         refAcc = Vacc_molAcc(acc, vx[0], srad);
01972         for (i=1; i<(dim+1); i++) {
01973             myAcc = Vacc_molAcc(acc, vx[i], srad);
01974             if (myAcc != refAcc) {
01975                 return 1;
01976             }
01977         }
01978         break;
01979     case VSM_SPLINE:
01980         refAcc = Vacc_splineAcc(acc, vx[0], swin, 0.0);
01981         for (i=1; i<(dim+1); i++) {
01982             myAcc = Vacc_splineAcc(acc, vx[i], swin, 0.0);
01983             if (myAcc != refAcc) {
01984                 return 1;
01985             }
01986         }
01987         break;
01988     default:
01989         VASSERT(0);
01990         break;
01991     }
01992     return 0;
01993 }
01994
01995 VPUBLIC void Vfetk_PDE_oneChart(int dim, int dimII, int objType, int chart[],
double vx[][3], int dimV) {
02000 }
02001 }
02002
02003 VPUBLIC double Vfetk_PDE_Ju(PDE *thee, int key) {
02004     int i, ichop;
02005     double dielE, qmE, coef2, u2;
02006     double value = 0.;
02007     Vhal_PBEType type;

```



```

02009
02010     type = var.fetk->type;
02011
02012     /* interior form case */
02013     if (key == 0) {
02014         dielE = 0;
02015         for (i=0; i<3; i++) dielE += VSQR(var.dU[0][i]);
02016         dielE = dielE*var.diel;
02017
02018         switch (type) {
02019             case PBE_LPBE:
02020                 if ((var.ionacc > VSMALL) && (var.zkappa2 > VSMALL)) {
02021                     qmE = var.ionacc*var.zkappa2*VSQR(var.U[0]);
02022                 } else qmE = 0;
02023                 break;
02024             case PBE_NPBE:
02025                 if ((var.ionacc > VSMALL) && (var.zks2 > VSMALL)) {
02026                     qmE = 0.;
02027                     for (i=0; i<var.nion; i++) {
02028                         coef2 = var.ionacc * var.zks2 * var.ionConc[i] * var.ionQ[i];
02029                         u2 = -1.0 * (var.U[0]) * var.ionQ[i];
02030                         qmE += (coef2 * (Vcap_exp(u2, &ichop) - 1.0));
02031                     }
02032                 } else qmE = 0;
02033                 break;
02034             case PBE_LRPBE:
02035                 if ((var.ionacc > VSMALL) && (var.zkappa2 > VSMALL)) {
02036                     qmE = var.ionacc*var.zkappa2*VSQR((var.U[0] + var.W));
02037                 } else qmE = 0;
02038                 break;
02039             case PBE_NRPBE:
02040                 if ((var.ionacc > VSMALL) && (var.zks2 > VSMALL)) {
02041                     qmE = 0.;
02042                     for (i=0; i<var.nion; i++) {
02043                         coef2 = var.ionacc * var.zks2 * var.ionConc[i] * var.ionQ[i];
02044                         u2 = -1.0 * (var.U[0] + var.W) * var.ionQ[i];
02045                         qmE += (coef2 * (Vcap_exp(u2, &ichop) - 1.0));
02046                     }
02047                 } else qmE = 0;
02048                 break;
02049             case PBE_SMPBE: /* SMPBE Temp */
02050                 if ((var.ionacc > VSMALL) && (var.zks2 > VSMALL)) {
02051                     qmE = 0.;
02052                     for (i=0; i<var.nion; i++) {
02053                         coef2 = var.ionacc * var.zks2 * var.ionConc[i] * var.ionQ[i];
02054                         u2 = -1.0 * (var.U[0]) * var.ionQ[i];
02055                         qmE += (coef2 * (Vcap_exp(u2, &ichop) - 1.0));
02056                     }
02057                 } else qmE = 0;
02058                 break;
02059             default:
02060                 Vnm_print(2, "Vfetk_PDE_Ju: Invalid PBE type (%d)!\n", type);
02061                 VASSERT(0);
02062                 break;
02063         }
02064
02065         value = 0.5*(dielE + qmE)/Vpbe_getZmagic(var.fetk->pbe);
02066
02067     /* boundary form case */
02068     } else if (key == 1) {
02069         value = 0.0;
02070
02071     /* how did we get here? */
02072     } else VASSERT(0);
02073
02074     return value;
02075 }
02076
02077
02078 VPUBLIC void Vfetk_externalUpdateFunction(SS **simps, int num) {
02079
02080     Vcsm *csm = VNULL;
02081     int rc;
02082
02083     VASSERT(var.fetk != VNULL);
02084     csm = Vfetk_getVcsm(var.fetk);
02085     VASSERT(csm != VNULL);
02086
02087     rc = Vcsm_update(csm, simps, num);
02088
02089     if (!rc) {

```

```

02090         Vnm_print(2, "Error while updating charge-simplex map!\n");
02091         VASSERT(0);
02092     }
02093 }
02094
02095 VPRIVATE void polyEval(int numP, double p[], double c[][VMAXP], double xv[]) {
02096     int i;
02097     double x, y, z;
02098
02099     x = xv[0];
02100     y = xv[1];
02101     z = xv[2];
02102     for (i=0; i<numP; i++) {
02103         p[i] = c[i][0]
02104             + c[i][1] * x
02105             + c[i][2] * y
02106             + c[i][3] * z
02107             + c[i][4] * x*x
02108             + c[i][5] * y*y
02109             + c[i][6] * z*z
02110             + c[i][7] * x*y
02111             + c[i][8] * x*z
02112             + c[i][9] * y*z
02113             + c[i][10] * x*x*x
02114             + c[i][11] * y*y*y
02115             + c[i][12] * z*z*z
02116             + c[i][13] * x*x*y
02117             + c[i][14] * x*x*z
02118             + c[i][15] * x*y*y
02119             + c[i][16] * y*y*z
02120             + c[i][17] * x*z*z
02121             + c[i][18] * y*z*z;
02122     }
02123 }
02124
02125 VPRIVATE void setCoef(int numP, double c[][VMAXP], double cx[][VMAXP],
02126     double cy[][VMAXP], double cz[][VMAXP], int ic[][VMAXP], int icx[][VMAXP],
02127     int icy[][VMAXP], int icz[][VMAXP]) {
02128
02129     int i, j;
02130     for (i=0; i<numP; i++) {
02131         for (j=0; j<VMAXP; j++) {
02132             c[i][j] = 0.5 * (double)ic[i][j];
02133             cx[i][j] = 0.5 * (double)icx[i][j];
02134             cy[i][j] = 0.5 * (double)icy[i][j];
02135             cz[i][j] = 0.5 * (double)icz[i][j];
02136         }
02137     }
02138 }
02139
02140 VPUBLIC int Vfetc_PDE_simplexBasisInit(int key, int dim, int comp, int *ndof,
02141     int dof[]) {
02142
02143     int qorder, bump, dimIS[VAPBS_NVS];
02144
02145     /* necessary quadrature order to return at the end */
02146     qorder = P_DEG;
02147
02148     /* deal with bump function requests */
02149     if ((key == 0) || (key == 1)) {
02150         bump = 0;
02151     } else if ((key == 2) || (key == 3)) {
02152         bump = 1;
02153     } else { VASSERT(0); }
02154
02155     /* for now use same element for all components, both trial and test */
02156     if (dim==2) {
02157         /* 2D simplex dimensions */
02158         dimIS[0] = 3; /* number of vertices */
02159         dimIS[1] = 3; /* number of edges */
02160         dimIS[2] = 0; /* number of faces (3D only) */
02161         dimIS[3] = 1; /* number of simplices (always=1) */
02162         if (bump==0) {
02163             if (P_DEG==1) {
02164                 init_2DPl(dimIS, ndof, dof, c, cx, cy, cz);
02165             } else if (P_DEG==2) {
02166                 init_2DPl(dimIS, ndof, dof, c, cx, cy, cz);
02167             } else if (P_DEG==3) {
02168                 init_2DPl(dimIS, ndof, dof, c, cx, cy, cz);
02169             } else Vnm_print(2, "..bad order..");
02170         } else if (bump==1) {

```

```

02171         if (P_DEG==1) {
02172             init_2DP1(dimIS, ndof, dof, c, cx, cy, cz);
02173         } else Vnm_print(2, "..bad order..");
02174     } else Vnm_print(2, "..bad bump..");
02175 } else if (dim==3) {
02176     /* 3D simplex dimensions */
02177     dimIS[0] = 4; /* number of vertices */
02178     dimIS[1] = 6; /* number of edges */
02179     dimIS[2] = 4; /* number of faces (3D only) */
02180     dimIS[3] = 1; /* number of simplices (always=1) */
02181     if (bump==0) {
02182         if (P_DEG==1) {
02183             init_3DP1(dimIS, ndof, dof, c, cx, cy, cz);
02184         } else if (P_DEG==2) {
02185             init_3DP1(dimIS, ndof, dof, c, cx, cy, cz);
02186         } else if (P_DEG==3) {
02187             init_3DP1(dimIS, ndof, dof, c, cx, cy, cz);
02188         } else Vnm_print(2, "..bad order..");
02189     } else if (bump==1) {
02190         if (P_DEG==1) {
02191             init_3DP1(dimIS, ndof, dof, c, cx, cy, cz);
02192         } else Vnm_print(2, "..bad order..");
02193     } else Vnm_print(2, "..bad bump..");
02194 } else Vnm_print(2, "..bad dimension..");
02195
02196 /* save number of DF */
02197 numP = *ndof;
02198
02199 /* return the required quarature order */
02200 return qorder;
02201 }
02202
02203 VPUBLIC void Vfetk_PDE_simplexBasisForm(int key, int dim, int comp, int pdkey,
02204 double xq[], double basis[]) {
02205
02206     if (pdkey == 0) {
02207         polyEval(numP, basis, c, xq);
02208     } else if (pdkey == 1) {
02209         polyEval(numP, basis, cx, xq);
02210     } else if (pdkey == 2) {
02211         polyEval(numP, basis, cy, xq);
02212     } else if (pdkey == 3) {
02213         polyEval(numP, basis, cz, xq);
02214     } else { VASSERT(0); }
02215 }
02216
02217 VPRIVATE void init_2DP1(int dimIS[], int *ndof, int dof[], double c[][VMAXP],
02218 double cx[][VMAXP], double cy[][VMAXP], double cz[][VMAXP]) {
02219
02220     int i;
02221
02222     /* dof number and locations */
02223     dof[0] = 1;
02224     dof[1] = 0;
02225     dof[2] = 0;
02226     dof[3] = 0;
02227     *ndof = 0;
02228     for (i=0; i<VAPBS_NVS; i++) *ndof += dimIS[i] * dof[i];
02229     VASSERT( *ndof == dim_2DP1 );
02230     VASSERT( *ndof <= VMAXP );
02231
02232     /* coefficients of the polynomials */
02233     setCoef( *ndof, c, cx, cy, cz, lgr_2DP1x, lgr_2DP1y, lgr_2DP1z );
02234 }
02235
02236 VPRIVATE void init_3DP1(int dimIS[], int *ndof, int dof[], double c[][VMAXP],
02237 double cx[][VMAXP], double cy[][VMAXP], double cz[][VMAXP]) {
02238
02239     int i;
02240
02241     /* dof number and locations */
02242     dof[0] = 1;
02243     dof[1] = 0;
02244     dof[2] = 0;
02245     dof[3] = 0;
02246     *ndof = 0;
02247     for (i=0; i<VAPBS_NVS; i++) *ndof += dimIS[i] * dof[i];
02248     VASSERT( *ndof == dim_3DP1 );
02249     VASSERT( *ndof <= VMAXP );
02250
02251     /* coefficients of the polynomials */

```

```

02252     setCoef( *ndof, c, cx, cy, cz, lgr_3DP1, lgr_3DP1x, lgr_3DP1y, lgr_3DP1z );
02253 }
02254
02255 VPUBLIC void Vfetc_dumpLocalVar() {
02256
02257     int i;
02258
02259     Vnm_print(1, "DEBUG: nvec = (%g, %g, %g)\n", var.nvec[0], var.nvec[1],
02260               var.nvec[2]);
02261     Vnm_print(1, "DEBUG: nverts = %d\n", var.nverts);
02262     for (i=0; i<var.nverts; i++) {
02263         Vnm_print(1, "DEBUG: verts[%d] ID = %d\n", i, VV_id(var.verts[i]));
02264         Vnm_print(1, "DEBUG: vx[%d] = (%g, %g, %g)\n", i, var.vx[i][0],
02265               var.vx[i][1], var.vx[i][2]);
02266     }
02267     Vnm_print(1, "DEBUG: simp ID = %d\n", SS_id(var.simp));
02268     Vnm_print(1, "DEBUG: sType = %d\n", var.sType);
02269     Vnm_print(1, "DEBUG: fType = %d\n", var.fType);
02270     Vnm_print(1, "DEBUG: xq = (%g, %g, %g)\n", var.xq[0], var.xq[1], var.xq[2]);
02271     Vnm_print(1, "DEBUG: U[0] = %g\n", var.U[0]);
02272     Vnm_print(1, "DEBUG: dU[0] = (%g, %g, %g)\n", var.dU[0][0], var.dU[0][1],
02273               var.dU[0][2]);
02274     Vnm_print(1, "DEBUG: W = %g\n", var.W);
02275     Vnm_print(1, "DEBUG: d2W = %g\n", var.d2W);
02276     Vnm_print(1, "DEBUG: dW = (%g, %g, %g)\n", var.dW[0], var.dW[1], var.dW[2]);
02277     Vnm_print(1, "DEBUG: diel = %g\n", var.diel);
02278     Vnm_print(1, "DEBUG: ionacc = %g\n", var.ionacc);
02279     Vnm_print(1, "DEBUG: A = %g\n", var.A);
02280     Vnm_print(1, "DEBUG: F = %g\n", var.F);
02281     Vnm_print(1, "DEBUG: B = %g\n", var.B);
02282     Vnm_print(1, "DEBUG: DB = %g\n", var.DB);
02283     Vnm_print(1, "DEBUG: nion = %d\n", var.nion);
02284     for (i=0; i<var.nion; i++) {
02285         Vnm_print(1, "DEBUG: ionConc[%d] = %g\n", i, var.ionConc[i]);
02286         Vnm_print(1, "DEBUG: ionQ[%d] = %g\n", i, var.ionQ[i]);
02287         Vnm_print(1, "DEBUG: ionRadii[%d] = %g\n", i, var.ionRadii[i]);
02288     }
02289     Vnm_print(1, "DEBUG: zkappa2 = %g\n", var.zkappa2);
02290     Vnm_print(1, "DEBUG: zks2 = %g\n", var.zks2);
02291     Vnm_print(1, "DEBUG: Fu_v = %g\n", var.Fu_v);
02292     Vnm_print(1, "DEBUG: DFu_wv = %g\n", var.DFu_wv);
02293     Vnm_print(1, "DEBUG: delta = %g\n", var.delta);
02294     Vnm_print(1, "DEBUG: u_D = %g\n", var.u_D);
02295     Vnm_print(1, "DEBUG: u_T = %g\n", var.u_T);
02296
02297 };
02298
02299 VPUBLIC int Vfetc_fillArray(Vfetc *thee, Bvec *vec, Vdata_Type type) {
02300
02301     int i, j, ichop;
02302     double coord[3], chi, q, conc, val;
02303     VV *vert;
02304     Bvec *u, *u_d;
02305     AM *am;
02306     Gem *gm;
02307     PBEparm *pbeparm;
02308     Vacc *acc;
02309     Vpbe *pbe;
02310
02311     gm = thee->gm;
02312     am = thee->am;
02313     pbe = thee->pbe;
02314     pbeparm = thee->pbeparm;
02315     acc = pbe->acc;
02316
02317     /* Make sure vec has enough rows to accomodate the vertex data */
02318     if (Bvec_numRB(vec, 0) != Gem_numVV(gm)) {
02319         Vnm_print(2, "Vfetc_fillArray: insufficient space in Bvec!\n");
02320         Vnm_print(2, "Vfetc_fillArray: Have %d, need %d!\n", Bvec_numRB(vec, 0),
02321               Gem_numVV(gm));
02322         return 0;
02323     }
02324
02325     switch (type) {
02326
02327     case VDT_CHARGE:
02328         Vnm_print(2, "Vfetc_fillArray: can't write out charge distribution!\n");
02329         return 0;
02330         break;
02331
02332     case VDT_POT:

```

```

02333     u = am->u;
02334     u_d = am->ud;
02335     /* Copy in solution */
02336     Bvec_copy(vec, u);
02337     /* Add dirichlet condition */
02338     Bvec_axpy(vec, u_d, 1.0);
02339     break;
02340
02341 case VDT_SMOL:
02342     for (i=0; i<Gem_numVV(gm); i++) {
02343         vert = Gem_VV(gm, i);
02344         for (j=0; j<3; j++) coord[j] = VV_coord(vert, j);
02345         chi = Vacc_molAcc(acc, coord, pbe->solventRadius);
02346         Bvec_set(vec, i, chi);
02347     }
02348     break;
02349
02350 case VDT_SSPL:
02351     for (i=0; i<Gem_numVV(gm); i++) {
02352         vert = Gem_VV(gm, i);
02353         for (j=0; j<3; j++) coord[j] = VV_coord(vert, j);
02354         chi = Vacc_splineAcc(acc, coord, pbeparm->swin, 0.0);
02355         Bvec_set(vec, i, chi);
02356     }
02357     break;
02358
02359 case VDT_VDW:
02360     for (i=0; i<Gem_numVV(gm); i++) {
02361         vert = Gem_VV(gm, i);
02362         for (j=0; j<3; j++) coord[j] = VV_coord(vert, j);
02363         chi = Vacc_vdwAcc(acc, coord);
02364         Bvec_set(vec, i, chi);
02365     }
02366     break;
02367
02368 case VDT_IVDW:
02369     for (i=0; i<Gem_numVV(gm); i++) {
02370         vert = Gem_VV(gm, i);
02371         for (j=0; j<3; j++) coord[j] = VV_coord(vert, j);
02372         chi = Vacc_ivdwAcc(acc, coord, pbe->maxIonRadius);
02373         Bvec_set(vec, i, chi);
02374     }
02375     break;
02376
02377 case VDT_LAP:
02378     Vnm_print(2, "Vfetk_fillArray: can't write out Laplacian!\n");
02379     return 0;
02380     break;
02381
02382 case VDT_EDENS:
02383     Vnm_print(2, "Vfetk_fillArray: can't write out energy density!\n");
02384     return 0;
02385     break;
02386
02387 case VDT_NDENS:
02388     u = am->u;
02389     u_d = am->ud;
02390     /* Copy in solution */
02391     Bvec_copy(vec, u);
02392     /* Add dirichlet condition */
02393     Bvec_axpy(vec, u_d, 1.0);
02394     /* Load up ions */
02395     ichop = 0;
02396     for (i=0; i<Gem_numVV(gm); i++) {
02397         val = 0;
02398         for (j=0; j<pbe->numIon; j++) {
02399             q = pbe->ionQ[j];
02400             conc = pbe->ionConc[j];
02401             if (thee->type == PBE_NPBE || thee->type == PBE_SMPBE /* SMPBE Added */) {
02402                 val += (conc*Vcap_exp(-q*Bvec_val(vec, i), &ichop));
02403             } else if (thee->type == PBE_LPBE) {
02404                 val += (conc * (1 - q*Bvec_val(vec, i)));
02405             }
02406         }
02407         Bvec_set(vec, i, val);
02408     }
02409     break;
02410
02411 case VDT_QDENS:
02412     u = am->u;
02413     u_d = am->ud;

```

```

02414         /* Copy in solution */
02415         Bvec_copy(vec, u);
02416         /* Add dirichlet condition */
02417         Bvec_axpy(vec, u_d, 1.0);
02418         /* Load up ions */
02419         ichop = 0;
02420         for (i=0; i<Gem_numVV(gm); i++) {
02421             val = 0;
02422             for (j=0; j<pbe->numIon; j++) {
02423                 q = pbe->ionQ[j];
02424                 conc = pbe->ionConc[j];
02425                 if (thee->type == PBE_NPBE || thee->type == PBE_SMPBE /* SMPBE Added */) {
02426                     val += (q*conc*Vcap_exp(-q*Bvec_val(vec, i), &ichop));
02427                 } else if (thee->type == PBE_LPBE) {
02428                     val += (q*conc*(1 - q*Bvec_val(vec, i)));
02429                 }
02430             }
02431             Bvec_set(vec, i, val);
02432         }
02433         break;
02434
02435     case VDT_DIELX:
02436         Vnm_print(2, "Vfetc_fillArray: can't write out x-shifted diel!\n");
02437         return 0;
02438         break;
02439
02440     case VDT_DIELY:
02441         Vnm_print(2, "Vfetc_fillArray: can't write out y-shifted diel!\n");
02442         return 0;
02443         break;
02444
02445     case VDT_DIELZ:
02446         Vnm_print(2, "Vfetc_fillArray: can't write out z-shifted diel!\n");
02447         return 0;
02448         break;
02449
02450     case VDT_KAPPA:
02451         Vnm_print(2, "Vfetc_fillArray: can't write out kappa!\n");
02452         return 0;
02453         break;
02454
02455     default:
02456         Vnm_print(2, "Vfetc_fillArray: invalid data type (%d)!\n", type);
02457         return 0;
02458         break;
02459 }
02460
02461 return 1;
02462 }
02463
02464 VPUBLIC int Vfetc_write(Vfetc *thee, const char *iodev, const char *iofmt,
02465     const char *thost, const char *fname, Bvec *vec, Vdata_Format format) {
02466     int i, j, ichop;
02467     Aprx *aprx;
02468     Gem *gm;
02469     Vio *sock;
02470
02471     VASSERT(thee != VNULL);
02472     aprx = thee->aprx;
02473     gm = thee->gm;
02474
02475     sock = Vio_ctor(iodev, iofmt, thost, fname, "w");
02476     if (sock == VNULL) {
02477         Vnm_print(2, "Vfetc_write: Problem opening virtual socket %s\n",
02478             fname);
02479         return 0;
02480     }
02481     if (Vio_connect(sock, 0) < 0) {
02482         Vnm_print(2, "Vfetc_write: Problem connecting to virtual socket %s\n",
02483             fname);
02484         return 0;
02485     }
02486
02487     /* Make sure vec has enough rows to accomodate the vertex data */
02488     if (Bvec_numRB(vec, 0) != Gem_numVV(gm)) {
02489         Vnm_print(2, "Vfetc_fillArray: insufficient space in Bvec!\n");
02490         Vnm_print(2, "Vfetc_fillArray: Have %d, need %d!\n", Bvec_numRB(vec, 0),
02491             Gem_numVV(gm));
02492         return 0;
02493     }
02494 }

```

```

02495
02496     switch (format) {
02497
02498         case VDF_DX:
02499             Aprx_writeSQL(aprx, sock, vec, "DX");
02500             break;
02501         case VDF_AVS:
02502             Aprx_writeSQL(aprx, sock, vec, "UCD");
02503             break;
02504         case VDF_UHBD:
02505             Vnm_print(2, "Vfetk_write:  UHBD format not supported!\n");
02506             return 0;
02507         default:
02508             Vnm_print(2, "Vfetk_write:  Invalid data format (%d)!\n", format);
02509             return 0;
02510     }
02511
02512
02513     Vio_connectFree(sock);
02514     Vio_dtor(&sock);
02515
02516     return 1;
02517 }

```

9.10 src/fem/vfetk.h File Reference

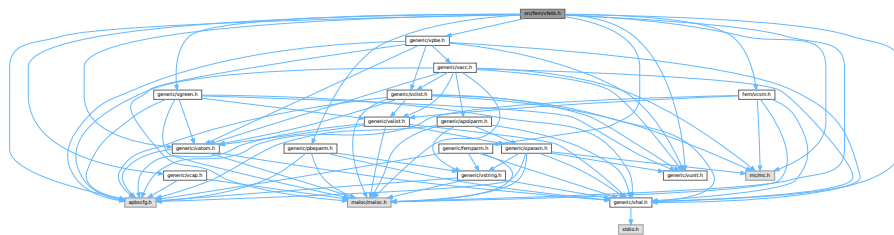
Contains declarations for class Vfetk.

```

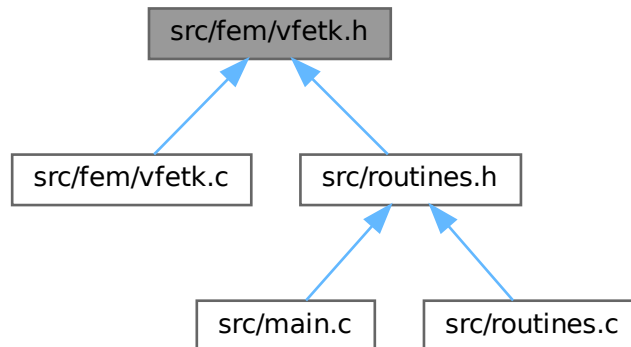
#include "apbscfg.h"
#include "maloc/maloc.h"
#include "mc/mc.h"
#include "generic/vhal.h"
#include "generic/vatom.h"
#include "generic/vpbe.h"
#include "generic/vunit.h"
#include "generic/vgreen.h"
#include "generic/vcap.h"
#include "generic/pbeparm.h"
#include "generic/femparm.h"
#include "fem/vcsm.h"

```

Include dependency graph for vfetk.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVfetc](#)
Contains public data members for Vfetc class/module.
- struct [sVfetc_LocalVar](#)
Vfetc LocalVar subclass.

Typedefs

- typedef enum [eVfetc_LsolvType](#) [Vfetc_LsolvType](#)
Declare FEMparm_LsolvType type.
- typedef enum [eVfetc_MeshLoad](#) [Vfetc_MeshLoad](#)
Declare FEMparm_GuessType type.
- typedef enum [eVfetc_NsolvType](#) [Vfetc_NsolvType](#)
Declare FEMparm_NsolvType type.
- typedef enum [eVfetc_GuessType](#) [Vfetc_GuessType](#)
Declare FEMparm_GuessType type.
- typedef enum [eVfetc_PrecType](#) [Vfetc_PrecType](#)
Declare FEMparm_GuessType type.
- typedef struct [sVfetc](#) [Vfetc](#)
Declaration of the Vfetc class as the Vfetc structure.
- typedef struct [sVfetc_LocalVar](#) [Vfetc_LocalVar](#)
Declaration of the Vfetc_LocalVar subclass as the Vfetc_LocalVar structure.

Enumerations

- enum [eVfetc_LsolvType](#) { [VLT_SLU](#) =0 , [VLT_MG](#) =1 , [VLT_CG](#) =2 , [VLT_BCG](#) =3 }
Linear solver type.
- enum [eVfetc_MeshLoad](#) { [VML_DIRICUBE](#) , [VML_NEUMCUBE](#) , [VML_EXTERNAL](#) }
Mesh loading operation.

- enum `eVfetk_NsolvType` { `VNT_NEW` =0 , `VNT_INC` =1 , `VNT_ARC` =2 }
Non-linear solver type.
- enum `eVfetk_GuessType` { `VG_T_ZERO` =0 , `VG_T_DIRI` =1 , `VG_T_PREV` =2 }
Initial guess type.
- enum `eVfetk_PrecType` { `VPT_IDEN` =0 , `VPT_DIAG` =1 , `VPT_MG` =2 }
Preconditioner type.

Functions

- VEXTERNC Gem * `Vfetk_getGem` (`Vfetk` *thee)
Get a pointer to the Gem (grid manager) object.
- VEXTERNC AM * `Vfetk_getAM` (`Vfetk` *thee)
Get a pointer to the AM (algebra manager) object.
- VEXTERNC `Vpbe` * `Vfetk_getVpbe` (`Vfetk` *thee)
Get a pointer to the Vpbe (PBE manager) object.
- VEXTERNC `Vcsm` * `Vfetk_getVcsm` (`Vfetk` *thee)
Get a pointer to the Vcsm (charge-simplex map) object.
- VEXTERNC int `Vfetk_getAtomColor` (`Vfetk` *thee, int iatom)
Get the partition information for a particular atom.
- VEXTERNC `Vfetk` * `Vfetk_ctor` (`Vpbe` *pbe, `Vhal_PBEType` type)
Constructor for Vfetk object.
- VEXTERNC int `Vfetk_ctor2` (`Vfetk` *thee, `Vpbe` *pbe, `Vhal_PBEType` type)
FORTTRAN stub constructor for Vfetk object.
- VEXTERNC void `Vfetk_dtor` (`Vfetk` **thee)
Object destructor.
- VEXTERNC void `Vfetk_dtor2` (`Vfetk` *thee)
FORTTRAN stub object destructor.
- VEXTERNC double * `Vfetk_getSolution` (`Vfetk` *thee, int *length)
Create an array containing the solution (electrostatic potential in units of $k_B T/e$) at the finest mesh level.
- VEXTERNC void `Vfetk_setParameters` (`Vfetk` *thee, `PBEparm` *pbeparm, `FEMparm` *feparm)
Set the parameter objects.
- VPUBLIC double `Vfetk_energy` (`Vfetk` *thee, int color, int nonlin)
Return the total electrostatic energy.
- VEXTERNC double `Vfetk_dqmEnergy` (`Vfetk` *thee, int color)
Get the "mobile charge" and "polarization" contributions to the electrostatic energy.
- VEXTERNC double `Vfetk_qfEnergy` (`Vfetk` *thee, int color)
Get the "fixed charge" contribution to the electrostatic energy.
- VEXTERNC unsigned long int `Vfetk_memChk` (`Vfetk` *thee)
Return the memory used by this structure (and its contents) in bytes.
- VEXTERNC void `Vfetk_setAtomColors` (`Vfetk` *thee)
Transfer color (partition ID) information frmo a partitioned mesh to the atoms.
- VEXTERNC void `Bmat_printHB` (`Bmat` *thee, char *fname)
Writes a Bmat to disk in Harwell-Boeing sparse matrix format.
- VEXTERNC `Vrc_Codes` `Vfetk_genCube` (`Vfetk` *thee, double center[3], double length[3], `Vfetk_MeshLoad` meshType)
Construct a rectangular mesh (in the current Vfetk object)
- VEXTERNC `Vrc_Codes` `Vfetk_loadMesh` (`Vfetk` *thee, double center[3], double length[3], `Vfetk_MeshLoad` meshType, `Vio` *sock)

- Loads a mesh into the Vfetk (and associated) object(s).*

 - VEXTERNC PDE * [Vfetk_PDE_ctor](#) (Vfetk *fetk)
- Constructs the FEtk PDE object.*

 - VEXTERNC int [Vfetk_PDE_ctor2](#) (PDE *thee, Vfetk *fetk)
- Initializes the FEtk PDE object.*

 - VEXTERNC void [Vfetk_PDE_dtor](#) (PDE **thee)
- Destroys FEtk PDE object.*

 - VEXTERNC void [Vfetk_PDE_dtor2](#) (PDE *thee)
- FORTTRAN stub: destroys FEtk PDE object.*

 - VEXTERNC void [Vfetk_PDE_initAssemble](#) (PDE *thee, int ip[], double rp[])
- Do once-per-assembly initialization.*

 - VEXTERNC void [Vfetk_PDE_initElement](#) (PDE *thee, int elementType, int chart, double txx[][[VAPBS_DIM](#)], void *data)
- Do once-per-element initialization.*

 - VEXTERNC void [Vfetk_PDE_initFace](#) (PDE *thee, int faceType, int chart, double tnvex[])
- Do once-per-face initialization.*

 - VEXTERNC void [Vfetk_PDE_initPoint](#) (PDE *thee, int pointType, int chart, double txq[], double tU[], double tdU[][[VAPBS_DIM](#)])
- Do once-per-point initialization.*

 - VEXTERNC void [Vfetk_PDE_Fu](#) (PDE *thee, int key, double F[])
- Evaluate strong form of PBE. For interior points, this is:*

 - VEXTERNC double [Vfetk_PDE_Fu_v](#) (PDE *thee, int key, double V[], double dV[][[VAPBS_DIM](#)])
- This is the weak form of the PBE; i.e. the strong form integrated with a test function to give:*

 - VEXTERNC double [Vfetk_PDE_DF_u_wv](#) (PDE *thee, int key, double W[], double dW[][[VAPBS_DIM](#)], double V[], double dV[][[VAPBS_DIM](#)])
- This is the linearization of the weak form of the PBE; e.g., for use in a Newton iteration. This is the functional linearization of the strong form integrated with a test function to give:*

 - VEXTERNC void [Vfetk_PDE_delta](#) (PDE *thee, int type, int chart, double txq[], void *user, double F[])
- Evaluate a (discretized) delta function source term at the given point.*

 - VEXTERNC void [Vfetk_PDE_u_D](#) (PDE *thee, int type, int chart, double txq[], double F[])
- Evaluate the Dirichlet boundary condition at the given point.*

 - VEXTERNC void [Vfetk_PDE_u_T](#) (PDE *thee, int type, int chart, double txq[], double F[])
- Evaluate the "true solution" at the given point for comparison with the numerical solution.*

 - VEXTERNC void [Vfetk_PDE_bisectEdge](#) (int dim, int dimII, int edgeType, int chart[], double vx[][[VAPBS_DIM](#)])
- Define the way manifold edges are bisected.*

 - VEXTERNC void [Vfetk_PDE_mapBoundary](#) (int dim, int dimII, int vertexType, int chart, double vx[[VAPBS_DIM](#)])
- Map a boundary point to some pre-defined shape.*

 - VEXTERNC int [Vfetk_PDE_markSimplex](#) (int dim, int dimII, int simplexType, int faceType[[VAPBS_NVS](#)], int vertexType[[VAPBS_NVS](#)], int chart[], double vx[][[VAPBS_DIM](#)], void *simplex)
- User-defined error estimator – in our case, a geometry-based refinement method; forcing simplex refinement at the dielectric boundary and (for non-regularized PBE) the charges.*

 - VEXTERNC void [Vfetk_PDE_oneChart](#) (int dim, int dimII, int objType, int chart[], double vx[][[VAPBS_DIM](#)], int dimV)
- Unify the chart for different coordinate systems – a no-op for us.*

 - VEXTERNC double [Vfetk_PDE_Ju](#) (PDE *thee, int key)
- Energy functional. This returns the energy (less delta function terms) in the form:*

 - VEXTERNC void [Vfetk_externalUpdateFunction](#) (SS **simps, int num)

External hook to simplex subdivision routines in Gem. Called each time a simplex is subdivided (we use it to update the charge-simplex map)

- VEXTERNC int [Vfetc_PDE_simplexBasisInit](#) (int key, int dim, int comp, int *ndof, int dof[])
Initialize the bases for the trial or the test space, for a particular component of the system, at all quadrature points on the master simplex element.
- VEXTERNC void [Vfetc_PDE_simplexBasisForm](#) (int key, int dim, int comp, int pdkey, double xq[], double basis[])
Evaluate the bases for the trial or test space, for a particular component of the system, at all quadrature points on the master simplex element.
- VEXTERNC void [Vfetc_readMesh](#) (Vfetc *thee, int skey, Vio *sock)
Read in mesh and initialize associated internal structures.
- VEXTERNC void [Vfetc_dumpLocalVar](#) ()
Debugging routine to print out local variables used by PDE object.
- VEXTERNC int [Vfetc_fillArray](#) (Vfetc *thee, Bvec *vec, [Vdata_Type](#) type)
Fill an array with the specified data.
- VEXTERNC int [Vfetc_write](#) (Vfetc *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, Bvec *vec, [Vdata_Format](#) format)
Write out data.
- VEXTERNC Vrc_Codes [Vfetc_loadGem](#) (Vfetc *thee, Gem *gm)
Load a Gem geometry manager object into Vfetc.

9.10.1 Detailed Description

Contains declarations for class Vfetc.

Version

\$Id\$

Author

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Attention

```
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*
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*
*

```

Definition in file [vfetk.h](#).

9.11 vfetk.h

[Go to the documentation of this file.](#)

```

00001
00062 #ifndef _VFETK_H_
00063 #define _VFETK_H_
00064
00065 #include "apbscfg.h"
00066
00067 #include "maloc/maloc.h"
00068 #include "mc/mc.h"
00069
00070 #include "generic/vhal.h"
00071 #include "generic/vatom.h"
00072 // #include "generic/valist.h"
00073 #include "generic/vpbe.h"
00074 #include "generic/vunit.h"
00075 #include "generic/vgreen.h"
00076 #include "generic/vcap.h"
00077 #include "generic/pbeparm.h"
00078 #include "generic/femparm.h"
00079 #include "fem/vcsm.h"
00080
00086 enum eVfetk_LsolvType {
00087     VLT_SLU=0,
00088     VLT_MG=1,
00089     VLT_CG=2,
00090     VLT_BCG=3
00091 };
00092
00097 typedef enum eVfetk_LsolvType Vfetk_LsolvType;
00098
00099
00104 enum eVfetk_MeshLoad {
00105     VML_DIRICUBE,
00106     VML_NEUMCUBE,
00107     VML_EXTERNAL
00108 };
00109
00114 typedef enum eVfetk_MeshLoad Vfetk_MeshLoad;
00115
00121 enum eVfetk_NsolvType {
00122     VNT_NEW=0,
00123     VNT_INC=1,
00124     VNT_ARC=2
00125 };
00126
00131 typedef enum eVfetk_NsolvType Vfetk_NsolvType;
00132
00138 enum eVfetk_GuessType {

```

```

00139     VGT_ZERO=0,
00140     VGT_DIRI=1,
00141     VGT_PREV=2
00142 };
00143
00148 typedef enum eVfetk_GuessType Vfetk_GuessType;
00149
00155 enum eVfetk_PrecType {
00156     VPT_IDEN=0,
00157     VPT_DIAG=1,
00158     VPT_MG=2
00159 };
00160
00165 typedef enum eVfetk_PrecType Vfetk_PrecType;
00166
00176 struct sVfetk {
00177
00178     Vmem *vmem;
00179     Gem *gm;
00182     AM *am;
00183     Aprx *aprx;
00184     PDE *pde;
00185     Vpbe *pbe;
00186     Vcsm *csm;
00187     Vfetk_LsolvType lkey;
00188     int lmax;
00189     double ltol;
00190     Vfetk_NsolvType nkey;
00191     int nmax;
00192     double ntol;
00193     Vfetk_GuessType gues;
00194     Vfetk_PrecType lprec;
00195     int pjac;
00197     PBEparm *pbeparm;
00198     FEMParm *feparm;
00199     Vhal_PBEType type;
00200     int level;
00202 };
00203
00207 typedef struct sVfetk Vfetk;
00208
00215 struct sVfetk_LocalVar {
00216     double nvec[VAPBS_DIM];
00217     double vx[4][VAPBS_DIM];
00218     double xq[VAPBS_DIM];
00219     double U[MAXV];
00220     double dU[MAXV][VAPBS_DIM];
00221     double W;
00222     double dW[VAPBS_DIM];
00223     double d2W;
00224     int sType;
00225     int fType;
00226     double diel;
00227     double ionacc;
00228     double A;
00229     double F;
00230     double B;
00231     double DB;
00232     double jumpDiel;
00233     Vfetk *fetk;
00234     Vgreen *green;
00235     int initGreen;
00237     SS *simp;
00239     VV *verts[4];
00240     int nverts;
00241     double ionConc[MAXION];
00242     double ionQ[MAXION];
00243     double ionRadii[MAXION];
00244     double zkappa2;
00245     double zks2;
00246     double ionstr;
00247     int nion;
00248     double Fu_v;
00249     double DFu_wv;
00250     double delta;
00251     double u_D;
00252     double u_T;
00253 };
00254
00259 typedef struct sVfetk_LocalVar Vfetk_LocalVar;
00260

```

```

00261 #if !defined(VINLINE_VFETK)
00262
00268     VEXTERNC Gem* Vfetk_getGem(
00269         Vfetk *thee
00270     );
00271
00277     VEXTERNC AM* Vfetk_getAM(
00278         Vfetk *thee
00279     );
00280
00286     VEXTERNC Vpbe* Vfetk_getVpbe(
00287         Vfetk *thee
00288     );
00289
00295     VEXTERNC Vcsm* Vfetk_getVcsm(
00296         Vfetk *thee
00297     );
00298
00305     VEXTERNC int Vfetk_getAtomColor(
00306         Vfetk *thee,
00307         int iatom
00308     );
00309
00310 #else /* if defined(VINLINE_VFETK) */
00311 #   define Vfetk_getGem(thee) ((thee)->gm)
00312 #   define Vfetk_getAM(thee) ((thee)->am)
00313 #   define Vfetk_getVpbe(thee) ((thee)->pbe)
00314 #   define Vfetk_getVcsm(thee) ((thee)->csm)
00315 #   define Vfetk_getAtomColor(thee, iatom) (Vatom_getPartID(Valist_getAtom(Vpbe_getValist(thee->pbe),
00316     iatom)))
00317 #endif /* if !defined(VINLINE_VFETK) */
00318 /* ////////////////////////////////////// */
00319 // Class Vfetk: Non-Inlineable methods (vfetk.c)
00321
00331 VEXTERNC Vfetk* Vfetk_ctor(
00332     Vpbe *pbe, /**< Vpbe (PBE manager object) */
00333     Vhal_PBEType type
00334 );
00335
00345 VEXTERNC int Vfetk_ctor2(
00346     Vfetk *thee,
00347     Vpbe *pbe,
00348     Vhal_PBEType type
00349 );
00350
00356 VEXTERNC void Vfetk_dtor(
00357     Vfetk **thee
00358 );
00359
00365 VEXTERNC void Vfetk_dtor2(
00366     Vfetk *thee
00367 );
00368
00378 VEXTERNC double* Vfetk_getSolution(
00379     Vfetk *thee,
00380     int *length
00381 );
00382
00388 VEXTERNC void Vfetk_setParameters(
00389     Vfetk *thee,
00390     PBEparm *pbeparm,
00391     FEMparm *feparm
00392 );
00393
00412 VEXTERNC double Vfetk_energy(
00413     Vfetk *thee,
00414     int color,
00418     int nonlin
00420 );
00421
00451 VEXTERNC double Vfetk_dqmEnergy(
00452     Vfetk *thee,
00453     int color
00457 );
00458
00476 VEXTERNC double Vfetk_qfEnergy(
00477     Vfetk *thee,
00478     int color
00480 );
00481

```

```
00489 VEXTERNC unsigned long int Vfetk_memChk(
00490     Vfetk *thee
00491 );
00492
00508 VEXTERNC void Vfetk_setAtomColors(
00509     Vfetk *thee
00510 );
00511
00520 VEXTERNC void Bmat_printHB(
00521     Bmat *thee,
00522     char *fname
00523 );
00524
00530 VEXTERNC Vrc_Codes Vfetk_genCube(
00531     Vfetk *thee,
00532     double center[3],
00533     double length[3],
00534     Vfetk_MeshLoad meshType
00535 );
00536
00542 VEXTERNC Vrc_Codes Vfetk_loadMesh(
00543     Vfetk *thee,
00544     double center[3],
00545     double length[3],
00546     Vfetk_MeshLoad meshType,
00547     Vio *sock
00548 );
00549
00556 VEXTERNC PDE* Vfetk_PDE_ctor(
00557     Vfetk *fetk
00558 );
00559
00566 VEXTERNC int Vfetk_PDE_ctor2(
00567     PDE *thee,
00568     Vfetk *fetk
00569 );
00570
00577 VEXTERNC void Vfetk_PDE_dtor(
00578     PDE **thee
00579 );
00580
00587 VEXTERNC void Vfetk_PDE_dtor2(
00588     PDE *thee
00589 );
00590
00596 VEXTERNC void Vfetk_PDE_initAssemble(
00597     PDE *thee,
00598     int ip[],
00599     double rp[]
00600 );
00601
00608 VEXTERNC void Vfetk_PDE_initElement(
00609     PDE *thee,
00610     int elementType,
00611     int chart,
00614     double tvx[][VAPBS_DIM],
00615     void *data
00616 );
00617
00623 VEXTERNC void Vfetk_PDE_initFace(
00624     PDE *thee,
00625     int faceType,
00627     int chart,
00629     double tnvect[]
00630 );
00631
00639 VEXTERNC void Vfetk_PDE_initPoint(
00640     PDE *thee,
00641     int pointType,
00642     int chart,
00644     double txq[],
00645     double tU[],
00646     double tdU[][VAPBS_DIM]
00647 );
00648
00666 VEXTERNC void Vfetk_PDE_Fu(
00667     PDE *thee,
00668     int key,
00670     double F[]
00671 );
00672
```

```

00683 VEXTERNC double Vfetk_PDE_Fu_v(
00684     PDE *thee,
00685     int key,
00687     double V[],
00688     double dv[][VAPBS_DIM]
00689 );
00690
00702 VEXTERNC double Vfetk_PDE_DFu_wv(
00703     PDE *thee,
00704     int key,
00706     double W[],
00707     double dw[][VAPBS_DIM],
00708     double V[],
00709     double dv[][VAPBS_DIM]
00710 );
00711
00718 VEXTERNC void Vfetk_PDE_delta(
00719     PDE *thee,
00720     int type,
00721     int chart,
00722     double txq[],
00723     void *user,
00724     double F[]
00725 );
00726
00734 VEXTERNC void Vfetk_PDE_u_D(
00735     PDE *thee,
00736     int type,
00737     int chart,
00738     double txq[],
00739     double F[]
00740 );
00741
00749 VEXTERNC void Vfetk_PDE_u_T(
00750     PDE *thee,
00751     int type,
00752     int chart,
00753     double txq[],
00754     double F[]
00755 );
00756
00762 VEXTERNC void Vfetk_PDE_bisectEdge(
00763     int dim,
00764     int dimII,
00765     int edgeType,
00766     int chart[],
00768     double vx[][VAPBS_DIM]
00769 );
00770
00776 VEXTERNC void Vfetk_PDE_mapBoundary(
00777     int dim,
00778     int dimII,
00779     int vertexType,
00780     int chart,
00781     double vx[VAPBS_DIM]
00782 );
00783
00792 VEXTERNC int Vfetk_PDE_markSimplex(
00793     int dim,
00794     int dimII,
00795     int simplexType,
00796     int faceType[VAPBS_NVS],
00797     int vertexType[VAPBS_NVS],
00798     int chart[],
00799     double vx[][VAPBS_DIM],
00800     void *simplex
00801 );
00802
00808 VEXTERNC void Vfetk_PDE_oneChart(
00809     int dim,
00810     int dimII,
00811     int objType,
00812     int chart[],
00813     double vx[][VAPBS_DIM],
00814     int dimV
00815 );
00816
00826 VEXTERNC double Vfetk_PDE_Ju(
00827     PDE *thee,
00828     int key
00829 );

```



```

00830
00838 VEXTERNC void Vfetc_externalUpdateFunction(
00839     SS **simps,
00841     int num
00842 );
00843
00844
00907 VEXTERNC int Vfetc_PDE_simplexBasisInit(
00908     int key,
00910     int dim,
00911     int comp,
00913     int *ndof,
00914     int dof[]
00915 );
00916
00924 VEXTERNC void Vfetc_PDE_simplexBasisForm(
00925     int key,
00927     int dim,
00928     int comp ,
00929     int pdkey,
00938     double xq[],
00939     double basis[]
00941 );
00942
00948 VEXTERNC void Vfetc_readMesh(
00949     Vfetc *thee,
00950     int skey,
00951     Vio *sock
00952 );
00953
00959 VEXTERNC void Vfetc_dumpLocalVar();
00960
00968 VEXTERNC int Vfetc_fillArray(
00969     Vfetc *thee,
00970     Bvec *vec,
00971     Vdata_Type type
00972 );
00973
00988 VEXTERNC int Vfetc_write(
00989     Vfetc *thee,
00990     const char *iodev,
00992     const char *iofmt,
00994     const char *thost,
00995     const char *fname,
00996     Bvec *vec,
00997     Vdata_Format format
00998 );
00999
01005 VEXTERNC Vrc_Codes Vfetc_loadGem(
01006     Vfetc *thee,
01007     Gem *gm
01008 );
01009
01010
01011 #endif /* ifndef _VFETK_H_ */

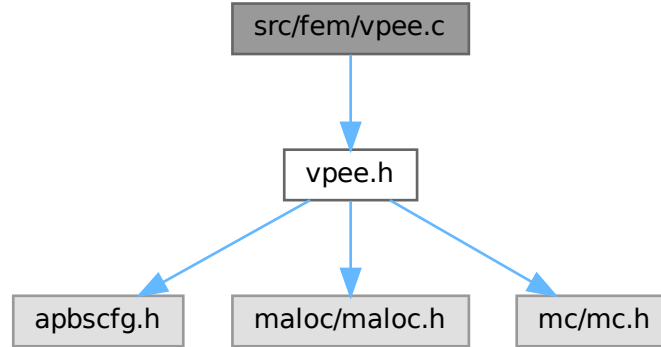
```

9.12 src/fem/vpee.c File Reference

Class Vpee methods.

```
#include "vpee.h"
```

Include dependency graph for vpee.c:



Functions

- VPRIVATE int [Vpee_userDefined](#) ([Vpee](#) *thee, SS *sm)
- VPRIVATE int [Vpee_ourSimp](#) ([Vpee](#) *thee, SS *sm, int rcol)
- VEXTERNC double [Aprx_estNonlinResid](#) ([Aprx](#) *thee, SS *sm, Bvec *u, Bvec *ud, Bvec *f)
- VEXTERNC double [Aprx_estLocalProblem](#) ([Aprx](#) *thee, SS *sm, Bvec *u, Bvec *ud, Bvec *f)
- VEXTERNC double [Aprx_estDualProblem](#) ([Aprx](#) *thee, SS *sm, Bvec *u, Bvec *ud, Bvec *f)
- VPUBLIC [Vpee](#) * [Vpee_ctor](#) ([Gem](#) *gm, int localPartID, int killFlag, double killParam)
Construct the Vpee object.
- VPUBLIC int [Vpee_ctor2](#) ([Vpee](#) *thee, [Gem](#) *gm, int localPartID, int killFlag, double killParam)
FORTTRAN stub to construct the Vpee object.
- VPUBLIC void [Vpee_dtor](#) ([Vpee](#) **thee)
Object destructor.
- VPUBLIC void [Vpee_dtor2](#) ([Vpee](#) *thee)
FORTTRAN stub object destructor.
- VPUBLIC int [Vpee_markRefine](#) ([Vpee](#) *thee, [AM](#) *am, int level, int akey, int rcol, double etol, int bkey)
Mark simplices for refinement based on attenuated error estimates.
- VPUBLIC int [Vpee_numSS](#) ([Vpee](#) *thee)
Returns the number of simplices in the local partition.

9.12.1 Detailed Description

Class Vpee methods.

Author

Nathan Baker

Version`Id`**Attention**

```

*
* APBS -- Adaptive Poisson-Boltzmann Solver
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*
*

```

Definition in file [vpee.c](#).

9.12.2 Function Documentation**9.12.2.1 Vpee_ourSimp()**

```

VPRIVATE int Vpee_ourSimp (
    Vpee * thee,
    SS * sm,
    int rcol )

```

Definition at line 532 of file [vpee.c](#).

9.12.2.2 Vpee_userDefined()

```
VPRIVATE int Vpee_userDefined (
    Vpee * thee,
    SS * sm )
```

Definition at line 498 of file [vpee.c](#).

9.13 vpee.c

[Go to the documentation of this file.](#)

```
00001
00057 #include "vpee.h"
00058
00059 VPRIVATE int Vpee_userDefined(Vpee *thee,
00060                               SS *sm
00061                               );
00062 VPRIVATE int Vpee_ourSimp(Vpee *thee,
00063                           SS *sm,
00064                           int rcol
00065                           );
00066 VEXTERNC double Aprx_estNonlinResid(Aprx *thee,
00067                                     SS *sm,
00068                                     Bvec *u,
00069                                     Bvec *ud,
00070                                     Bvec *f
00071                                     );
00072 VEXTERNC double Aprx_estLocalProblem(Aprx *thee,
00073                                     SS *sm,
00074                                     Bvec *u,
00075                                     Bvec *ud,
00076                                     Bvec *f);
00077 VEXTERNC double Aprx_estDualProblem(Aprx *thee,
00078                                     SS *sm,
00079                                     Bvec *u,
00080                                     Bvec *ud,
00081                                     Bvec *f
00082                                     );
00083
00084 /* ////////////////////////////////////////
00085 // Class Vpee: Non-inlineable methods
00086
00087 /* ////////////////////////////////////////
00088 // Routine: Vpee_ctor
00089 //
00090 //
00091 // Author: Nathan Baker
00093 VPUBLIC Vpee* Vpee_ctor(Gem *gm,
00094                       int localPartID,
00095                       int killFlag,
00096                       double killParam
00097                       ) {
00098
00099     Vpee *thee = VNULL;
00100
00101     /* Set up the structure */
00102     thee = Vmem_malloc(VNULL, 1, sizeof(Vpee) );
00103     VASSERT( thee != VNULL);
00104     VASSERT( Vpee_ctor2(thee, gm, localPartID, killFlag, killParam));
00105
00106     return thee;
00107 }
00108
00109 /* ////////////////////////////////////////
00110 // Routine: Vpee_ctor2
00111 //
00112 // Author: Nathan Baker
00114 VPUBLIC int Vpee_ctor2(Vpee *thee,
00115                      Gem *gm,
00116                      int localPartID,
00117                      int killFlag,
00118                      double killParam
00119                      ) {
```

```

00120
00121     int ivert,
00122         nLocalVerts;
00123     SS *simp;
00124     VV *vert;
00125     double radius,
00126         dx,
00127         dy,
00128         dz;
00129
00130     VASSERT(thee != VNULL);
00131
00132     /* Sanity check on input values */
00133     if (killFlag == 0) {
00134         Vnm_print(0, "Vpee_ctor2: No error attenuation outside partition.\n");
00135     } else if (killFlag == 1) {
00136         Vnm_print(0, "Vpee_ctor2: Error outside local partition ignored.\n");
00137     } else if (killFlag == 2) {
00138         Vnm_print(0, "Vpee_ctor2: Error ignored outside sphere with radius %4.3f times the radius of the
circumscribing sphere\n", killParam);
00139         if (killParam < 1.0) {
00140             Vnm_print(2, "Vpee_ctor2: Warning! Parameter killParam = %4.3 < 1.0!\n",
killParam);
00141             Vnm_print(2, "Vpee_ctor2: This may result in non-optimal marking and refinement!\n");
00142         }
00143     } else if (killFlag == 3) {
00144         Vnm_print(0, "Vpee_ctor2: Error outside local partition and immediate neighbors ignored [NOT
IMPLEMENTED].\n");
00145     } else {
00146         Vnm_print(2, "Vpee_ctor2: UNRECOGNIZED killFlag PARAMETER! BAILING!\n");
00147         VASSERT(0);
00148     }
00149
00150
00151     thee->gm = gm;
00152     thee->localPartID = localPartID;
00153     thee->killFlag = killFlag;
00154     thee->killParam = killParam;
00155     thee->mem = Vmem_ctor("APBS::VPEE");
00156
00157     /* Now, figure out the center of geometry for the local partition. The
00158      * general plan is to loop through the vertices, loop through the
00159      * vertices' simplex lists and find the vertices with simplices containing
00160      * chart values we're interested in. */
00161     thee->localPartCenter[0] = 0.0;
00162     thee->localPartCenter[1] = 0.0;
00163     thee->localPartCenter[2] = 0.0;
00164     nLocalVerts = 0;
00165     for (ivert=0; ivert<Gem_numVV(thee->gm); ivert++) {
00166         vert = Gem_VV(thee->gm, ivert);
00167         simp = VV_firstSS(vert);
00168         VASSERT(simp != VNULL);
00169         while (simp != VNULL) {
00170             if (SS_chart(simp) == thee->localPartID) {
00171                 thee->localPartCenter[0] += VV_coord(vert, 0);
00172                 thee->localPartCenter[1] += VV_coord(vert, 1);
00173                 thee->localPartCenter[2] += VV_coord(vert, 2);
00174                 nLocalVerts++;
00175                 break;
00176             }
00177             simp = SS_link(simp, vert);
00178         }
00179     }
00180     VASSERT(nLocalVerts > 0);
00181     thee->localPartCenter[0] =
00182         thee->localPartCenter[0]/((double) (nLocalVerts));
00183     thee->localPartCenter[1] =
00184         thee->localPartCenter[1]/((double) (nLocalVerts));
00185     thee->localPartCenter[2] =
00186         thee->localPartCenter[2]/((double) (nLocalVerts));
00187     Vnm_print(0, "Vpee_ctor2: Part %d centered at (%4.3f, %4.3f, %4.3f)\n",
00188         thee->localPartID, thee->localPartCenter[0], thee->localPartCenter[1],
00189         thee->localPartCenter[2]);
00190
00191
00192     /* Now, figure out the radius of the sphere circumscribing the local
00193      * partition. We need to keep track of vertices so we don't double count
00194      * them. */
00195     thee->localPartRadius = 0.0;
00196     for (ivert=0; ivert<Gem_numVV(thee->gm); ivert++) {
00197         vert = Gem_VV(thee->gm, ivert);
00198         simp = VV_firstSS(vert);

```

```

00199     VASSERT(simp != VNULL);
00200     while (simp != VNULL) {
00201         if (SS_chart(simp) == thee->localPartID) {
00202             dx = thee->localPartCenter[0] - VV_coord(vert, 0);
00203             dy = thee->localPartCenter[1] - VV_coord(vert, 1);
00204             dz = thee->localPartCenter[2] - VV_coord(vert, 2);
00205             radius = dx*dx + dy*dy + dz*dz;
00206             if (radius > thee->localPartRadius) thee->localPartRadius =
00207                 radius;
00208             break;
00209         }
00210         simp = SS_link(simp, vert);
00211     }
00212 }
00213 thee->localPartRadius = VSQRT(thee->localPartRadius);
00214 Vnm_print(0, "Vpee_ctor2: Part %d has circumscribing sphere of radius %4.3f\n",
00215     thee->localPartID, thee->localPartRadius);
00216
00217 return 1;
00218 }
00219
00220 /* ////////////////////////////////////////////////////////////////////
00221 // Routine: Vpee_dtor
00222 //
00223 // Author: Nathan Baker
00225 VPUBLIC void Vpee_dtor(Vpee **thee) {
00226
00227     if ((*thee) != VNULL) {
00228         Vpee_dtor2(*thee);
00229         Vmem_free(VNULL, 1, sizeof(Vpee), (void **)thee);
00230         (*thee) = VNULL;
00231     }
00232 }
00233 }
00234
00235 /* ////////////////////////////////////////////////////////////////////
00236 // Routine: Vpee_dtor2
00237 //
00238 // Author: Nathan Baker
00240 VPUBLIC void Vpee_dtor2(Vpee *thee) {
00241     Vmem_dtor(&(thee->mem));
00242 }
00243
00244 /* ////////////////////////////////////////////////////////////////////
00245 // Routine: Vpee_markRefine
00246 //
00247 // Author: Nathan Baker (and Michael Holst: the author of AM_markRefine, on
00248 // which this is based)
00250 VPUBLIC int Vpee_markRefine(Vpee *thee,
00251     AM *am,
00252     int level,
00253     int akey,
00254     int rcol,
00255     double etol,
00256     int bkey
00257 ) {
00258
00259     Aprx *aprx;
00260     int marked = 0,
00261         markMe,
00262         i,
00263         smid,
00264         count,
00265         currentQ;
00266     double minError = 0.0,
00267         maxError = 0.0,
00268         errEst = 0.0,
00269         mlevel,
00270         barrier;
00271     SS *sm;
00272
00273
00274     VASSERT(thee != VNULL);
00275
00276     /* Get the Aprx object from AM */
00277     aprx = am->aprx;
00278
00279     /* input check and some i/o */
00280     if ( ! ((-1 <= akey) && (akey <= 4)) ) {
00281         Vnm_print(0, "Vpee_markRefine: bad refine key; simplices marked = %d\n",
00282             marked);

```

```

00283         return marked;
00284     }
00285
00286     /* For uniform markings, we have no effect */
00287     if ((-1 <= akey) && (akey <= 0)) {
00288         marked = Gem_markRefine(thee->gm, akey, rcol);
00289         return marked;
00290     }
00291
00292     /* Informative I/O */
00293     if (akey == 2) {
00294         Vnm_print(0, "Vpee_estRefine: using Aprx_estNonlinResid().\n");
00295     } else if (akey == 3) {
00296         Vnm_print(0, "Vpee_estRefine: using Aprx_estLocalProblem().\n");
00297     } else if (akey == 4) {
00298         Vnm_print(0, "Vpee_estRefine: using Aprx_estDualProblem().\n");
00299     } else {
00300         Vnm_print(0, "Vpee_estRefine: bad key given; simplices marked = %d\n",
00301             marked);
00302         return marked;
00303     }
00304     if (thee->killFlag == 0) {
00305         Vnm_print(0, "Vpee_markRefine: No error attenuation -- simplices in all partitions will be
marked.\n");
00306     } else if (thee->killFlag == 1) {
00307         Vnm_print(0, "Vpee_markRefine: Maximum error attenuation -- only simplices in local partition will
be marked.\n");
00308     } else if (thee->killFlag == 2) {
00309         Vnm_print(0, "Vpee_markRefine: Spherical error attenuation -- simplices within a sphere of %4.3f
times the size of the partition will be marked\n",
00310             thee->killParam);
00311     } else if (thee->killFlag == 2) {
00312         Vnm_print(0, "Vpee_markRefine: Neighbor-based error attenuation -- simplices in the local and
neighboring partitions will be marked [NOT IMPLEMENTED]!\n");
00313         VASSERT(0);
00314     } else {
00315         Vnm_print(2, "Vpee_markRefine: bogus killFlag given; simplices marked = %d\n",
00316             marked);
00317         return marked;
00318     }
00319
00320     /* set the barrier type */
00321     mlevel = (etol*etol) / Gem_numSS(thee->gm);
00322     if (bkey == 0) {
00323         barrier = (etol*etol);
00324         Vnm_print(0, "Vpee_estRefine: forcing [err per S] < [TOL] = %g\n",
00325             barrier);
00326     } else if (bkey == 1) {
00327         barrier = mlevel;
00328         Vnm_print(0, "Vpee_estRefine: forcing [err per S] < [(TOL^2/numS)^(1/2)] = %g\n",
00329             VSQRT(barrier));
00330     } else {
00331         Vnm_print(0, "Vpee_estRefine: bad bkey given; simplices marked = %d\n",
00332             marked);
00333         return marked;
00334     }
00335
00336     /* timer */
00337     Vnm_tstart(30, "error estimation");
00338
00339     /* count = num generations to produce from marked simplices (minimally) */
00340     count = 1; /* must be >= 1 */
00341
00342     /* check the refinement Q for emptiness */
00343     currentQ = 0;
00344     if (Gem_numSQ(thee->gm, currentQ) > 0) {
00345         Vnm_print(0, "Vpee_markRefine: non-empty refinement Q%d....clearing..",
00346             currentQ);
00347         Gem_resetSQ(thee->gm, currentQ);
00348         Vnm_print(0, "..done.\n");
00349     }
00350     if (Gem_numSQ(thee->gm, !currentQ) > 0) {
00351         Vnm_print(0, "Vpee_markRefine: non-empty refinement Q%d....clearing..",
00352             !currentQ);
00353         Gem_resetSQ(thee->gm, !currentQ);
00354         Vnm_print(0, "..done.\n");
00355     }
00356     VASSERT( Gem_numSQ(thee->gm, currentQ) == 0 );
00357     VASSERT( Gem_numSQ(thee->gm, !currentQ) == 0 );
00358
00359     /* clear everyone's refinement flags */

```

```

00360 Vnm_print(0,"Vpee_markRefine: clearing all simplex refinement flags..");
00361 for (i=0; i<Gem_numSS(thee->gm); i++) {
00362     if ( (i>0) && (i % VPRTKEY) == 0 ) Vnm_print(0,"[MS:%d]",i);
00363     sm = Gem_SS(thee->gm,i);
00364     SS_setRefineKey(sm,currentQ,0);
00365     SS_setRefineKey(sm,!currentQ,0);
00366     SS_setRefinementCount(sm,0);
00367 }
00368 Vnm_print(0,"..done.\n");
00369
00370 /* NON-ERROR-BASED METHODS */
00371 /* Simplex flag clearing */
00372 if (akey == -1) return marked;
00373 /* Uniform & user-defined refinement*/
00374 if ((akey == 0) || (akey == 1)) {
00375     smid = 0;
00376     while ( smid < Gem_numSS(thee->gm)) {
00377         /* Get the simplex and find out if it's markable */
00378         sm = Gem_SS(thee->gm,smid);
00379         markMe = Vpee_ourSimp(thee, sm, rcol);
00380         if (markMe) {
00381             if (akey == 0) {
00382                 marked++;
00383                 Gem_appendSQ(thee->gm,currentQ, sm);
00384                 SS_setRefineKey(sm,currentQ,1);
00385                 SS_setRefinementCount(sm,count);
00386             } else if (Vpee_userDefined(thee, sm)) {
00387                 marked++;
00388                 Gem_appendSQ(thee->gm,currentQ, sm);
00389                 SS_setRefineKey(sm,currentQ,1);
00390                 SS_setRefinementCount(sm,count);
00391             }
00392             smid++;
00393         }
00394     }
00395 }
00396
00397 /* ERROR-BASED METHODS */
00398 /* gerror = global error accumulation */
00399 aprx->gerror = 0.;
00400
00401 /* traverse the simplices and process the error estimates */
00402 Vnm_print(0,"Vpee_markRefine: estimating error..");
00403 smid = 0;
00404 while ( smid < Gem_numSS(thee->gm)) {
00405
00406     /* Get the simplex and find out if it's markable */
00407     sm = Gem_SS(thee->gm,smid);
00408     markMe = Vpee_ourSimp(thee, sm, rcol);
00409
00410     if ( (smid>0) && (smid % VPRTKEY) == 0 ) Vnm_print(0,"[MS:%d]",smid);
00411
00412     /* Produce an error estimate for this element if it is in the set */
00413     if (markMe) {
00414         if (akey == 2) {
00415             errEst = Aprx_estNonlinResid(aprx, sm, am->u,am->ud,am->f);
00416         } else if (akey == 3) {
00417             errEst = Aprx_estLocalProblem(aprx, sm, am->u,am->ud,am->f);
00418         } else if (akey == 4) {
00419             errEst = Aprx_estDualProblem(aprx, sm, am->u,am->ud,am->f);
00420         }
00421         VASSERT( errEst >= 0. );
00422
00423         /* if error estimate above tol, mark element for refinement */
00424         if ( errEst > barrier ) {
00425             marked++;
00426             Gem_appendSQ(thee->gm,currentQ, sm); /*add to refinement Q*/
00427             SS_setRefineKey(sm,currentQ,1);      /* note now on refine Q */
00428             SS_setRefinementCount(sm,count);      /* refine X many times? */
00429         }
00430
00431         /* keep track of min/max errors over the mesh */
00432         minError = VMIN2( VSQRT(VABS(errEst)), minError );
00433         maxError = VMAX2( VSQRT(VABS(errEst)), maxError );
00434
00435         /* store the estimate */
00436         Bvec_set( aprx->wev, smid, errEst );
00437
00438         /* accumulate into global error (errEst is SQUARED already) */
00439         aprx->gerror += errEst;
00440

```



```

00441      /* otherwise store a zero for the estimate */
00442      } else {
00443          Bvec_set( aprx->wev, smid, 0. );
00444      }
00445
00446      smid++;
00447  }
00448
00449      /* do some i/o */
00450      Vnm_print(0, "..done.  [marked=<%d/%d>]\n", marked, Gem_numSS( thee->gm ));
00451      Vnm_print(0, "Vpee_estRefine: TOL=<%g>  Global_Error=<%g>\n",
00452          etol, aprx->gerror);
00453      Vnm_print(0, "Vpee_estRefine: (TOL^2/numS)^(1/2)=<%g>  Max_Ele_Error=<%g>\n",
00454          VSQRT(mlevel), maxError);
00455      Vnm_tstop(30, "error estimation");
00456
00457      /* check for making the error tolerance */
00458      if ((bkey == 1) && (aprx->gerror <= etol)) {
00459          Vnm_print(0,
00460              "Vpee_estRefine: *****\n");
00461          Vnm_print(0,
00462              "Vpee_estRefine: Global Error criterion met; setting marked=0.\n");
00463          Vnm_print(0,
00464              "Vpee_estRefine: *****\n");
00465          marked = 0;
00466      }
00467
00468
00469      /* return */
00470      return marked;
00471  }
00472 }
00473
00474 /* ////////////////////////////////////////
00475 // Routine:  Vpee_numSS
00476 //
00477 // Author:   Nathan Baker
00479 VPUBLIC int Vpee_numSS(Vpee *thee) {
00480     int num = 0;
00481     int isimp;
00482
00483     for (isimp=0; isimp<Gem_numSS(thee->gm); isimp++) {
00484         if (SS_chart(Gem_SS(thee->gm, isimp)) == thee->localPartID) num++;
00485     }
00486
00487     return num;
00488 }
00489
00490 /* ////////////////////////////////////////
00491 // Routine:  Vpee_userDefined
00492 //
00493 // Purpose:  Reduce code bloat by wrapping up the common steps for getting the
00494 //            user-defined error estimate
00495 //
00496 // Author:   Nathan Baker
00498 VPRIVATE int Vpee_userDefined(Vpee *thee,
00499                             SS *sm
00500                             ) {
00501
00502     int ivert,
00503         icoord,
00504         chart[4],
00505         fType[4],
00506         vType[4];
00507     double vx[4][3];
00508
00509     for (ivert=0; ivert<Gem_dimVV(thee->gm); ivert++) {
00510         fType[ivert] = SS_faceType(sm, ivert);
00511         vType[ivert] = VV_type(SS_vertex(sm, ivert) );
00512         chart[ivert] = VV_chart(SS_vertex(sm, ivert) );
00513         for (icoord=0; icoord<Gem_dimII(thee->gm); icoord++) {
00514             vx[ivert][icoord] = VV_coord(SS_vertex(sm, ivert), icoord );
00515         }
00516     }
00517     return thee->gm->pde->markSimplex(Gem_dim(thee->gm), Gem_dimII(thee->gm),
00518         SS_type(sm), fType, vType, chart, vx, sm);
00519 }
00520
00521 /* ////////////////////////////////////////
00522 // Routine:  Vpee_ourSimp
00523 //

```

```

00524 // Purpose: Reduce code bloat by wrapping up the common steps for determining
00525 //           whether the given simplex can be marked (i.e., belongs to our
00526 //           partition or overlap region)
00527 //
00528 // Returns: 1 if could be marked, 0 otherwise
00529 //
00530 // Author: Nathan Baker
00531 VPRIVATE int Vpee_ourSimp(Vpee *thee,
00532                          SS *sm,
00533                          int rcol
00534                          ) {
00535
00536
00537     int ivert;
00538     double dist,
00539           dx,
00540           dy,
00541           dz;
00542
00543     if (thee->killFlag == 0) return 1;
00544     else if (thee->killFlag == 1) {
00545         if ((SS_chart(sm) == rcol) || (rcol < 0)) return 1;
00546     } else if (thee->killFlag == 2) {
00547         if (rcol < 0) return 1;
00548     } else {
00549         /* We can only do distance-based searches on the local partition */
00550         VASSERT(rcol == thee->localPartID);
00551         /* Find the closest distance between this simplex and the
00552          * center of the local partition and check it against
00553          * (thee->localPartRadius*thee->killParam) */
00554         dist = 0;
00555         for (ivert=0; ivert<SS_dimVV(sm); ivert++) {
00556             dx = VV_coord(SS_vertex(sm, ivert), 0) -
00557                 thee->localPartCenter[0];
00558             dy = VV_coord(SS_vertex(sm, ivert), 1) -
00559                 thee->localPartCenter[1];
00560             dz = VV_coord(SS_vertex(sm, ivert), 2) -
00561                 thee->localPartCenter[2];
00562             dist = VSQRT((dx*dx + dy*dy + dz*dz));
00563         }
00564         if (dist < thee->localPartRadius*thee->killParam) return 1;
00565     }
00566     } else if (thee->killFlag == 3) VASSERT(0);
00567     else VASSERT(0);
00568
00569     return 0;
00570
00571 }

```

9.14 src/fem/vpee.h File Reference

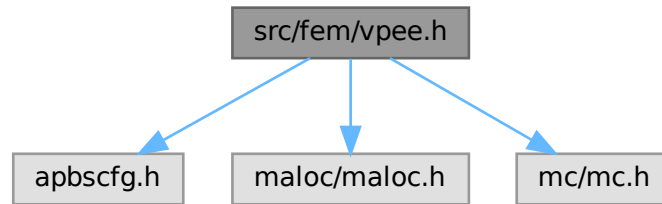
Contains declarations for class Vpee.

```

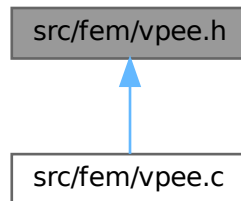
#include "apbscfg.h"
#include "maloc/maloc.h"
#include "mc/mc.h"

```

Include dependency graph for vpee.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVpee](#)
Contains public data members for Vpee class/module.

Typedefs

- typedef struct [sVpee](#) [Vpee](#)
Declaration of the Vpee class as the Vpee structure.

Functions

- VEXTERNC [Vpee](#) * [Vpee_ctor](#) (Gem *gm, int localPartID, int killFlag, double killParam)
Construct the Vpee object.
- VEXTERNC int [Vpee_ctor2](#) ([Vpee](#) *thee, Gem *gm, int localPartID, int killFlag, double killParam)
FORTTRAN stub to construct the Vpee object.
- VEXTERNC void [Vpee_dtor](#) ([Vpee](#) **thee)
Object destructor.
- VEXTERNC void [Vpee_dtor2](#) ([Vpee](#) *thee)

FORTTRAN stub object destructor.

- VEXTERNC int [Vpee_markRefine](#) ([Vpee](#) *thee, AM *am, int level, int akey, int rcol, double etol, int bkey)

Mark simplices for refinement based on attenuated error estimates.

- VEXTERNC int [Vpee_numSS](#) ([Vpee](#) *thee)

Returns the number of simplices in the local partition.

9.14.1 Detailed Description

Contains declarations for class [Vpee](#).

Version

\$Id\$

Author

Nathan A. Baker

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
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* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
*
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* THE POSSIBILITY OF SUCH DAMAGE.
*
*
```

Definition in file [vpee.h](#).

9.15 vpee.h

[Go to the documentation of this file.](#)

```

00001
00076 #ifndef _VPEE_H
00077 #define _VPEE_H
00078
00079 #include "apbscfg.h"
00080
00081 #include "malloc/malloc.h"
00082 #include "mc/mc.h"
00083
00089 struct sVpee {
00090
00091     Gem *gm;
00092     int localPartID;
00095     double localPartCenter[3];
00097     double localPartRadius;
00099     int killFlag;
00102     double killParam;
00104     Vmem *mem;
00106 };
00107
00112 typedef struct sVpee Vpee;
00113
00114 /* ////////////////////////////////////////
00115 // Class Vpee Inlineable methods
00116
00117 #if !defined(VINLINE_VPEE)
00118 #else /* if defined(VINLINE_VPEE) */
00120 #endif /* if !defined(VINLINE_VPEE) */
00121
00122 /* ////////////////////////////////////////
00123 // Class Vpee: Non-Inlineable methods (vpee.c)
00124
00125 VEXTERNC Vpee* Vpee_ctor(
00132     Gem *gm, /**< FEtk geometry manager object */
00133     int localPartID,
00134     int killFlag,
00135     double killParam
00146 );
00147
00148 VEXTERNC int Vpee_ctor2(
00155     Vpee *thee,
00156     Gem *gm,
00157     int localPartID,
00158     int killFlag,
00159     double killParam
00170 );
00171
00172 VEXTERNC void Vpee_dtor(
00177     Vpee **thee
00178 );
00179
00180 VEXTERNC void Vpee_dtor2(
00185     Vpee *thee
00186 );
00187
00188 VEXTERNC int Vpee_markRefine(
00204     Vpee *thee,
00205     AM *am,
00206     int level,
00207     int akey,
00208     int rcol,
00216     double etol,
00219     int bkey
00220 );
00224
00225 VEXTERNC int Vpee_numSS(
00231     Vpee *thee
00232 );
00233
00234 #endif /* ifndef _VPEE_H_ */

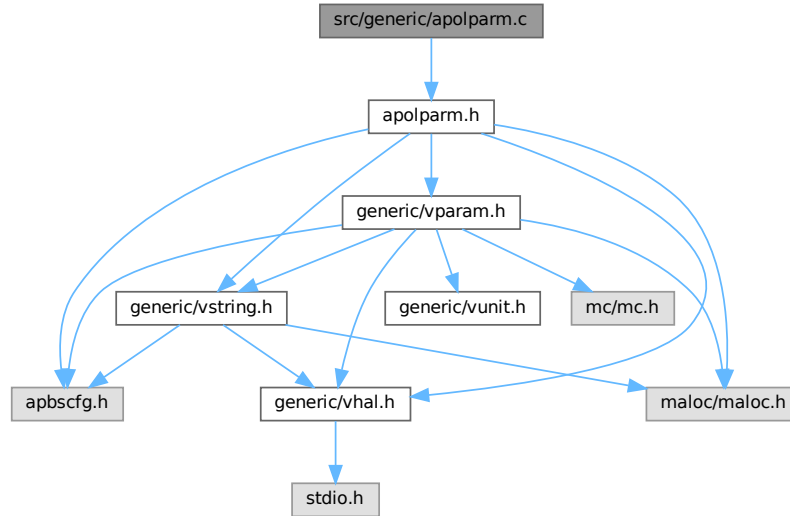
```

9.16 src/generic/apolparm.c File Reference

Class APOLparm methods.

```
#include "apolparm.h"
```

Include dependency graph for apolparm.c:



Functions

- VPUBLIC [APOLparm](#) * [APOLparm_ctor](#) ()
Construct APOLparm.
- VPUBLIC Vrc_Codes [APOLparm_ctor2](#) ([APOLparm](#) *thee)
FORTTRAN stub to construct APOLparm.
- VPUBLIC void [APOLparm_copy](#) ([APOLparm](#) *thee, [APOLparm](#) *source)
Copy target object into thee.
- VPUBLIC void [APOLparm_dtor](#) ([APOLparm](#) **thee)
Object destructor.
- VPUBLIC void [APOLparm_dtor2](#) ([APOLparm](#) *thee)
FORTTRAN stub for object destructor.
- VPUBLIC Vrc_Codes [APOLparm_check](#) ([APOLparm](#) *thee)
Consistency check for parameter values stored in object.
- VPRIVATE Vrc_Codes [APOLparm_parseGRID](#) ([APOLparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parseMOL](#) ([APOLparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parseSRFM](#) ([APOLparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parseSRAD](#) ([APOLparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parseSWIN](#) ([APOLparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parseTEMP](#) ([APOLparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parseGAMMA](#) ([APOLparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parseCALCENERGY](#) ([APOLparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parseCALCFORCE](#) ([APOLparm](#) *thee, Vio *sock)

- VPRIVATE Vrc_Codes [APOLparm_parseBCONC](#) (APOLparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parseSDENS](#) (APOLparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parseDPOS](#) (APOLparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parsePRESS](#) (APOLparm *thee, Vio *sock)
- VPUBLIC Vrc_Codes [APOLparm_parseToken](#) (APOLparm *thee, char tok[VMAX_BUFSIZE], Vio *sock)

Parse an MG keyword from an input file.

9.16.1 Detailed Description

Class APOLparm methods.

Author

David Gohara

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
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```

```
* THE POSSIBILITY OF SUCH DAMAGE.  
*  
*
```

Definition in file [apolparm.c](#).

9.16.2 Function Documentation

9.16.2.1 APOLparm_parseBCONC()

```
VPRIVATE Vrc_Codes APOLparm_parseBCONC (  
    APOLparm * thee,  
    Vio * sock )
```

Definition at line 491 of file [apolparm.c](#).

9.16.2.2 APOLparm_parseCALCENERGY()

```
VPRIVATE Vrc_Codes APOLparm_parseCALCENERGY (  
    APOLparm * thee,  
    Vio * sock )
```

Definition at line 385 of file [apolparm.c](#).

9.16.2.3 APOLparm_parseCALCFORCE()

```
VPRIVATE Vrc_Codes APOLparm_parseCALCFORCE (  
    APOLparm * thee,  
    Vio * sock )
```

Definition at line 438 of file [apolparm.c](#).

9.16.2.4 APOLparm_parseDPOS()

```
VPRIVATE Vrc_Codes APOLparm_parseDPOS (  
    APOLparm * thee,  
    Vio * sock )
```

Definition at line 529 of file [apolparm.c](#).

9.16.2.5 APOLparm_parseGAMMA()

```
VPRIVATE Vrc_Codes APOLparm_parseGAMMA (  
    APOLparm * thee,  
    Vio * sock )
```

Definition at line 366 of file [apolparm.c](#).

9.16.2.6 APOLparm_parseGRID()

```
VPRIVATE Vrc_Codes APOLparm_parseGRID (  
    APOLparm * thee,  
    Vio * sock )
```

Definition at line 237 of file [apolparm.c](#).

9.16.2.7 APOLparm_parseMOL()

```
VPRIVATE Vrc_Codes APOLparm_parseMOL (
    APOLparm * thee,
    Vio * sock )
```

Definition at line 268 of file [apolparm.c](#).

9.16.2.8 APOLparm_parsePRESS()

```
VPRIVATE Vrc_Codes APOLparm_parsePRESS (
    APOLparm * thee,
    Vio * sock )
```

Definition at line 558 of file [apolparm.c](#).

9.16.2.9 APOLparm_parseSDENS()

```
VPRIVATE Vrc_Codes APOLparm_parseSDENS (
    APOLparm * thee,
    Vio * sock )
```

Definition at line 510 of file [apolparm.c](#).

9.16.2.10 APOLparm_parseSRAD()

```
VPRIVATE Vrc_Codes APOLparm_parseSRAD (
    APOLparm * thee,
    Vio * sock )
```

Definition at line 309 of file [apolparm.c](#).

9.16.2.11 APOLparm_parseSRFM()

```
VPRIVATE Vrc_Codes APOLparm_parseSRFM (
    APOLparm * thee,
    Vio * sock )
```

Definition at line 287 of file [apolparm.c](#).

9.16.2.12 APOLparm_parseSWIN()

```
VPRIVATE Vrc_Codes APOLparm_parseSWIN (
    APOLparm * thee,
    Vio * sock )
```

Definition at line 328 of file [apolparm.c](#).

9.16.2.13 APOLparm_parseTEMP()

```
VPRIVATE Vrc_Codes APOLparm_parseTEMP (
    APOLparm * thee,
    Vio * sock )
```

Definition at line 347 of file [apolparm.c](#).

9.17 apolparm.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "apolparm.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 #if !defined(VINLINE_MGPARM)
00062
00063 #endif /* if !defined(VINLINE_MGPARM) */
00064
00065 VPUBLIC APOLparm* APOLparm_ctor() {
00066
00067     /* Set up the structure */
00068     APOLparm *thee = VNULL;
00069     thee = (APOLparm*)Vmem_malloc(VNULL, 1, sizeof(APOLparm));
00070     VASSERT( thee != VNULL);
00071     VASSERT( APOLparm_ctor2(thee) == VRC_SUCCESS );
00072
00073     return thee;
00074 }
00075
00076 VPUBLIC Vrc_Codes APOLparm_ctor2(APOLparm *thee) {
00077
00078     int i;
00079
00080     if (thee == VNULL) return VRC_FAILURE;
00081
00082     thee->parsed = 0;
00083
00084     thee->setgrid = 0;
00085     thee->setmolid = 0;
00086     thee->setbconc = 0;
00087     thee->setsdens = 0;
00088     thee->setdpos = 0;
00089     thee->setpress = 0;
00090     thee->setsrfm = 0;
00091     thee->setsrad = 0;
00092     thee->setswin = 0;
00093
00094     thee->settemp = 0;
00095     thee->setgamma = 0;
00096
00097     thee->setwat = 0;
00098
00099     thee->sav = 0.0;
00100     thee->sasa = 0.0;
00101     thee->wcaEnergy = 0.0;
00102
00103     for(i=0;i<3;i++) thee->totForce[i] = 0.0;
00104
00105     return VRC_SUCCESS;
00106 }
00107
00108 VPUBLIC void APOLparm_copy(
00109     APOLparm *thee,
00110     APOLparm *source
00111 ) {
00112
00113     int i;
00114
00115     thee->parsed = source->parsed;
00116
00117     for (i=0; i<3; i++) thee->grid[i] = source->grid[i];
00118     thee->setgrid = source->setgrid;
00119
00120     thee->molid = source->molid;
00121     thee->setmolid = source->setmolid;
00122
00123     thee->bconc = source->bconc ;
00124     thee->setbconc= source->setbconc ;
00125
00126     thee->sdens = source->sdens ;
00127     thee->setsdens= source->setsdens ;
00128
00129     thee->dpos = source->dpos ;
00130     thee->setdpos= source->setdpos ;
00131
00132     thee->press = source->press ;

```

```

00133     thee->setpress = source->setpress ;
00134
00135     thee->srfm = source->srfm ;
00136     thee->setsrfm = source->setsrfm ;
00137
00138     thee->srاد = source->srاد ;
00139     thee->setsrad = source->setsrad ;
00140
00141     thee->swin = source->swin ;
00142     thee->setswin = source->setswin ;
00143
00144     thee->temp = source->temp ;
00145     thee->settemp = source->settemp ;
00146
00147     thee->gamma = source->gamma ;
00148     thee->setgamma = source->setgamma ;
00149
00150     thee->calcenergy = source->calcenergy ;
00151     thee->setcalcenergy = source->setcalcenergy ;
00152
00153     thee->calcforce = source->calcforce ;
00154     thee->setcalcforce = source->setcalcforce ;
00155
00156     thee->setwat = source->setwat ;
00157
00158     thee->sav = source->sav;
00159     thee->sasa = source->sasa;
00160     thee->wcaEnergy = source->wcaEnergy;
00161
00162     for(i=0;i<3;i++) thee->totForce[i] = source->totForce[i];
00163
00164     return;
00165 }
00166
00167 VPUBLIC void APOLparm_dtor(APOLparm **thee) {
00168     if ((*thee) != VNULL) {
00169         APOLparm_dtor2(*thee);
00170         Vmem_free(VNULL, 1, sizeof(APOLparm), (void **)thee);
00171         (*thee) = VNULL;
00172     }
00173
00174     return;
00175 }
00176
00177 VPUBLIC void APOLparm_dtor2(APOLparm *thee) { ; }
00178
00179 VPUBLIC Vrc_Codes APOLparm_check(APOLparm *thee) {
00180
00181     Vrc_Codes rc;
00182     rc = VRC_SUCCESS;
00183
00184     if (!thee->parsed) {
00185         Vnm_print(2, "APOLparm_check: not filled!\n");
00186         return VRC_FAILURE;
00187     }
00188     if (!thee->setgrid) {
00189         Vnm_print(2, "APOLparm_check: grid not set!\n");
00190         rc = VRC_FAILURE;
00191     }
00192     if (!thee->setmolid) {
00193         Vnm_print(2, "APOLparm_check: molid not set!\n");
00194         rc = VRC_FAILURE;
00195     }
00196     if (!thee->setbconc) {
00197         Vnm_print(2, "APOLparm_check: bconc not set!\n");
00198         rc = VRC_FAILURE;
00199     }
00200     if (!thee->setsdens) {
00201         Vnm_print(2, "APOLparm_check: sdens not set!\n");
00202         rc = VRC_FAILURE;
00203     }
00204     if (!thee->setdpos) {
00205         Vnm_print(2, "APOLparm_check: dpos not set!\n");
00206         rc = VRC_FAILURE;
00207     }
00208     if (!thee->setpress) {
00209         Vnm_print(2, "APOLparm_check: press not set!\n");
00210         rc = VRC_FAILURE;
00211     }
00212     if (!thee->setsrfm) {

```

```

00214         Vnm_print(2, "APOLparm_check:  srfm not set!\n");
00215         rc = VRC_FAILURE;
00216     }
00217     if (!thee->setsrad) {
00218         Vnm_print(2, "APOLparm_check:  srad not set!\n");
00219         rc = VRC_FAILURE;
00220     }
00221     if (!thee->setswin) {
00222         Vnm_print(2, "APOLparm_check:  swin not set!\n");
00223         rc = VRC_FAILURE;
00224     }
00225     if (!thee->settemp) {
00226         Vnm_print(2, "APOLparm_check:  temp not set!\n");
00227         rc = VRC_FAILURE;
00228     }
00229     if (!thee->setgamma) {
00230         Vnm_print(2, "APOLparm_check:  gamma not set!\n");
00231         rc = VRC_FAILURE;
00232     }
00233     return rc;
00234 }
00235 }
00236
00237 VPRIVATE Vrc_Codes APOLparm_parseGRID(APOLparm *thee, Vio *sock) {
00238     char tok[VMAX_BUFSIZE];
00239     double tf;
00240
00241     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00242     if (sscanf(tok, "%lf", &tf) == 0) {
00243         Vnm_print(2, "Nosh:  Read non-float (%s) while parsing GRID \
00244 keyword!\n", tok);
00245         return VRC_WARNING;
00246     } else thee->grid[0] = tf;
00247     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00248     if (sscanf(tok, "%lf", &tf) == 0) {
00249         Vnm_print(2, "Nosh:  Read non-float (%s) while parsing GRID \
00250 keyword!\n", tok);
00251         return VRC_WARNING;
00252     } else thee->grid[1] = tf;
00253     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00254     if (sscanf(tok, "%lf", &tf) == 0) {
00255         Vnm_print(2, "Nosh:  Read non-float (%s) while parsing GRID \
00256 keyword!\n", tok);
00257         return VRC_WARNING;
00258     } else thee->grid[2] = tf;
00259     thee->setgrid = 1;
00260     return VRC_SUCCESS;
00261 }
00262
00263 VERROR1:
00264     Vnm_print(2, "parseAPOL:  ran out of tokens!\n");
00265     return VRC_WARNING;
00266 }
00267
00268 VPRIVATE Vrc_Codes APOLparm_parseMOL(APOLparm *thee, Vio *sock) {
00269     int ti;
00270     char tok[VMAX_BUFSIZE];
00271
00272     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00273     if (sscanf(tok, "%d", &ti) == 0) {
00274         Vnm_print(2, "Nosh:  Read non-int (%s) while parsing MOL \
00275 keyword!\n", tok);
00276         return VRC_WARNING;
00277     }
00278     thee->molid = ti;
00279     thee->setmolid = 1;
00280     return VRC_SUCCESS;
00281 }
00282 VERROR1:
00283     Vnm_print(2, "parseAPOL:  ran out of tokens!\n");
00284     return VRC_WARNING;
00285 }
00286
00287 VPRIVATE Vrc_Codes APOLparm_parseSRFM(APOLparm *thee, Vio *sock) {
00288     char tok[VMAX_BUFSIZE];
00289
00290     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00291
00292     if (Vstring_strcasecmp(tok, "sacc") == 0) {
00293         thee->srfm = VSM_MOL;
00294         thee->setsrfm = 1;

```

```

00295         return VRC_SUCCESS;
00296     } else {
00297         Vnm_print(2, "parseAPOL: Unrecongized keyword (%s) when parsing srfm!\n", tok);
00298         Vnm_print(2, "parseAPOL: Accepted values for srfm = sacc\n");
00299         return VRC_WARNING;
00300     }
00301
00302     return VRC_FAILURE;
00303
00304 ERROR1:
00305     Vnm_print(2, "parseAPOL: ran out of tokens!\n");
00306     return VRC_WARNING;
00307 }
00308
00309 VPRIVATE Vrc_Codes APOLparm_parseSRAD(APOLparm *thee, Vio *sock) {
00310     char tok[VMAX_BUFSIZE];
00311     double tf;
00312
00313     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00314     if (sscanf(tok, "%lf", &tf) == 0) {
00315         Vnm_print(2, "Nosh: Read non-float (%s) while parsing SRAD \
00316 keyword!\n", tok);
00317         return VRC_WARNING;
00318     }
00319     thee->srad = tf;
00320     thee->setsrad = 1;
00321     return VRC_SUCCESS;
00322
00323 ERROR1:
00324     Vnm_print(2, "parseAPOL: ran out of tokens!\n");
00325     return VRC_WARNING;
00326 }
00327
00328 VPRIVATE Vrc_Codes APOLparm_parseSWIN(APOLparm *thee, Vio *sock) {
00329     char tok[VMAX_BUFSIZE];
00330     double tf;
00331
00332     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00333     if (sscanf(tok, "%lf", &tf) == 0) {
00334         Vnm_print(2, "Nosh: Read non-float (%s) while parsing SWIN \
00335 keyword!\n", tok);
00336         return VRC_WARNING;
00337     }
00338     thee->swin = tf;
00339     thee->setswin = 1;
00340     return VRC_SUCCESS;
00341
00342 ERROR1:
00343     Vnm_print(2, "parseAPOL: ran out of tokens!\n");
00344     return VRC_WARNING;
00345 }
00346
00347 VPRIVATE Vrc_Codes APOLparm_parseTEMP(APOLparm *thee, Vio *sock) {
00348     char tok[VMAX_BUFSIZE];
00349     double tf;
00350
00351     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00352     if (sscanf(tok, "%lf", &tf) == 0) {
00353         Vnm_print(2, "Nosh: Read non-float (%s) while parsing TEMP \
00354 keyword!\n", tok);
00355         return VRC_WARNING;
00356     }
00357     thee->temp = tf;
00358     thee->settemp = 1;
00359     return VRC_SUCCESS;
00360
00361 ERROR1:
00362     Vnm_print(2, "parseAPOL: ran out of tokens!\n");
00363     return VRC_WARNING;
00364 }
00365
00366 VPRIVATE Vrc_Codes APOLparm_parseGAMMA(APOLparm *thee, Vio *sock) {
00367     char tok[VMAX_BUFSIZE];
00368     double tf;
00369
00370     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00371     if (sscanf(tok, "%lf", &tf) == 0) {
00372         Vnm_print(2, "Nosh: Read non-float (%s) while parsing GAMMA \
00373 keyword!\n", tok);
00374         return VRC_WARNING;
00375     }

```

```

00376     thee->gamma = tf;
00377     thee->setgamma = 1;
00378     return VRC_SUCCESS;
00379
00380 VERROR1:
00381     Vnm_print(2, "parseAPOL:  ran out of tokens!\n");
00382     return VRC_WARNING;
00383 }
00384
00385 VPRIVATE Vrc_Codes APOLparm_parseCALCENERGY(APOLparm *thee, Vio *sock) {
00386     char tok[VMAX_BUFSIZE];
00387     int ti;
00388
00389     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00390     /* Parse number */
00391     if (sscanf(tok, "%d", &ti) == 1) {
00392         thee->calcenergy = (APOLparm_calcEnergy)ti;
00393         thee->setcalcenergy = 1;
00394
00395         Vnm_print(2, "parseAPOL:  Warning -- parsed deprecated \"calcenergy \
00396 %d\" statement.\n", ti);
00397         Vnm_print(2, "parseAPOL:  Please use \"calcenergy \");
00398         switch (thee->calcenergy) {
00399             case ACE_NO:
00400                 Vnm_print(2, "no");
00401                 break;
00402             case ACE_TOTAL:
00403                 Vnm_print(2, "total");
00404                 break;
00405             case ACE_COMPS:
00406                 Vnm_print(2, "comps");
00407                 break;
00408             default:
00409                 Vnm_print(2, "UNKNOWN");
00410                 break;
00411         }
00412         Vnm_print(2, "\" instead.\n");
00413         return VRC_SUCCESS;
00414     } else if (Vstring_strcasecmp(tok, "no") == 0) {
00415         thee->calcenergy = ACE_NO;
00416         thee->setcalcenergy = 1;
00417         return VRC_SUCCESS;
00418     } else if (Vstring_strcasecmp(tok, "total") == 0) {
00419         thee->calcenergy = ACE_TOTAL;
00420         thee->setcalcenergy = 1;
00421         return VRC_SUCCESS;
00422     } else if (Vstring_strcasecmp(tok, "comps") == 0) {
00423         thee->calcenergy = ACE_COMPS;
00424         thee->setcalcenergy = 1;
00425         return VRC_SUCCESS;
00426     } else {
00427         Vnm_print(2, "Nosh:  Unrecognized parameter (%s) while parsing \
00428 calcenergy!\n", tok);
00429         return VRC_WARNING;
00430     }
00431     return VRC_FAILURE;
00432
00433 VERROR1:
00434     Vnm_print(2, "parseAPOL:  ran out of tokens!\n");
00435     return VRC_WARNING;
00436 }
00437
00438 VPRIVATE Vrc_Codes APOLparm_parseCALCFORCE(APOLparm *thee, Vio *sock) {
00439     char tok[VMAX_BUFSIZE];
00440     int ti;
00441
00442     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00443     /* Parse number */
00444     if (sscanf(tok, "%d", &ti) == 1) {
00445         thee->calcforce = (APOLparm_calcForce)ti;
00446         thee->setcalcforce = 1;
00447
00448         Vnm_print(2, "parseAPOL:  Warning -- parsed deprecated \"calcforce \
00449 %d\" statement.\n", ti);
00450         Vnm_print(2, "parseAPOL:  Please use \"calcforce \");
00451         switch (thee->calcenergy) {
00452             case ACF_NO:
00453                 Vnm_print(2, "no");
00454                 break;
00455             case ACF_TOTAL:
00456                 Vnm_print(2, "total");

```

```

00457         break;
00458     case ACF_COMPS:
00459         Vnm_print(2, "comps");
00460         break;
00461     default:
00462         Vnm_print(2, "UNKNOWN");
00463         break;
00464     }
00465     Vnm_print(2, "\"" instead.\n");
00466     return VRC_SUCCESS;
00467 } else if (Vstring_strcasecmp(tok, "no") == 0) {
00468     thee->calcforce = ACF_NO;
00469     thee->setcalcforce = 1;
00470     return VRC_SUCCESS;
00471 } else if (Vstring_strcasecmp(tok, "total") == 0) {
00472     thee->calcforce = ACF_TOTAL;
00473     thee->setcalcforce = 1;
00474     return VRC_SUCCESS;
00475 } else if (Vstring_strcasecmp(tok, "comps") == 0) {
00476     thee->calcforce = ACF_COMPS;
00477     thee->setcalcforce = 1;
00478     return VRC_SUCCESS;
00479 } else {
00480     Vnm_print(2, "Nosh: Unrecognized parameter (%s) while parsing \
00481 calcforce!\n", tok);
00482     return VRC_WARNING;
00483 }
00484 return VRC_FAILURE;
00485
00486 ERROR1:
00487     Vnm_print(2, "parseAPOL: ran out of tokens!\n");
00488     return VRC_WARNING;
00489 }
00490
00491 VPRIVATE Vrc_Codes APOLparm_parseBCONC(APOLparm *thee, Vio *sock) {
00492     char tok[VMAX_BUFSIZE];
00493     double tf;
00494
00495     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00496     if (sscanf(tok, "%lf", &tf) == 0) {
00497         Vnm_print(2, "Nosh: Read non-float (%s) while parsing BCONC \
00498 keyword!\n", tok);
00499         return VRC_WARNING;
00500     }
00501     thee->bconc = tf;
00502     thee->setbconc = 1;
00503     return VRC_SUCCESS;
00504
00505 ERROR1:
00506     Vnm_print(2, "parseAPOL: ran out of tokens!\n");
00507     return VRC_WARNING;
00508 }
00509
00510 VPRIVATE Vrc_Codes APOLparm_parseSDENS(APOLparm *thee, Vio *sock) {
00511     char tok[VMAX_BUFSIZE];
00512     double tf;
00513
00514     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00515     if (sscanf(tok, "%lf", &tf) == 0) {
00516         Vnm_print(2, "Nosh: Read non-float (%s) while parsing SDENS \
00517 keyword!\n", tok);
00518         return VRC_WARNING;
00519     }
00520     thee->sdens = tf;
00521     thee->setsdens = 1;
00522     return VRC_SUCCESS;
00523
00524 ERROR1:
00525     Vnm_print(2, "parseAPOL: ran out of tokens!\n");
00526     return VRC_WARNING;
00527 }
00528
00529 VPRIVATE Vrc_Codes APOLparm_parseDPOS(APOLparm *thee, Vio *sock) {
00530     char tok[VMAX_BUFSIZE];
00531     double tf;
00532
00533     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00534     if (sscanf(tok, "%lf", &tf) == 0) {
00535         Vnm_print(2, "Nosh: Read non-float (%s) while parsing SDENS \
00536 keyword!\n", tok);
00537         return VRC_WARNING;

```

```

00538     }
00539     thee->dpos = tf;
00540     thee->setdpos = 1;
00541
00542     if(thee->dpos < 0.001){
00543         Vnm_print(1, "\nWARNING WARNING WARNING WARNING\n");
00544         Vnm_print(1, "Nosh: dpos is set to a very small value.\n");
00545         Vnm_print(1, "Nosh: If you are not using a PQR file, you can \
00546 safely ignore this message.\n");
00547         Vnm_print(1, "Nosh: Otherwise please choose a value greater than \
00548 or equal to 0.001.\n\n");
00549     }
00550
00551     return VRC_SUCCESS;
00552
00553 ERROR1:
00554     Vnm_print(2, "parseAPOL: ran out of tokens!\n");
00555     return VRC_WARNING;
00556 }
00557
00558 VPRIVATE Vrc_Codes APOLparm_parsePRESS(APOLparm *thee, Vio *sock) {
00559     char tok[VMAX_BUFSIZE];
00560     double tf;
00561
00562     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00563     if (sscanf(tok, "%lf", &tf) == 0) {
00564         Vnm_print(2, "Nosh: Read non-float (%s) while parsing PRESS \
00565 keyword!\n", tok);
00566         return VRC_WARNING;
00567     }
00568     thee->press = tf;
00569     thee->setpress = 1;
00570     return VRC_SUCCESS;
00571
00572 ERROR1:
00573     Vnm_print(2, "parseAPOL: ran out of tokens!\n");
00574     return VRC_WARNING;
00575 }
00576
00577 VPUBLIC Vrc_Codes APOLparm_parseToken(APOLparm *thee, char tok[VMAX_BUFSIZE],
00578     Vio *sock) {
00579
00580     if (thee == VNULL) {
00581         Vnm_print(2, "parseAPOL: got NULL thee!\n");
00582         return VRC_WARNING;
00583     }
00584
00585     if (sock == VNULL) {
00586         Vnm_print(2, "parseAPOL: got NULL socket!\n");
00587         return VRC_WARNING;
00588     }
00589
00590     if (Vstring_strcasecmp(tok, "mol") == 0) {
00591         return APOLparm_parseMOL(thee, sock);
00592     } else if (Vstring_strcasecmp(tok, "grid") == 0) {
00593         return APOLparm_parseGRID(thee, sock);
00594     } else if (Vstring_strcasecmp(tok, "dime") == 0) {
00595         Vnm_print(2, "APOLparm_parseToken: The DIME and GLEN keywords for APOLAR have been replaced with
00596 GRID.\n");
00597         Vnm_print(2, "APOLparm_parseToken: Please see the APBS User Guide for more information.\n");
00598         return VRC_WARNING;
00599     } else if (Vstring_strcasecmp(tok, "glen") == 0) {
00600         Vnm_print(2, "APOLparm_parseToken: The DIME and GLEN keywords for APOLAR have been replaced with
00601 GRID.\n");
00602         Vnm_print(2, "APOLparm_parseToken: Please see the APBS User Guide for more information.\n");
00603         return VRC_WARNING;
00604     } else if (Vstring_strcasecmp(tok, "bconc") == 0) {
00605         return APOLparm_parseBCONC(thee, sock);
00606     } else if (Vstring_strcasecmp(tok, "sdens") == 0) {
00607         return APOLparm_parseSDENS(thee, sock);
00608     } else if (Vstring_strcasecmp(tok, "dpos") == 0) {
00609         return APOLparm_parseDPOS(thee, sock);
00610     } else if (Vstring_strcasecmp(tok, "srfm") == 0) {
00611         return APOLparm_parseSRFM(thee, sock);
00612     } else if (Vstring_strcasecmp(tok, "srad") == 0) {
00613         return APOLparm_parseSRAD(thee, sock);
00614     } else if (Vstring_strcasecmp(tok, "swin") == 0) {
00615         return APOLparm_parseSWIN(thee, sock);
00616     } else if (Vstring_strcasecmp(tok, "temp") == 0) {
00617         return APOLparm_parseTEMP(thee, sock);
00618     } else if (Vstring_strcasecmp(tok, "gamma") == 0) {

```



```

00617         return APOLparm_parseGAMMA(thee, sock);
00618     } else if (Vstring_strcasecmp(tok, "press") == 0) {
00619         return APOLparm_parsePRESS(thee, sock);
00620     } else if (Vstring_strcasecmp(tok, "calcenergy") == 0) {
00621         return APOLparm_parseCALCENERGY(thee, sock);
00622     } else if (Vstring_strcasecmp(tok, "calcforce") == 0) {
00623         return APOLparm_parseCALCFORCE(thee, sock);
00624     }
00625
00626     return VRC_FAILURE;
00627 }
00628 }

```

9.18 apolparm.h

```

00001
00063 #ifndef _APOLPARAM_H_
00064 #define _APOLPARAM_H_
00065
00066 /* Generic header files */
00067 #include "apbscfg.h"
00068
00069 #include "malloc/malloc.h"
00070
00071 #include "generic/vhal.h"
00072 #include "generic/vstring.h"
00073 #include "generic/vparam.h"
00074
00079 enum eAPOLparm_calcEnergy {
00080     ACE_NO=0,
00081     ACE_TOTAL=1,
00082     ACE_COMPS=2
00083 };
00084
00089 typedef enum eAPOLparm_calcEnergy APOLparm_calcEnergy;
00090
00095 enum eAPOLparm_calcForce {
00096     ACF_NO=0,
00097     ACF_TOTAL=1,
00098     ACF_COMPS=2
00099 };
00100
00105 typedef enum eAPOLparm_calcForce APOLparm_calcForce;
00106
00111 enum eAPOLparm_doCalc {
00112     ACD_NO=0,
00113     ACD_YES=1,
00114     ACD_ERROR=2
00115 };
00116
00121 typedef enum eAPOLparm_doCalc APOLparm_doCalc;
00122
00123
00129 struct sAPOLparm {
00130
00131     int parsed;
00133     double grid[3];
00134     int setgrid;
00136     int molid;
00137     int setmolid;
00139     double bconc;
00140     int setbconc;
00142     double sdens;
00143     int setsdens;
00145     double dpos;
00146     int setdpos;
00148     double press;
00149     int setpress;
00151     Vsurf_Meth srfm;
00152     int setsrfm;
00154     double srad;
00155     int setsrad;
00157     double swin;
00158     int setswin;
00160     double temp;
00161     int settemp;
00163     double gamma;
00165     int setgamma;

```

```

00167     APOLparm_calcEnergy calcenergy;
00168     int setcalcenergy;
00170     APOLparm_calcForce calcforce;
00171     int setcalcforce;
00173     double watsigma;
00174     double watepsilon;
00175     double sasa;
00176     double sav;
00177     double wcaEnergy;
00178     double totForce[3];
00180     int setwat;
00182 };
00183
00188 typedef struct sAPOLparm APOLparm;
00189
00190 /* ////////////////////////////////////////
00191 // Class Nosh: Non-inlineable methods (nosh.c)
00193
00199 VEXTERNC APOLparm* APOLparm_ctor();
00200
00207 VEXTERNC Vrc_Codes APOLparm_ctor2(APOLparm *thee);
00208
00214 VEXTERNC void APOLparm_dtor(APOLparm **thee);
00215
00221 VEXTERNC void APOLparm_dtor2(APOLparm *thee);
00222
00230 VEXTERNC Vrc_Codes APOLparm_check(APOLparm *thee);
00231
00238 VEXTERNC void APOLparm_copy(APOLparm *thee, APOLparm *source);
00239
00250 VEXTERNC Vrc_Codes APOLparm_parseToken(APOLparm *thee, char tok[VMAX_BUFSIZE],
00251     Vio *sock);
00252
00253 #endif
00254

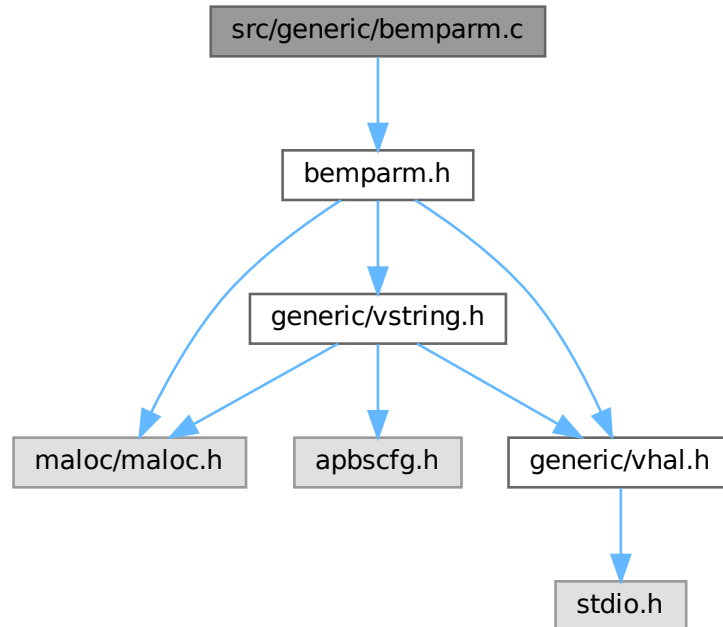
```

9.19 src/generic/bemparm.c File Reference

Class BEMparm methods.

```
#include "bemparm.h"
```

Include dependency graph for bemparm.c:



Functions

- VPUBLIC BEMparm * BEMparm_ctor (BEMparm_CalcType type)
Construct BEMparm object.
- VPUBLIC Vrc_Codes BEMparm_ctor2 (BEMparm *thee, BEMparm_CalcType type)
FORTTRAN stub to construct BEMparm object.
- VPUBLIC void BEMparm_dtor (BEMparm **thee)
Object destructor.
- VPUBLIC void BEMparm_dtor2 (BEMparm *thee)
FORTTRAN stub for object destructor.
- VPUBLIC Vrc_Codes BEMparm_check (BEMparm *thee)
Consistency check for parameter values stored in object.
- VPUBLIC void BEMparm_copy (BEMparm *thee, BEMparm *parm)
Copy object info into thee.
- VPRIVATE Vrc_Codes BEMparm_parseTREE_ORDER (BEMparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes BEMparm_parseTREE_N0 (BEMparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes BEMparm_parseMAC (BEMparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes BEMparm_parseMESH (BEMparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes BEMparm_parseOUTDATA (BEMparm *thee, Vio *sock)
- VPUBLIC Vrc_Codes BEMparm_parseToken (BEMparm *thee, char tok[VMAX_BUFSIZE], Vio *sock)
Parse an MG keyword from an input file.

9.19.1 Detailed Description

Class BEMparm methods.

Author

Nathan A. Baker, Weihua Geng, and Andrew J. Stevens

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
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*   Pacific Northwest National Laboratory
*
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*
*
```

Definition in file [bemparm.c](#).

9.19.2 Function Documentation

9.19.2.1 BEMparm_copy()

```
VPUBLIC void BEMparm_copy (
    BEMparm * thee,
    BEMparm * parm )
```

Copy object info into thee.

Author

Nathan Baker

Parameters

<i>thee</i>	destination object
<i>parm</i>	source object

Definition at line 174 of file [bemparm.c](#).

9.19.2.2 BEMparm_parseMAC()

```
VPRIVATE Vrc_Codes BEMparm_parseMAC (
    BEMparm * thee,
    Vio * sock )
```

Definition at line 256 of file [bemparm.c](#).

9.19.2.3 BEMparm_parseMESH()

```
VPRIVATE Vrc_Codes BEMparm_parseMESH (
    BEMparm * thee,
    Vio * sock )
```

Definition at line 279 of file [bemparm.c](#).

9.19.2.4 BEMparm_parseOUTDATA()

```
VPRIVATE Vrc_Codes BEMparm_parseOUTDATA (
    BEMparm * thee,
    Vio * sock )
```

Definition at line 308 of file [bemparm.c](#).

9.19.2.5 BEMparm_parseTREE_N0()

```
VPRIVATE Vrc_Codes BEMparm_parseTREE_N0 (
    BEMparm * thee,
    Vio * sock )
```

Definition at line 233 of file [bemparm.c](#).

9.19.2.6 BEMparm_parseTREE_ORDER()

```
VPRIVATE Vrc_Codes BEMparm_parseTREE_ORDER (
    BEMparm * thee,
    Vio * sock )
```

Definition at line 210 of file [bemparm.c](#).

9.20 bemparm.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "bemparm.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 #if !defined(VINLINE_MGPARM)
00062
00063 #endif /* if !defined(VINLINE_MGPARM) */
00064
00065
00066 VPUBLIC BEmparm* BEmparm_ctor(BEmparm_CalcType type) {
00067
00068     /* Set up the structure */
00069     BEmparm *thee = VNULL;
00070     thee = (BEmparm*)Vmem_malloc(VNULL, 1, sizeof(BEmparm));
00071     VASSERT( thee != VNULL);
00072     VASSERT( BEmparm_ctor2(thee, type) == VRC_SUCCESS );
00073
00074     return thee;
00075 }
00076
00077 VPUBLIC Vrc_Codes BEmparm_ctor2(BEmparm *thee, BEmparm_CalcType type) {
00078
00079     int i;
00080
00081     if (thee == VNULL) return VRC_FAILURE;
00082
00083     thee->parsed = 0;
00084     thee->type = type;
00085
00086     /* *** GENERIC PARAMETERS *** */
00087
00088     /* *** TYPE 0 PARAMETERS *** */
00089     thee->tree_order = 1;
00090     thee->settree_order = 0;
00091     thee->tree_n0 = 500;
00092     thee->settree_n0 = 0;
00093     thee->mac = 0.8;
00094     thee->setmac = 0;
00095
00096     thee->mesh = 0;
00097     thee->setmesh = 0;
00098
00099     thee->outdata = 0;
00100     thee->setoutdata = 0;
00101
00102     /* *** TYPE 1 & 2 PARAMETERS *** */
00103
00104     /* *** TYPE 2 PARAMETERS *** */
00105     thee->nonlintype = 0;
00106     thee->setnonlintype = 0;
00107
00108     /* *** Default parameters for TINKER *** */
00109     thee->chgs = VCM_CHARGE;
00110
00111     return VRC_SUCCESS;
00112 }
00113
00114 VPUBLIC void BEmparm_dtor(BEmparm **thee) {
00115     if ((*thee) != VNULL) {
00116         BEmparm_dtor2(*thee);
00117         Vmem_free(VNULL, 1, sizeof(BEmparm), (void **)thee);
00118         (*thee) = VNULL;
00119     }
00120 }
00121
00122 VPUBLIC void BEmparm_dtor2(BEmparm *thee) { ; }
00123
00124 VPUBLIC Vrc_Codes BEmparm_check(BEmparm *thee) {
00125
00126     Vrc_Codes rc;
00127     int i, tdime[3], ti, tnlev[3], nlev;
00128

```

```

00129     rc = VRC_SUCCESS;
00130
00131     Vnm_print(0, "BEMparm_check: checking BEMparm object of type %d.\n",
00132             thee->type);
00133
00134     /* Check to see if we were even filled... */
00135     if (!thee->parsed) {
00136         Vnm_print(2, "BEMparm_check: not filled!\n");
00137         return VRC_FAILURE;
00138     }
00139
00140
00141     /* Check type settings */
00142     if ((thee->type != BCT_MANUAL) && (thee->type != BCT_NONE)) {
00143         Vnm_print(2, "BEMparm_check: type not set");
00144         rc = VRC_FAILURE;
00145     }
00146
00147     /* Check treecode setting */
00148     if (thee->tree_order < 1) {
00149         Vnm_print(2, "BEMparm_check: treecode order is less than 1");
00150         rc = VRC_FAILURE;
00151     }
00152     if (thee->tree_n0 < 1) {
00153         Vnm_print(2, "BEMparm_check: treecode leaf size is less than 1");
00154         rc = VRC_FAILURE;
00155     }
00156     if (thee->mac > 1 || thee->mac <= 0) {
00157         Vnm_print(2, "BEMparm_check: MAC criterion fails");
00158         rc = VRC_FAILURE;
00159     }
00160
00161     if (thee->mesh > 2 || thee->mesh < 0) {
00162         Vnm_print(2, "BEMparm_check: mesh must be 0 (msms) or 1 and 2 (NanoShaper)");
00163         rc = VRC_FAILURE;
00164     }
00165
00166     if (thee->outdata > 2 || thee->outdata < 0) {
00167         Vnm_print(2, "BEMparm_check: outdata must be 0, 1 (vtk), or 2 (not specified)");
00168         rc = VRC_FAILURE;
00169     }
00170
00171     return rc;
00172 }
00173
00174 VPUBLIC void BEMparm_copy(BEMparm *thee, BEMparm *parm) {
00175
00176     int i;
00177
00178     VASSERT(thee != VNULL);
00179     VASSERT(parm != VNULL);
00180
00181
00182     thee->type = parm->type;
00183     thee->parsed = parm->parsed;
00184
00185     /* *** GENERIC PARAMETERS *** */
00186
00187     /* *** TYPE 0 PARMS *** */
00188
00189     thee->tree_order = parm->tree_order;
00190     thee->settree_order = parm->settree_order;
00191     thee->tree_n0 = parm->tree_n0;
00192     thee->settree_n0 = parm->settree_n0;
00193     thee->mac = parm->mac;
00194     thee->setmac = parm->setmac;
00195
00196     thee->mesh = parm->mesh;
00197     thee->setmesh = parm->setmesh;
00198
00199     thee->outdata = parm->outdata;
00200     thee->setoutdata = parm->setoutdata;
00201
00202     /* *** TYPE 1 & 2 PARMS *** */
00203
00204     /* *** TYPE 2 PARMS *** */
00205     thee->nonlintype = parm->nonlintype;
00206     thee->setnonlintype = parm->setnonlintype;
00207 }
00208
00209

```

```

00210 VPRIVATE Vrc_Codes BEMparm_parseTREE_ORDER(BEMparm *thee, Vio *sock) {
00211     char tok[VMAX_BUFSIZE];
00212     int ti;
00213
00214     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00215     if (sscanf(tok, "%d", &ti) == 0) {
00216         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing TREE_ORDER \
00217 keyword!\n", tok);
00218         return VRC_WARNING;
00219     } else if (ti <= 0) {
00220         Vnm_print(2, "parseBEM: tree_order must be greater than 0!\n");
00221         return VRC_WARNING;
00222     } else thee->tree_order = ti;
00223     thee->settree_order = 1;
00224     return VRC_SUCCESS;
00225
00226     ERROR1:
00227     Vnm_print(2, "parseBEM: ran out of tokens!\n");
00228     return VRC_WARNING;
00229 }
00230
00231
00232 VPRIVATE Vrc_Codes BEMparm_parseTREE_N0(BEMparm *thee, Vio *sock) {
00233     char tok[VMAX_BUFSIZE];
00234     int ti;
00235
00236     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00237     if (sscanf(tok, "%d", &ti) == 0) {
00238         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing TREE_N0 \
00239 keyword!\n", tok);
00240         return VRC_WARNING;
00241     } else if (ti <= 0) {
00242         Vnm_print(2, "parseBEM: tree_n0 must be greater than 0!\n");
00243         return VRC_WARNING;
00244     } else thee->tree_n0 = ti;
00245     thee->settree_n0 = 1;
00246     return VRC_SUCCESS;
00247
00248     ERROR1:
00249     Vnm_print(2, "parseBEM: ran out of tokens!\n");
00250     return VRC_WARNING;
00251 }
00252
00253
00254 VPRIVATE Vrc_Codes BEMparm_parseMAC(BEMparm *thee, Vio *sock) {
00255     char tok[VMAX_BUFSIZE];
00256     double tf;
00257
00258     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00259     if (sscanf(tok, "%lf", &tf) == 0) {
00260         Vnm_print(2, "Nosh: Read non-float (%s) while parsing mac \
00261 keyword!\n", tok);
00262         return VRC_WARNING;
00263     } else if (tf <= 0.0 || tf > 1.0) {
00264         Vnm_print(2, "parseBEM: mac must be between 0 and 1!\n");
00265         return VRC_WARNING;
00266     } else thee->mac = tf;
00267     thee->setmac = 1;
00268     return VRC_SUCCESS;
00269
00270     ERROR1:
00271     Vnm_print(2, "parseBEM: ran out of tokens!\n");
00272     return VRC_WARNING;
00273 }
00274
00275
00276 VPRIVATE Vrc_Codes BEMparm_parseMESH(BEMparm *thee, Vio *sock) {
00277     char tok[VMAX_BUFSIZE];
00278
00279     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00280     if (strcmp(tok, "msms") == 0) {
00281         thee->mesh = 0;
00282     }
00283     else if (strcmp(tok, "ses") == 0) {
00284         thee->mesh = 1;
00285     }
00286     else if (strcmp(tok, "skin") == 0) {
00287

```



```

00291     thee->mesh = 2;
00292 }
00293 else{
00294     Vnm_print(2, "parseBEM: mesh option %s is not recognized! It must be one of msms, \
00295         ses, or skin.\n", tok);
00296     return VRC_WARNING;
00297 }
00298
00299 thee->setmesh = 1;
00300 return VRC_SUCCESS;
00301
00302 VERROR1:
00303     Vnm_print(2, "parseBEM: ran out of tokens!\n");
00304     return VRC_WARNING;
00305 }
00306
00307
00308 VPRIVATE Vrc_Codes BEMparm_parseOUTDATA(BEMparm *thee, Vio *sock) {
00309
00310     char tok[VMAX_BUFSIZE];
00311     int ti;
00312
00313     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00314     if (sscanf(tok, "%d", &ti) == 0) {
00315         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing OUTDATA \
00316             keyword!\n", tok);
00317         return VRC_WARNING;
00318     } else if (ti < 0 || ti > 2) {
00319         Vnm_print(2, "parseBEM: outdata must be 0, 1 (vtk), \
00320             or 2 (unspecified)!\n");
00321         return VRC_WARNING;
00322     } else thee->outdata = ti;
00323     thee->setoutdata = 1;
00324     return VRC_SUCCESS;
00325
00326 VERROR1:
00327     Vnm_print(2, "parseBEM: ran out of tokens!\n");
00328     return VRC_WARNING;
00329 }
00330
00331
00332 VPUBLIC Vrc_Codes BEMparm_parseToken(BEMparm *thee, char tok[VMAX_BUFSIZE],
00333     Vio *sock) {
00334
00335     if (thee == VNULL) {
00336         Vnm_print(2, "parseBEM: got NULL thee!\n");
00337         return VRC_WARNING;
00338     }
00339     if (sock == VNULL) {
00340         Vnm_print(2, "parseBEM: got NULL socket!\n");
00341         return VRC_WARNING;
00342     }
00343
00344     Vnm_print(0, "BEMparm_parseToken: trying %s...\n", tok);
00345
00346     if (Vstring_strcasecmp(tok, "tree_order") == 0) {
00347         return BEMparm_parseTREE_ORDER(thee, sock);
00348     } else if (Vstring_strcasecmp(tok, "tree_n0") == 0) {
00349         return BEMparm_parseTREE_N0(thee, sock);
00350     } else if (Vstring_strcasecmp(tok, "mac") == 0) {
00351         return BEMparm_parseMAC(thee, sock);
00352     } else if (Vstring_strcasecmp(tok, "mesh") == 0) {
00353         return BEMparm_parseMESH(thee, sock);
00354     } else if (Vstring_strcasecmp(tok, "outdata") == 0) {
00355         return BEMparm_parseOUTDATA(thee, sock);
00356     } else {
00357         Vnm_print(2, "parseBEM: Unrecognized keyword (%s)!\n", tok);
00358         return VRC_WARNING;
00359     }
00360 }
00361
00362 return VRC_FAILURE;
00363
00364 }

```

9.21 bemparm.h

00001

```

00064 #ifndef _BEMPARM_H_
00065 #define _BEMPARM_H_
00066
00067 /* Generic header files */
00068 #include "malloc/malloc.h"
00069
00070 #include "generic/vhal.h"
00071 #include "generic/vstring.h"
00072
00077 enum eBEMparm_CalcType {
00078     BCT_MANUAL=0,
00079     BCT_NONE=1
00080 };
00081
00086 typedef enum eBEMparm_CalcType BEMparm_CalcType;
00087
00096 typedef struct sBEMparm {
00097
00098     BEMparm_CalcType type;
00099     int parsed;
00101     /* *** GENERIC PARAMETERS *** */
00102     Vchrg_Src chgs;
00104     int tree_order;
00105     int settree_order;
00106     int tree_n0;
00107     int settree_n0;
00108     double mac;
00109     int setmac;
00110     int nonlintype;
00111     int setnonlintype;
00113     int mesh;
00114     int setmesh;
00116     int outdata;
00117     int setoutdata;
00119 } BEMparm;
00120
00127 VEXTERNC BEMparm* BEMparm_ctor(BEMparm_CalcType type);
00128
00136 VEXTERNC Vrc_Codes BEMparm_ctor2(BEMparm *thee, BEMparm_CalcType type);
00137
00143 VEXTERNC void BEMparm_dtor(BEMparm **thee);
00144
00150 VEXTERNC void BEMparm_dtor2(BEMparm *thee);
00151
00158 VEXTERNC Vrc_Codes BEMparm_check(BEMparm *thee);
00159
00166 VEXTERNC void BEMparm_copy(BEMparm *thee, BEMparm *parm);
00167
00177 VEXTERNC Vrc_Codes BEMparm_parseToken(BEMparm *thee, char tok[VMAX_BUFSIZE],
00178                                         Vio *sock);
00179
00180 #endif

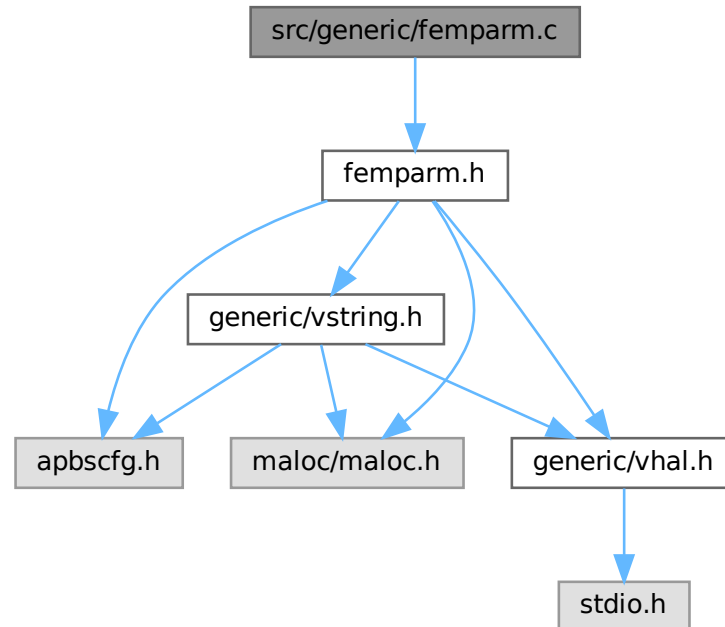
```

9.22 src/generic/femparm.c File Reference

Class FEMparm methods.

```
#include "femparm.h"
```

Include dependency graph for femparm.c:



Functions

- VPUBLIC [FEMparm](#) * [FEMparm_ctor](#) ([FEMparm_CalcType](#) type)
Construct FEMparm.
- VPUBLIC int [FEMparm_ctor2](#) ([FEMparm](#) *thee, [FEMparm_CalcType](#) type)
FORTTRAN stub to construct FEMparm.
- VPUBLIC void [FEMparm_copy](#) ([FEMparm](#) *thee, [FEMparm](#) *source)
Copy target object into thee.
- VPUBLIC void [FEMparm_dtor](#) ([FEMparm](#) **thee)
Object destructor.
- VPUBLIC void [FEMparm_dtor2](#) ([FEMparm](#) *thee)
FORTTRAN stub for object destructor.
- VPUBLIC int [FEMparm_check](#) ([FEMparm](#) *thee)
Consistency check for parameter values stored in object.
- VPRIVATE Vrc_Codes [FEMparm_parseDOMAINLENGTH](#) ([FEMparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [FEMparm_parseETOL](#) ([FEMparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [FEMparm_parseEKEY](#) ([FEMparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [FEMparm_parseAKEYPRE](#) ([FEMparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [FEMparm_parseAKEYSOLVE](#) ([FEMparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [FEMparm_parseTARGETNUM](#) ([FEMparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [FEMparm_parseTARGETRES](#) ([FEMparm](#) *thee, Vio *sock)

- VPRIVATE Vrc_Codes [FEMparm_parseMAXSOLVE](#) (FEMparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [FEMparm_parseMAXVERT](#) (FEMparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [FEMparm_parseUSEMESH](#) (FEMparm *thee, Vio *sock)
- VPUBLIC Vrc_Codes [FEMparm_parseToken](#) (FEMparm *thee, char tok[VMAX_BUFSIZE], Vio *sock)

Parse an MG keyword from an input file.

9.22.1 Detailed Description

Class FEMparm methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
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*   Pacific Northwest National Laboratory
*
*   Additional contributing authors listed in the code documentation.
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*
*
```

Definition in file [femparm.c](#).

9.22.2 Function Documentation

9.22.2.1 FEMparm_parseAKEYPRE()

```
VPRIVATE Vrc_Codes FEMparm_parseAKEYPRE (
    FEMparm * thee,
    Vio * sock )
```

Definition at line 276 of file [femparm.c](#).

9.22.2.2 FEMparm_parseAKEYSOLVE()

```
VPRIVATE Vrc_Codes FEMparm_parseAKEYSOLVE (
    FEMparm * thee,
    Vio * sock )
```

Definition at line 303 of file [femparm.c](#).

9.22.2.3 FEMparm_parseDOMAINLENGTH()

```
VPRIVATE Vrc_Codes FEMparm_parseDOMAINLENGTH (
    FEMparm * thee,
    Vio * sock )
```

Definition at line 196 of file [femparm.c](#).

9.22.2.4 FEMparm_parseEKEY()

```
VPRIVATE Vrc_Codes FEMparm_parseEKEY (
    FEMparm * thee,
    Vio * sock )
```

Definition at line 244 of file [femparm.c](#).

9.22.2.5 FEMparm_parseETOL()

```
VPRIVATE Vrc_Codes FEMparm_parseETOL (
    FEMparm * thee,
    Vio * sock )
```

Definition at line 221 of file [femparm.c](#).

9.22.2.6 FEMparm_parseMAXSOLVE()

```
VPRIVATE Vrc_Codes FEMparm_parseMAXSOLVE (
    FEMparm * thee,
    Vio * sock )
```

Definition at line 372 of file [femparm.c](#).

9.22.2.7 FEMparm_parseMAXVERT()

```
VPRIVATE Vrc_Codes FEMparm_parseMAXVERT (
    FEMparm * thee,
    Vio * sock )
```

Definition at line 391 of file [femparm.c](#).

9.22.2.8 FEMparm_parseTARGETNUM()

```
VPRIVATE Vrc_Codes FEMparm_parseTARGETNUM (
    FEMparm * thee,
    Vio * sock )
```

Definition at line 333 of file [femparm.c](#).

9.22.2.9 FEMparm_parseTARGETRES()

```
VPRIVATE Vrc_Codes FEMparm_parseTARGETRES (
    FEMparm * thee,
    Vio * sock )
```

Definition at line 352 of file [femparm.c](#).

9.22.2.10 FEMparm_parseUSEMESH()

```
VPRIVATE Vrc_Codes FEMparm_parseUSEMESH (
    FEMparm * thee,
    Vio * sock )
```

Definition at line 411 of file [femparm.c](#).

9.23 femparm.c

[Go to the documentation of this file.](#)

```
00001
00057 #include "femparm.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 #if !defined(VINLINE_MGPARM)
00062
00063 #endif /* if !defined(VINLINE_MGPARM) */
00064
00065 VPUBLIC FEMparm* FEMparm_ctor(FEMparm_CalcType type) {
00066
00067     /* Set up the structure */
00068     FEMparm *thee = VNULL;
00069     thee = (FEMparm*)Vmem_malloc(VNULL, 1, sizeof(FEMparm));
00070     VASSERT( thee != VNULL);
00071     VASSERT( FEMparm_ctor2(thee, type) );
00072
00073     return thee;
00074 }
00075
00076 VPUBLIC int FEMparm_ctor2(FEMparm *thee,
00077                          FEMparm_CalcType type
00078                          ) {
00079
00080     if (thee == VNULL) return 0;
00081
00082     thee->parsed = 0;
00083     thee->type = type;
00084     thee->settype = 1;
00085
00086     thee->setglen = 0;
```

```

00087     thee->setetol = 0;
00088     thee->setekey = 0;
00089     thee->setakeyPRE = 0;
00090     thee->setakeySOLVE = 0;
00091     thee->settargetNum = 0;
00092     thee->settargetRes = 0;
00093     thee->setmaxsolve = 0;
00094     thee->setmaxvert = 0;
00095     thee->useMesh = 0;
00096
00097     return 1;
00098 }
00099
00100 VPUBLIC void FEMparm_copy(
00101     FEMparm *thee,
00102     FEMparm *source
00103 ) {
00104
00105     int i;
00106
00107     thee->parsed = source->parsed;
00108     thee->type = source->type;
00109     thee->settype = source->settype;
00110     for (i=0; i<3; i++) thee->glen[i] = source->glen[i];
00111     thee->setglen = source->setglen;
00112     thee->etol = source->etol;
00113     thee->setetol = source->setetol;
00114     thee->ekey = source->ekey;
00115     thee->setekey = source->setekey;
00116     thee->akeyPRE = source->akeyPRE;
00117     thee->setakeyPRE = source->setakeyPRE;
00118     thee->akeySOLVE = source->akeySOLVE;
00119     thee->setakeySOLVE = source->setakeySOLVE;
00120     thee->targetNum = source->targetNum;
00121     thee->settargetNum = source->settargetNum;
00122     thee->targetRes = source->targetRes;
00123     thee->settargetRes = source->settargetRes;
00124     thee->maxsolve = source->maxsolve;
00125     thee->setmaxsolve = source->setmaxsolve;
00126     thee->maxvert = source->maxvert;
00127     thee->setmaxvert = source->setmaxvert;
00128     thee->pkey = source->pkey;
00129     thee->useMesh = source->useMesh;
00130     thee->meshID = source->meshID;
00131 }
00132
00133 VPUBLIC void FEMparm_dtor(FEMparm **thee) {
00134     if ((*thee) != VNULL) {
00135         FEMparm_dtor2(*thee);
00136         Vmem_free(VNULL, 1, sizeof(FEMparm), (void **)thee);
00137         (*thee) = VNULL;
00138     }
00139 }
00140
00141 VPUBLIC void FEMparm_dtor2(FEMparm *thee) { ; }
00142
00143 VPUBLIC int FEMparm_check(FEMparm *thee) {
00144     int rc;
00145     rc = 1;
00146
00147     if (!thee->parsed) {
00148         Vnm_print(2, "FEMparm_check: not filled!\n");
00149         return 0;
00150     }
00151     if (!thee->settype) {
00152         Vnm_print(2, "FEMparm_check: type not set!\n");
00153         rc = 0;
00154     }
00155     if (!thee->setglen) {
00156         Vnm_print(2, "FEMparm_check: glen not set!\n");
00157         rc = 0;
00158     }
00159     if (!thee->setetol) {
00160         Vnm_print(2, "FEMparm_check: etol not set!\n");
00161         rc = 0;
00162     }
00163     if (!thee->setekey) {
00164         Vnm_print(2, "FEMparm_check: ekey not set!\n");
00165         rc = 0;
00166     }
00167 }

```

```

00168     if (!thee->setakeyPRE) {
00169         Vnm_print(2, "FEMparm_check: akeyPRE not set!\n");
00170         rc = 0;
00171     }
00172     if (!thee->setakeySOLVE) {
00173         Vnm_print(2, "FEMparm_check: akeySOLVE not set!\n");
00174         rc = 0;
00175     }
00176     if (!thee->settargetNum) {
00177         Vnm_print(2, "FEMparm_check: targetNum not set!\n");
00178         rc = 0;
00179     }
00180     if (!thee->settargetRes) {
00181         Vnm_print(2, "FEMparm_check: targetRes not set!\n");
00182         rc = 0;
00183     }
00184     if (!thee->setmaxsolve) {
00185         Vnm_print(2, "FEMparm_check: maxsolve not set!\n");
00186         rc = 0;
00187     }
00188     if (!thee->setmaxvert) {
00189         Vnm_print(2, "FEMparm_check: maxvert not set!\n");
00190         rc = 0;
00191     }
00192     return rc;
00193 }
00194
00195 VPRIVATE Vrc_Codes FEMparm_parseDOMAINLENGTH(FEMparm *thee,
00196                                               Vio *sock
00197                                               ) {
00198     int i;
00199     double tf;
00200     char tok[VMAX_BUFSIZE];
00201
00202     for (i=0; i<3; i++) {
00203         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00204         if (sscanf(tok, "%lf", &tf) == 0) {
00205             Vnm_print(2, "parseFE: Read non-double (%s) while parsing \
00206 DOMAINLENGTH keyword!\n", tok);
00207             return VRC_FAILURE;
00208         }
00209         thee->glen[i] = tf;
00210     }
00211     thee->setglen = 1;
00212     return VRC_SUCCESS;
00213 }
00214 VERROR1:
00215 Vnm_print(2, "parseFE: ran out of tokens!\n");
00216 return VRC_FAILURE;
00217
00218 }
00219
00220 VPRIVATE Vrc_Codes FEMparm_parseETOL(FEMparm *thee,
00221                                     Vio *sock
00222                                     ) {
00223     double tf;
00224     char tok[VMAX_BUFSIZE];
00225
00226     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00227     if (sscanf(tok, "%lf", &tf) == 0) {
00228         Vnm_print(2, "parseFE: Read non-double (%s) while parsing \
00229 ETOL keyword!\n", tok);
00230         return VRC_FAILURE;
00231     }
00232     thee->etol = tf;
00233     thee->setetol = 1;
00234     return VRC_SUCCESS;
00235 }
00236 VERROR1:
00237 Vnm_print(2, "parseFE: ran out of tokens!\n");
00238 return VRC_FAILURE;
00239
00240 }
00241
00242 VPRIVATE Vrc_Codes FEMparm_parseEKEY(FEMparm *thee,
00243                                     Vio *sock
00244                                     ) {
00245     char tok[VMAX_BUFSIZE];

```



```

00249     Vrc_Codes vrc = VRC_FAILURE;
00250
00251     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00252     if (Vstring_strcasecmp(tok, "simp") == 0) {
00253         thee->ekey = FET_SIMP;
00254         thee->setekey = 1;
00255         vrc = VRC_SUCCESS;
00256     } else if (Vstring_strcasecmp(tok, "glob") == 0) {
00257         thee->ekey = FET_GLOB;
00258         thee->setekey = 1;
00259         vrc = VRC_SUCCESS;
00260     } else if (Vstring_strcasecmp(tok, "frac") == 0) {
00261         thee->ekey = FET_FRAC;
00262         thee->setekey = 1;
00263         vrc = VRC_SUCCESS;
00264     } else {
00265         Vnm_print(2, "parseFE: undefined value (%s) for ekey!\n", tok);
00266         vrc = VRC_FAILURE;
00267     }
00268
00269     return vrc;
00270 ERROR1:
00271     Vnm_print(2, "parseFE: ran out of tokens!\n");
00272     return VRC_FAILURE;
00273 }
00274 }
00275
00276 VPRIVATE Vrc_Codes FEMparm_parseAKEYPRE(FEMparm *thee, Vio *sock) {
00277
00278     char tok[VMAX_BUFSIZE];
00279     Vrc_Codes vrc = VRC_FAILURE;
00280
00281     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00282     if (Vstring_strcasecmp(tok, "unif") == 0) {
00283         thee->akeyPRE = FRT_UNIF;
00284         thee->setakeyPRE = 1;
00285         vrc = VRC_SUCCESS;
00286     } else if (Vstring_strcasecmp(tok, "geom") == 0) {
00287         thee->akeyPRE = FRT_GEOM;
00288         thee->setakeyPRE = 1;
00289         vrc = VRC_SUCCESS;
00290     } else {
00291         Vnm_print(2, "parseFE: undefined value (%s) for akeyPRE!\n", tok);
00292         vrc = VRC_FAILURE;
00293     }
00294
00295     return vrc;
00296
00297 ERROR1:
00298     Vnm_print(2, "parseFE: ran out of tokens!\n");
00299     return VRC_FAILURE;
00300 }
00301 }
00302
00303 VPRIVATE Vrc_Codes FEMparm_parseAKEYSOLVE(FEMparm *thee, Vio *sock) {
00304
00305     char tok[VMAX_BUFSIZE];
00306     Vrc_Codes vrc = VRC_FAILURE;
00307
00308     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00309     if (Vstring_strcasecmp(tok, "resi") == 0) {
00310         thee->akeySOLVE = FRT_RESI;
00311         thee->setakeySOLVE = 1;
00312         vrc = VRC_SUCCESS;
00313     } else if (Vstring_strcasecmp(tok, "dual") == 0) {
00314         thee->akeySOLVE = FRT_DUAL;
00315         thee->setakeySOLVE = 1;
00316         vrc = VRC_SUCCESS;
00317     } else if (Vstring_strcasecmp(tok, "loca") == 0) {
00318         thee->akeySOLVE = FRT_LOCA;
00319         thee->setakeySOLVE = 1;
00320         vrc = VRC_SUCCESS;
00321     } else {
00322         Vnm_print(2, "parseFE: undefined value (%s) for akeyPRE!\n", tok);
00323         vrc = VRC_FAILURE;
00324     }
00325
00326     return vrc;
00327 ERROR1:
00328     Vnm_print(2, "parseFE: ran out of tokens!\n");
00329     return VRC_SUCCESS;

```

```

00330
00331 }
00332
00333 VPRIVATE Vrc_Codes FEMparm_parseTARGETNUM(FEMparm *thee, Vio *sock) {
00334
00335     char tok[VMAX_BUFSIZE];
00336     int ti;
00337
00338     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00339     if (sscanf(tok, "%d", &ti) == 0) {
00340         Vnm_print(2, "parseFE: read non-int (%s) for targetNum!\n", tok);
00341         return VRC_FAILURE;
00342     }
00343     thee->targetNum = ti;
00344     thee->settargetNum = 1;
00345     return VRC_SUCCESS;
00346 ERROR1:
00347     Vnm_print(2, "parseFE: ran out of tokens!\n");
00348     return VRC_FAILURE;
00349 }
00350
00351
00352 VPRIVATE Vrc_Codes FEMparm_parseTARGETRES(FEMparm *thee, Vio *sock) {
00353
00354     char tok[VMAX_BUFSIZE];
00355     double tf;
00356
00357     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00358     if (sscanf(tok, "%lf", &tf) == 0) {
00359         Vnm_print(2, "parseFE: read non-double (%s) for targetNum!\n",
00360             tok);
00361         return VRC_FAILURE;
00362     }
00363     thee->targetRes = tf;
00364     thee->settargetRes = 1;
00365     return VRC_SUCCESS;
00366 ERROR1:
00367     Vnm_print(2, "parseFE: ran out of tokens!\n");
00368     return VRC_FAILURE;
00369 }
00370
00371
00372 VPRIVATE Vrc_Codes FEMparm_parseMAXSOLVE(FEMparm *thee, Vio *sock) {
00373
00374     char tok[VMAX_BUFSIZE];
00375     int ti;
00376
00377     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00378     if (sscanf(tok, "%d", &ti) == 0) {
00379         Vnm_print(2, "parseFE: read non-int (%s) for maxsolve!\n", tok);
00380         return VRC_FAILURE;
00381     }
00382     thee->maxsolve = ti;
00383     thee->setmaxsolve = 1;
00384     return VRC_SUCCESS;
00385 ERROR1:
00386     Vnm_print(2, "parseFE: ran out of tokens!\n");
00387     return VRC_FAILURE;
00388 }
00389
00390
00391 VPRIVATE Vrc_Codes FEMparm_parseMAXVERT(FEMparm *thee, Vio *sock) {
00392
00393     char tok[VMAX_BUFSIZE];
00394     int ti;
00395
00396     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00397     if (sscanf(tok, "%d", &ti) == 0) {
00398         Vnm_print(2, "parseFE: read non-int (%s) for maxvert!\n", tok);
00399         return VRC_FAILURE;
00400     }
00401     thee->maxvert = ti;
00402     thee->setmaxvert = 1;
00403     return VRC_SUCCESS;
00404
00405 ERROR1:
00406     Vnm_print(2, "parseFE: ran out of tokens!\n");
00407     return VRC_FAILURE;
00408 }
00409 }
00410

```

```

00411 VPRIVATE Vrc_Codes FEMparm_parseUSEMESH(FEMparm *thee, Vio *sock) {
00412     char tok[VMAX_BUFSIZE];
00413     int ti;
00414
00415     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00416     if (sscanf(tok, "%d", &ti) == 0) {
00417         Vnm_print(2, "parseFE: read non-int (%s) for usemesh!\n", tok);
00418         return VRC_FAILURE;
00419     }
00420     thee->useMesh = 1;
00421     thee->meshID = ti;
00422
00423     return VRC_SUCCESS;
00424
00425 ERROR1:
00426     Vnm_print(2, "parsePBE: ran out of tokens!\n");
00427     return VRC_FAILURE;
00428 }
00429
00430
00431 VPUBLIC Vrc_Codes FEMparm_parseToken(FEMparm *thee, char tok[VMAX_BUFSIZE],
00432     Vio *sock) {
00433
00434     //int i, ti; // gcc says unused
00435     //double tf; // gcc says unused
00436
00437     if (thee == VNULL) {
00438         Vnm_print(2, "parseFE: got NULL thee!\n");
00439         return VRC_FAILURE;
00440     }
00441
00442     if (sock == VNULL) {
00443         Vnm_print(2, "parseFE: got NULL socket!\n");
00444         return VRC_FAILURE;
00445     }
00446
00447     if (Vstring_strcasecmp(tok, "domainLength") == 0) {
00448         return FEMparm_parseDOMAINLENGTH(thee, sock);
00449     } else if (Vstring_strcasecmp(tok, "etol") == 0) {
00450         return FEMparm_parseETOL(thee, sock);
00451     } else if (Vstring_strcasecmp(tok, "ekey") == 0) {
00452         return FEMparm_parseEKEY(thee, sock);
00453     } else if (Vstring_strcasecmp(tok, "akeyPRE") == 0) {
00454         return FEMparm_parseAKEYPRE(thee, sock);
00455     } else if (Vstring_strcasecmp(tok, "akeySOLVE") == 0) {
00456         return FEMparm_parseAKEYSOLVE(thee, sock);
00457     } else if (Vstring_strcasecmp(tok, "targetNum") == 0) {
00458         return FEMparm_parseTARGETNUM(thee, sock);
00459     } else if (Vstring_strcasecmp(tok, "targetRes") == 0) {
00460         return FEMparm_parseTARGETRES(thee, sock);
00461     } else if (Vstring_strcasecmp(tok, "maxsolve") == 0) {
00462         return FEMparm_parseMAXSOLVE(thee, sock);
00463     } else if (Vstring_strcasecmp(tok, "maxvert") == 0) {
00464         return FEMparm_parseMAXVERT(thee, sock);
00465     } else if (Vstring_strcasecmp(tok, "usemesh") == 0) {
00466         return FEMparm_parseUSEMESH(thee, sock);
00467     }
00468
00469     return VRC_WARNING;
00470
00471 }

```

9.24 src/generic/femparm.h File Reference

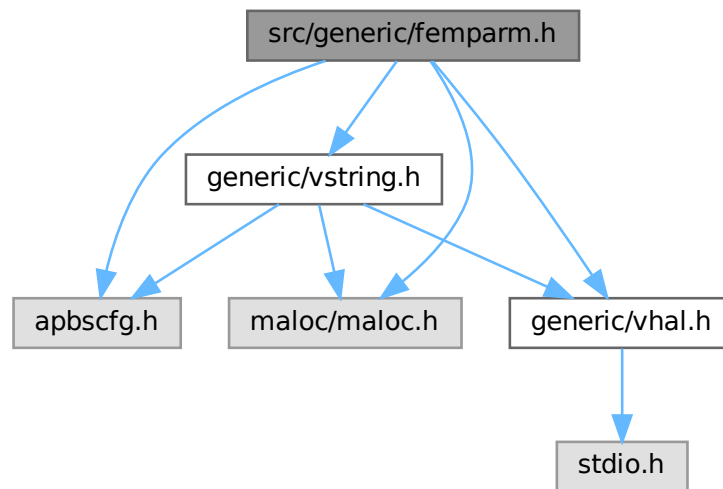
Contains declarations for class APOLparm.

```

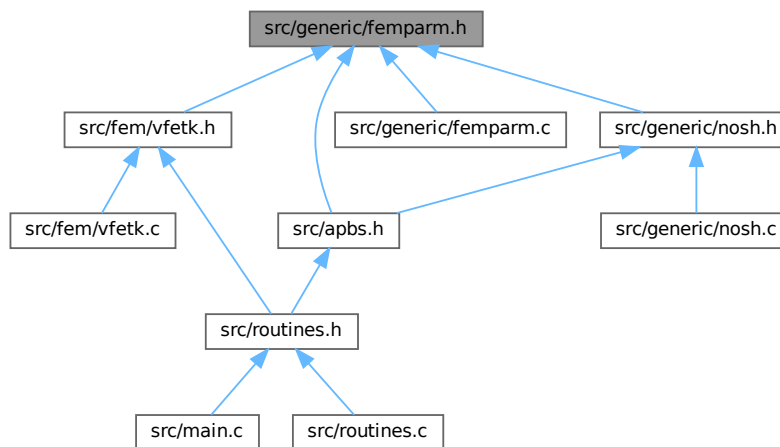
#include "apbscfg.h"
#include "maloc/maloc.h"
#include "generic/vhal.h"
#include "generic/vstring.h"

```

Include dependency graph for femparm.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sFEMparm](#)

Parameter structure for FEM-specific variables from input files.

Typedefs

- typedef enum [eFEMparm_EtolType](#) FEMparm_EtolType
Declare FEMparm_EtolType type.
- typedef enum [eFEMparm_EstType](#) FEMparm_EstType
Declare FEMparm_EstType type.
- typedef enum [eFEMparm_CalcType](#) FEMparm_CalcType
Declare FEMparm_CalcType type.
- typedef struct [sFEMparm](#) FEMparm
Declaration of the FEMparm class as the FEMparm structure.

Enumerations

- enum [eFEMparm_EtolType](#) { FET_SIMP =0 , FET_GLOB =1 , FET_FRAC =2 }
Adaptive refinement error estimate tolerance key.
- enum [eFEMparm_EstType](#) { FRT_UNIF =0 , FRT_GEOM =1 , FRT_RESI =2 , FRT_DUAL =3 , FRT_LOCA =4 }
Adaptive refinement error estimator method.
- enum [eFEMparm_CalcType](#) { FCT_MANUAL , FCT_NONE }
Calculation type.

Functions

- VEXTERNC [FEMparm](#) * [FEMparm_ctor](#) ([FEMparm_CalcType](#) type)
Construct FEMparm.
- VEXTERNC int [FEMparm_ctor2](#) ([FEMparm](#) *thee, [FEMparm_CalcType](#) type)
FORTTRAN stub to construct FEMparm.
- VEXTERNC void [FEMparm_dtor](#) ([FEMparm](#) **thee)
Object destructor.
- VEXTERNC void [FEMparm_dtor2](#) ([FEMparm](#) *thee)
FORTTRAN stub for object destructor.
- VEXTERNC int [FEMparm_check](#) ([FEMparm](#) *thee)
Consistency check for parameter values stored in object.
- VEXTERNC void [FEMparm_copy](#) ([FEMparm](#) *thee, [FEMparm](#) *source)
Copy target object into thee.
- VEXTERNC Vrc_Codes [FEMparm_parseToken](#) ([FEMparm](#) *thee, char tok[VMAX_BUFSIZE], Vio *sock)
Parse an MG keyword from an input file.

9.24.1 Detailed Description

Contains declarations for class APOLparm.

Contains declarations for class FEMparm.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```

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* Pacific Northwest National Laboratory
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* THE POSSIBILITY OF SUCH DAMAGE.
*
*

```

Definition in file [femparm.h](#).

9.25 femparm.h

[Go to the documentation of this file.](#)

```

00001
00063 #ifndef _FEMPARM_H_
00064 #define _FEMPARM_H_
00065
00066 /* Generic header files */
00067 #include "apbscfg.h"
00068
00069 #include "malloc/malloc.h"
00070
00071 #include "generic/vhal.h"
00072 #include "generic/vstring.h"
00073
00079 enum eFEMparm_EtolType {
00080     FET_SIMP=0,
00081     FET_GLOB=1,

```

```

00082     FET_FRAC=2
00083 };
00084
00090 typedef enum eFEMparm_EtolType FEMparm_EtolType;
00091
00098 enum eFEMparm_EstType {
00099     FRT_UNIF=0,
00100     FRT_GEOM=1,
00101     FRT_RESI=2,
00102     FRT_DUAL=3,
00104     FRT_LOCA=4
00105 };
00106
00111 typedef enum eFEMparm_EstType FEMparm_EstType;
00112
00117 enum eFEMparm_CalcType {
00118     FCT_MANUAL,
00119     FCT_NONE
00120 };
00121
00126 typedef enum eFEMparm_CalcType FEMparm_CalcType;
00127
00133 struct sFEMparm {
00134
00135     int parsed;
00138     FEMparm_CalcType type;
00139     int settype;
00140     double glen[3];
00141     int setglen;
00142     double etol;
00144     int setetol;
00145     FEMparm_EtolType ekey;
00147     int setekey;
00148     FEMparm_EstType akeyPRE;
00151     int setakeyPRE;
00152     FEMparm_EstType akeySOLVE;
00154     int setakeySOLVE;
00155     int targetNum;
00159     int settargetNum;
00160     double targetRes;
00164     int settargetRes;
00165     int maxsolve;
00166     int setmaxsolve;
00167     int maxvert;
00169     int setmaxvert;
00170     int pkey;
00173     int useMesh;
00174     int meshID;
00176 };
00177
00182 typedef struct sFEMparm FEMparm;
00183
00184 /* ////////////////////////////////////////
00185 // Class NOsh: Non-inlineable methods (nosh.c)
00187
00194 VEXTERNC FEMparm* FEMparm_ctor(FEMparm_CalcType type);
00195
00203 VEXTERNC int FEMparm_ctor2(FEMparm *thee, FEMparm_CalcType type);
00204
00210 VEXTERNC void FEMparm_dtor(FEMparm **thee);
00211
00217 VEXTERNC void FEMparm_dtor2(FEMparm *thee);
00218
00226 VEXTERNC int FEMparm_check(FEMparm *thee);
00227
00234 VEXTERNC void FEMparm_copy(FEMparm *thee, FEMparm *source);
00235
00246 VEXTERNC Vrc_Codes FEMparm_parseToken(FEMparm *thee, char tok[VMAX_BUFSIZE],
00247     Vio *sock);
00248
00249 #endif
00250

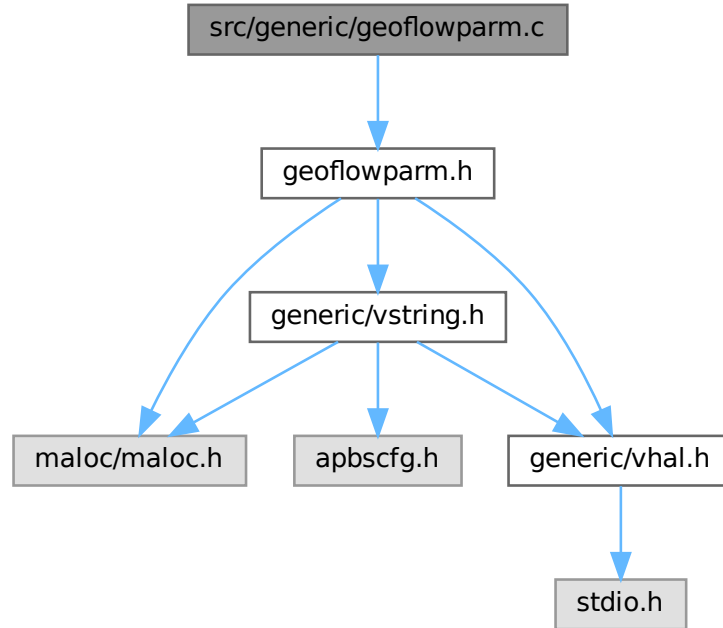
```

9.26 src/generic/geoflowparm.c File Reference

Class GEOFLOWparm methods.

```
#include "geoflowparm.h"
```

Include dependency graph for geoflowparm.c:



Functions

- `VPUBLIC GEOFLOWparm * GEOFLOWparm_ctor (GEOFLOWparm_CalcType type)`
Construct GEOFLOWparm object.
- `VPUBLIC Vrc_Codes GEOFLOWparm_ctor2 (GEOFLOWparm *thee, GEOFLOWparm_CalcType type)`
FORTTRAN stub to construct GEOFLOWparm object ?????????!!!!!!!
- `VPUBLIC void GEOFLOWparm_dtor (GEOFLOWparm **thee)`
Object destructor.
- `VPUBLIC void GEOFLOWparm_dtor2 (GEOFLOWparm *thee)`
FORTTRAN stub for object destructor ?????????!!!!!!!
- `VPUBLIC Vrc_Codes GEOFLOWparm_check (GEOFLOWparm *thee)`
Consistency check for parameter values stored in object.
- `VPUBLIC void GEOFLOWparm_copy (GEOFLOWparm *thee, GEOFLOWparm *parm)`
copy GEOFLOWparm object into thee.
- `Vrc_Codes FUBAR (const char *name)`
- `Vrc_Codes parseNonNeg (double *tf, double def, int *set, char *name, Vio *sock)`
- `VPRIVATE Vrc_Codes GEOFLOWparm_parseVDW (GEOFLOWparm *thee, Vio *sock)`
- `VPRIVATE Vrc_Codes GEOFLOWparm_parseETOL (GEOFLOWparm *thee, Vio *sock)`
- `VPUBLIC Vrc_Codes GEOFLOWparm_parseToken (GEOFLOWparm *thee, char tok[VMAX_BUFSIZE], Vio *sock)`
Parse an MG keyword from an input file.

9.26.1 Detailed Description

Class GEOFLOWparm methods.

Author

Andrew Stevens

Version

\$Id\$

Attention

```
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*
*
```

Definition in file [geoflowparm.c](#).

9.26.2 Function Documentation

9.26.2.1 FUBAR()

```
Vrc_Codes FUBAR (
    const char * name )
```

Definition at line 138 of file [geoflowparm.c](#).

9.26.2.2 GEOFLOWparm_parseETOL()

```
VPRIVATE Vrc_Codes GEOFLOWparm_parseETOL (
    GEOFLOWparm * thee,
    Vio * sock )
```

Definition at line 186 of file [geoflowparm.c](#).

9.26.2.3 GEOFLOWparm_parseVDW()

```
VPRIVATE Vrc_Codes GEOFLOWparm_parseVDW (
    GEOFLOWparm * thee,
    Vio * sock )
```

Definition at line 164 of file [geoflowparm.c](#).

9.26.2.4 parseNonNeg()

```
Vrc_Codes parseNonNeg (
    double * tf,
    double def,
    int * set,
    char * name,
    Vio * sock )
```

Definition at line 143 of file [geoflowparm.c](#).

9.27 geoflowparm.c

[Go to the documentation of this file.](#)

```
00001
00057 #include "geoflowparm.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 #if !defined(VINLINE_MGPARM)
00062
00063 #endif /* if !defined(VINLINE_MGPARM) */
00064
00065
00066 VPUBLIC GEOFLOWparm* GEOFLOWparm_ctor(GEOFLOWparm_CalcType type) {
00067
00068     /* Set up the structure */
00069     GEOFLOWparm *thee = VNULL;
00070     thee = (GEOFLOWparm*)Vmem_malloc(VNULL, 1, sizeof(GEOFLOWparm));
00071     VASSERT( thee != VNULL);
00072     VASSERT( GEOFLOWparm_ctor2(thee, type) == VRC_SUCCESS );
00073
00074     return thee;
00075 }
00076
00077 VPUBLIC Vrc_Codes GEOFLOWparm_ctor2(GEOFLOWparm *thee, GEOFLOWparm_CalcType type) {
00078
00079     int i;
00080
00081     if (thee == VNULL) return VRC_FAILURE;
00082
00083     thee->parsed = 0;
```

```

00084     thee->type = type;
00085     thee->vdw = 0;
00086     thee->etol = 1.0e-6;
00087
00088     return VRC_SUCCESS;
00089 }
00090
00091 VPUBLIC void GEOFLOWparm_dtor(GEOFLOWparm **thee) {
00092     if ((*thee) != VNULL) {
00093         GEOFLOWparm_dtor2(*thee);
00094         Vmem_free(VNULL, 1, sizeof(GEOFLOWparm), (void **)thee);
00095         (*thee) = VNULL;
00096     }
00097 }
00098
00099 VPUBLIC void GEOFLOWparm_dtor2(GEOFLOWparm *thee) { ; }
00100
00101 VPUBLIC Vrc_Codes GEOFLOWparm_check(GEOFLOWparm *thee) {
00102     Vrc_Codes rc;
00103
00104     rc = VRC_SUCCESS;
00105
00106     Vnm_print(0, "GEOFLOWparm_check: checking GEOFLOWparm object of type %d.\n",
00107         thee->type);
00108
00109     /* Check to see if we were even filled... */
00110     if (!thee->parsed) {
00111         Vnm_print(2, "GEOFLOWparm_check: not filled!\n");
00112         return VRC_FAILURE;
00113     }
00114
00115     /* Check type settings */
00116     //if ((thee->type != GFCT_MANUAL)&& (thee->type != GFCT_AUTO)&& (thee->type != GFCT_NONE)) {
00117     if (thee->type != GFCT_AUTO) {
00118         Vnm_print(2, "GEOFLOWparm_check: type not set");
00119         rc = VRC_FAILURE;
00120     }
00121
00122     return rc;
00123 }
00124
00125 }
00126
00127 VPUBLIC void GEOFLOWparm_copy(GEOFLOWparm *thee, GEOFLOWparm *parm) {
00128     VASSERT(thee != VNULL);
00129     VASSERT(parm != VNULL);
00130
00131     thee->type = parm->type;
00132     thee->parsed = parm->parsed;
00133
00134     thee->vdw = parm->vdw;
00135     thee->etol = parm->etol;
00136 }
00137
00138 Vrc_Codes FUBAR(const char* name){
00139     Vnm_print(2, "parseGEOFLOW: ran out of tokens on %s!\n", name);
00140     return VRC_WARNING;
00141 }
00142
00143 Vrc_Codes parseNonNeg(double* tf, double def, int* set, char* name, Vio* sock){
00144     char tok[VMAX_BUFSIZE];
00145     if (Vio_scanf(sock, "%s", tok) == 0) {
00146         *tf = def;
00147         return FUBAR(name);
00148     }
00149
00150     if (sscanf(tok, "%lf", tf) == 0){
00151         Vnm_print(2, "Nosh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00152         *tf = def;
00153         return VRC_WARNING;
00154     } else if (*tf < 0.0){
00155         Vnm_print(2, "parseGEOFLOW: %s must be greater than 0!\n", name);
00156         *tf = def;
00157         return VRC_WARNING;
00158     }
00159
00160     *set = 1;
00161     return VRC_SUCCESS;
00162 }
00163
00164 VPRIVATE Vrc_Codes GEOFLOWparm_parseVDW(GEOFLOWparm *thee, Vio *sock){

```

```

00165     const char* name = "vdw";
00166     char tok[VMAX_BUFSIZE];
00167     int tf;
00168     if(Vio_scanf(sock, "%s", tok) == 0) {
00169         return FUBAR(name);
00170     }
00171
00172
00173     if (sscanf(tok, "%u", &tf) == 0){
00174         Vnm_print(2, "NOsh: Read non-unsigned int (%s) while parsing %s keyword!\n", tok, name);
00175         return VRC_WARNING;
00176     }else if(tf != 0 && tf != 1){
00177         Vnm_print(2, "parseGEOFLOW: %s must be 0 or 1!\n", name);
00178         return VRC_WARNING;
00179     }else{
00180         thee->vdw = tf;
00181     }
00182     thee->setvdw = 1;
00183     return VRC_SUCCESS;
00184 }
00185
00186 VPRIVATE Vrc_Codes GEOFLOWparm_parseETOL(GEOFLOWparm *thee, Vio *sock){
00187
00188     char tok[VMAX_BUFSIZE];
00189     double tf;
00190
00191     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00192     if(sscanf(tok, "%lf", &tf) == 0){
00193         Vnm_print(2, "NOsh: Read non-float (%s) while parsing etol keyword!\n", tok);
00194         return VRC_WARNING;
00195     } else if(tf <= 0.0) {
00196         Vnm_print(2, "parseGEOFLOW: etol must be greater than 0!\n");
00197         return VRC_WARNING;
00198     } else {
00199         thee->etol = tf;
00200     }
00201
00202     return VRC_SUCCESS;
00203
00204
00205
00206 ERROR1:
00207     Vnm_print(2, "parseGEOFLOW: ran out of tokens!\n");
00208     return VRC_WARNING;
00209
00210 }
00211
00212 VPUBLIC Vrc_Codes GEOFLOWparm_parseToken(GEOFLOWparm *thee, char tok[VMAX_BUFSIZE],
00213     Vio *sock) {
00214
00215     if (thee == VNULL) {
00216         Vnm_print(2, "parseGEOFLOW: got NULL thee!\n");
00217         return VRC_WARNING;
00218     }
00219     if (sock == VNULL) {
00220         Vnm_print(2, "parseGEOFLOW: got NULL socket!\n");
00221         return VRC_WARNING;
00222     }
00223
00224     Vnm_print(0, "GEOFLOWparm_parseToken: trying %s...\n", tok);
00225
00226     if (Vstring_strcasecmp(tok, "vdwdisp") == 0) {
00227         return GEOFLOWparm_parseVDW(thee, sock);
00228     } else if(Vstring_strcasecmp(tok, "etol") == 0){
00229         return GEOFLOWparm_parseETOL(thee, sock);
00230     }else {
00231         Vnm_print(2, "parseGEOFLOW: Unrecognized keyword (%s)!\n", tok);
00232         return VRC_WARNING;
00233     }
00234
00235     return VRC_FAILURE;
00236
00237 }

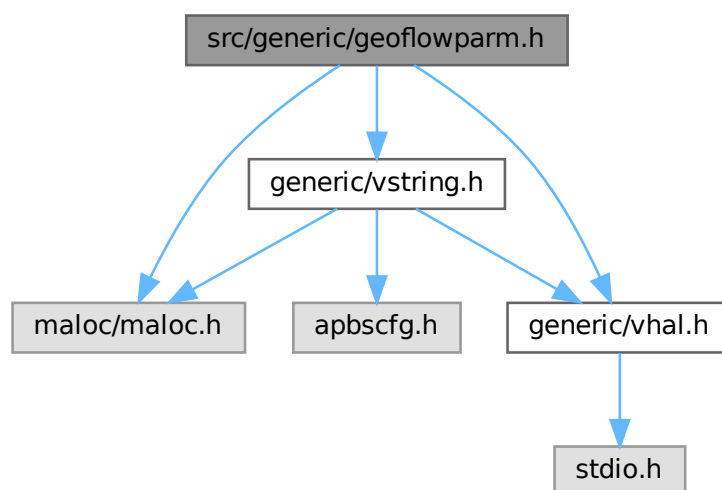
```

9.28 src/generic/geoflowparm.h File Reference

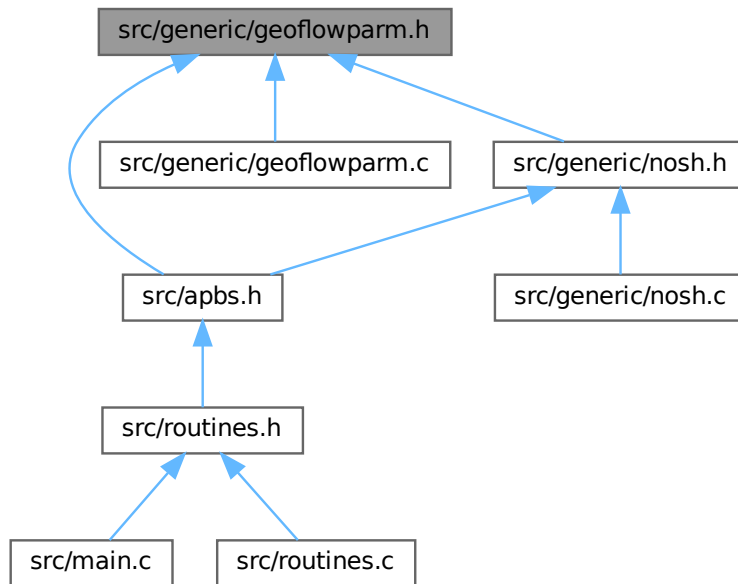
Contains declarations for class GEOFLOWparm.

```
#include "maloc/maloc.h"  
#include "generic/vhal.h"  
#include "generic/vstring.h"
```

Include dependency graph for geoflowparm.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sGEOFLOWparm](#)
Parameter structure for GEOFLOW-specific variables from input files.

Typedefs

- typedef enum [eGEOFLOWparm_CalcType](#) [GEOFLOWparm_CalcType](#)
Declare GEOFLOWparm_CalcType type.
- typedef struct [sGEOFLOWparm](#) [GEOFLOWparm](#)
Parameter structure for GEOFLOW-specific variables from input files.

Enumerations

- enum [eGEOFLOWparm_CalcType](#) { [GFCT_AUTO](#) =1 }
Calculation type.

Functions

- VEXTERNC [GEOFLOWparm](#) * [GEOFLOWparm_ctor](#) ([GEOFLOWparm_CalcType](#) type)
Construct GEOFLOWparm object.
- VEXTERNC Vrc_Codes [GEOFLOWparm_ctor2](#) ([GEOFLOWparm](#) *thee, [GEOFLOWparm_CalcType](#) type)
FORTTRAN stub to construct GEOFLOWparm object ?????????!!!!!!!
- VEXTERNC void [GEOFLOWparm_dtor](#) ([GEOFLOWparm](#) **thee)

Object destructor.

- VEXTERN void [GEOFLOWparm_dtor2](#) ([GEOFLOWparm](#) *thee)
FORTTRAN stub for object destructor ?????????!!!!!!!
- VEXTERN Vrc_Codes [GEOFLOWparm_check](#) ([GEOFLOWparm](#) *thee)
Consistency check for parameter values stored in object.
- VEXTERN Vrc_Codes [GEOFLOWparm_parseToken](#) ([GEOFLOWparm](#) *thee, char tok[VMAX_BUFSIZE], Vio *sock)
Parse an MG keyword from an input file.
- VEXTERN void [GEOFLOWparm_copy](#) ([GEOFLOWparm](#) *thee, [GEOFLOWparm](#) *parm)
copy GEOFLOWparm object into thee.
- VPRIVATE Vrc_Codes [GEOFLOWparm_parseVDW](#) ([GEOFLOWparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [GEOFLOWparm_parseETOL](#) ([GEOFLOWparm](#) *thee, Vio *sock)

9.28.1 Detailed Description

Contains declarations for class [GEOFLOWparm](#).

Version

\$Id\$

Author

Andrew Stevens

Attention

```
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*
*

```

Definition in file [geoflowparm.h](#).

9.28.2 Function Documentation

9.28.2.1 GEOFLOWparm_parseETOL()

```

VPRIVATE Vrc_Codes GEOFLOWparm_parseETOL (
    GEOFLOWparm * thee,
    Vio * sock )

```

Definition at line 186 of file [geoflowparm.c](#).

9.28.2.2 GEOFLOWparm_parseVDW()

```

VPRIVATE Vrc_Codes GEOFLOWparm_parseVDW (
    GEOFLOWparm * thee,
    Vio * sock )

```

Definition at line 164 of file [geoflowparm.c](#).

9.29 geoflowparm.h

[Go to the documentation of this file.](#)

```

00001
00064 #ifndef _GEOFLOWPARM_H_
00065 #define _GEOFLOWPARM_H_
00066
00067 /* Generic header files */
00068 #include "malloc/malloc.h"
00069
00070 #include "generic/vhal.h"
00071 #include "generic/vstring.h"
00072
00077 enum eGEOFLOWparm_CalcType {
00078     //other methods disabled for now only auto currently implemented.
00079     //GFCT_MANUAL=0,    /**< GEOFLOW-manual */
00080     GFCT_AUTO=1,
00081     //GFCT_NONE=2 /**< not defined */
00082 };
00083
00088 typedef enum eGEOFLOWparm_CalcType GEOFLOWparm_CalcType;
00089
00098 typedef struct sGEOFLOWparm {
00099
00100     GEOFLOWparm_CalcType type;
00101     int parsed;
00103     /* *** GENERIC PARAMETERS *** */
00104     int vdw;
00105     int setvdw;
00106     double etol;
00108 } GEOFLOWparm;
00109

```



```

00116 VEXTERNC GEOFLOWparm* GEOFLOWparm_ctor(GEOFLOWparm_CalcType type);
00117
00125 VEXTERNC Vrc_Codes GEOFLOWparm_ctor2(GEOFLOWparm *thee, GEOFLOWparm_CalcType type);
00126
00132 VEXTERNC void GEOFLOWparm_dtor(GEOFLOWparm **thee);
00133
00139 VEXTERNC void GEOFLOWparm_dtor2(GEOFLOWparm *thee);
00140
00147 VEXTERNC Vrc_Codes GEOFLOWparm_check(GEOFLOWparm *thee);
00148
00158 VEXTERNC Vrc_Codes GEOFLOWparm_parseToken(GEOFLOWparm *thee, char tok[VMAX_BUFSIZE],
00159 Vrc_Codes Vio *sock);
00167 VEXTERNC void GEOFLOWparm_copy(GEOFLOWparm *thee, GEOFLOWparm *parm);
00168
00169 VPRIVATE Vrc_Codes GEOFLOWparm_parseVDW(GEOFLOWparm *thee, Vio *sock);
00170
00171 VPRIVATE Vrc_Codes GEOFLOWparm_parseETOL(GEOFLOWparm *thee, Vio *sock);
00172
00173
00174
00175 #endif
00176

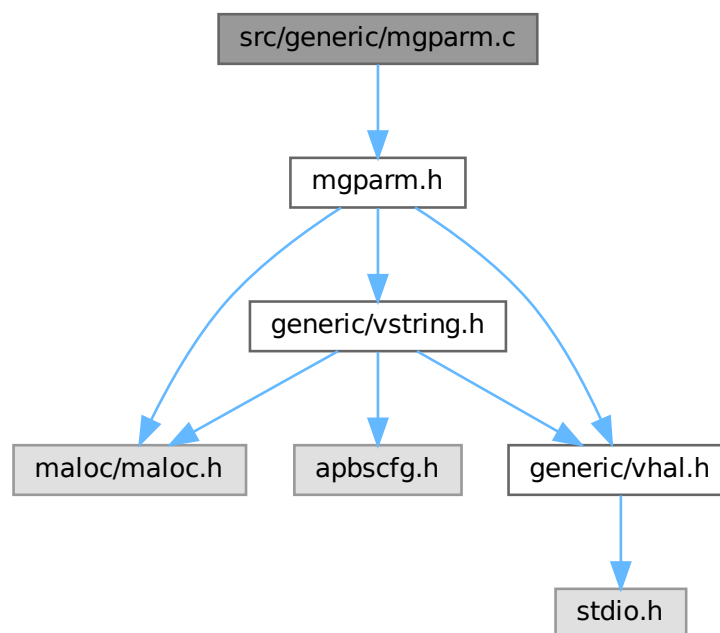
```

9.30 src/generic/mgparm.c File Reference

Class MGparm methods.

```
#include "mgparm.h"
```

Include dependency graph for mgparm.c:



Functions

- VPUBLIC void `MGparm_setCenterX` (`MGparm *thee`, double `x`)

- Set center x-coordinate.*

 - VPUBLIC void [MGparm_setCenterY](#) (MGparm *thee, double y)
- Set center y-coordinate.*

 - VPUBLIC void [MGparm_setCenterZ](#) (MGparm *thee, double z)
- Set center z-coordinate.*

 - VPUBLIC double [MGparm_getCenterX](#) (MGparm *thee)
- Get center x-coordinate.*

 - VPUBLIC double [MGparm_getCenterY](#) (MGparm *thee)
- Get center y-coordinate.*

 - VPUBLIC double [MGparm_getCenterZ](#) (MGparm *thee)
- Get center z-coordinate.*

 - VPUBLIC int [MGparm_getNx](#) (MGparm *thee)
- Get number of grid points in x direction.*

 - VPUBLIC int [MGparm_getNy](#) (MGparm *thee)
- Get number of grid points in y direction.*

 - VPUBLIC int [MGparm_getNz](#) (MGparm *thee)
- Get number of grid points in z direction.*

 - VPUBLIC double [MGparm_getHx](#) (MGparm *thee)
- Get grid spacing in x direction (Å)*

 - VPUBLIC double [MGparm_getHy](#) (MGparm *thee)
- Get grid spacing in y direction (Å)*

 - VPUBLIC double [MGparm_getHz](#) (MGparm *thee)
- Get grid spacing in z direction (Å)*

 - VPUBLIC MGparm * [MGparm_ctor](#) (MGparm_CalcType type)
- Construct MGparm object.*

 - VPUBLIC Vrc_Codes [MGparm_ctor2](#) (MGparm *thee, MGparm_CalcType type)
- FORTTRAN stub to construct MGparm object.*

 - VPUBLIC void [MGparm_dtor](#) (MGparm **thee)
- Object destructor.*

 - VPUBLIC void [MGparm_dtor2](#) (MGparm *thee)
- FORTTRAN stub for object destructor.*

 - VPUBLIC Vrc_Codes [MGparm_check](#) (MGparm *thee)
- Consistency check for parameter values stored in object.*

 - VPUBLIC void [MGparm_copy](#) (MGparm *thee, MGparm *parm)
- Copy MGparm object into thee.*

 - VPRIVATE Vrc_Codes [MGparm_parseDIME](#) (MGparm *thee, Vio *sock)
 - VPRIVATE Vrc_Codes [MGparm_parseCHGM](#) (MGparm *thee, Vio *sock)
 - VPRIVATE Vrc_Codes [MGparm_parseNLEV](#) (MGparm *thee, Vio *sock)
 - VPRIVATE Vrc_Codes [MGparm_parseETOL](#) (MGparm *thee, Vio *sock)
 - VPRIVATE Vrc_Codes [MGparm_parseGRID](#) (MGparm *thee, Vio *sock)
 - VPRIVATE Vrc_Codes [MGparm_parseGLEN](#) (MGparm *thee, Vio *sock)
 - VPRIVATE Vrc_Codes [MGparm_parseGAMMA](#) (MGparm *thee, Vio *sock)
 - VPRIVATE Vrc_Codes [MGparm_parseGCENT](#) (MGparm *thee, Vio *sock)
 - VPRIVATE Vrc_Codes [MGparm_parseCGLEN](#) (MGparm *thee, Vio *sock)
 - VPRIVATE Vrc_Codes [MGparm_parseFGLEN](#) (MGparm *thee, Vio *sock)
 - VPRIVATE Vrc_Codes [MGparm_parseCGCENT](#) (MGparm *thee, Vio *sock)
 - VPRIVATE Vrc_Codes [MGparm_parseFGCENT](#) (MGparm *thee, Vio *sock)
 - VPRIVATE Vrc_Codes [MGparm_parsePDIME](#) (MGparm *thee, Vio *sock)

- VPRIVATE Vrc_Codes [MGparm_parseOFRAC](#) ([MGparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [MGparm_parseASYNC](#) ([MGparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [MGparm_parseUSEAQUA](#) ([MGparm](#) *thee, Vio *sock)
- VPUBLIC Vrc_Codes [MGparm_parseToken](#) ([MGparm](#) *thee, char tok[VMAX_BUFSIZE], Vio *sock)

Parse an MG keyword from an input file.

9.30.1 Detailed Description

Class MGparm methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
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*
*
```

Definition in file [mgparm.c](#).

9.30.2 Function Documentation

9.30.2.1 MGparm_parseASYNC()

```
VPRIVATE Vrc_Codes MGparm_parseASYNC (  
    MGparm * thee,  
    Vio * sock )
```

Definition at line 892 of file [mgparm.c](#).

9.30.2.2 MGparm_parseCGCENT()

```
VPRIVATE Vrc_Codes MGparm_parseCGCENT (  
    MGparm * thee,  
    Vio * sock )
```

Definition at line 730 of file [mgparm.c](#).

9.30.2.3 MGparm_parseCGLEN()

```
VPRIVATE Vrc_Codes MGparm_parseCGLEN (  
    MGparm * thee,  
    Vio * sock )
```

Definition at line 668 of file [mgparm.c](#).

9.30.2.4 MGparm_parseCHGM()

```
VPRIVATE Vrc_Codes MGparm_parseCHGM (  
    MGparm * thee,  
    Vio * sock )
```

Definition at line 446 of file [mgparm.c](#).

9.30.2.5 MGparm_parseDIME()

```
VPRIVATE Vrc_Codes MGparm_parseDIME (  
    MGparm * thee,  
    Vio * sock )
```

Definition at line 415 of file [mgparm.c](#).

9.30.2.6 MGparm_parseETOL()

```
VPRIVATE Vrc_Codes MGparm_parseETOL (  
    MGparm * thee,  
    Vio * sock )
```

Definition at line 516 of file [mgparm.c](#).

9.30.2.7 MGparm_parseFGCENT()

```
VPRIVATE Vrc_Codes MGparm_parseFGCENT (  
    MGparm * thee,  
    Vio * sock )
```

Definition at line 782 of file [mgparm.c](#).

9.30.2.8 MGparm_parseFGLEN()

```
VPRIVATE Vrc_Codes MGparm_parseFGLEN (  
    MGparm * thee,  
    Vio * sock )
```

Definition at line 699 of file [mgparm.c](#).

9.30.2.9 MGparm_parseGAMMA()

```
VPRIVATE Vrc_Codes MGparm_parseGAMMA (  
    MGparm * thee,  
    Vio * sock )
```

Definition at line 601 of file [mgparm.c](#).

9.30.2.10 MGparm_parseGCENT()

```
VPRIVATE Vrc_Codes MGparm_parseGCENT (  
    MGparm * thee,  
    Vio * sock )
```

Definition at line 616 of file [mgparm.c](#).

9.30.2.11 MGparm_parseGLEN()

```
VPRIVATE Vrc_Codes MGparm_parseGLEN (  
    MGparm * thee,  
    Vio * sock )
```

Definition at line 570 of file [mgparm.c](#).

9.30.2.12 MGparm_parseGRID()

```
VPRIVATE Vrc_Codes MGparm_parseGRID (  
    MGparm * thee,  
    Vio * sock )
```

Definition at line 539 of file [mgparm.c](#).

9.30.2.13 MGparm_parseNLEV()

```
VPRIVATE Vrc_Codes MGparm_parseNLEV (  
    MGparm * thee,  
    Vio * sock )
```

Definition at line 497 of file [mgparm.c](#).

9.30.2.14 MGparm_parseOFRAC()

```
VPRIVATE Vrc_Codes MGparm_parseOFRAC (
    MGparm * thee,
    Vio * sock )
```

Definition at line 872 of file [mgparm.c](#).

9.30.2.15 MGparm_parsePDIME()

```
VPRIVATE Vrc_Codes MGparm_parsePDIME (
    MGparm * thee,
    Vio * sock )
```

Definition at line 834 of file [mgparm.c](#).

9.30.2.16 MGparm_parseUSEAQUA()

```
VPRIVATE Vrc_Codes MGparm_parseUSEAQUA (
    MGparm * thee,
    Vio * sock )
```

Definition at line 912 of file [mgparm.c](#).

9.31 mgparm.c

[Go to the documentation of this file.](#)

```
00001
00057 #include "mgparm.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 #if !defined(VINLINE_MGPARM)
00062
00063 #endif /* if !defined(VINLINE_MGPARM) */
00064
00065 VPUBLIC void MGparm_setCenterX(MGparm *thee, double x) {
00066     VASSERT(thee != VNULL);
00067     thee->center[0] = x;
00068 }
00069 VPUBLIC void MGparm_setCenterY(MGparm *thee, double y) {
00070     VASSERT(thee != VNULL);
00071     thee->center[1] = y;
00072 }
00073 VPUBLIC void MGparm_setCenterZ(MGparm *thee, double z) {
00074     VASSERT(thee != VNULL);
00075     thee->center[2] = z;
00076 }
00077 VPUBLIC double MGparm_getCenterX(MGparm *thee) {
00078     VASSERT(thee != VNULL);
00079     return thee->center[0];
00080 }
00081 VPUBLIC double MGparm_getCenterY(MGparm *thee) {
00082     VASSERT(thee != VNULL);
00083     return thee->center[1];
00084 }
00085 VPUBLIC double MGparm_getCenterZ(MGparm *thee) {
00086     VASSERT(thee != VNULL);
00087     return thee->center[2];
00088 }
00089 VPUBLIC int MGparm_getNx(MGparm *thee) {
00090     VASSERT(thee != VNULL);
00091     return thee->dime[0];
00092 }
00093 VPUBLIC int MGparm_getNy(MGparm *thee) {
00094     VASSERT(thee != VNULL);
00095     return thee->dime[1];
00096 }
00097 VPUBLIC int MGparm_getNz(MGparm *thee) {
```

```

00098     VASSERT(thee != VNULL);
00099     return thee->dime[2];
00100 }
00101 VPUBLIC double MGparm_getHx(MGparm *thee) {
00102     VASSERT(thee != VNULL);
00103     return thee->grid[0];
00104 }
00105 VPUBLIC double MGparm_getHy(MGparm *thee) {
00106     VASSERT(thee != VNULL);
00107     return thee->grid[1];
00108 }
00109 VPUBLIC double MGparm_getHz(MGparm *thee) {
00110     VASSERT(thee != VNULL);
00111     return thee->grid[2];
00112 }
00113
00114 VPUBLIC MGparm* MGparm_ctor(MGparm_CalcType type) {
00115
00116     /* Set up the structure */
00117     MGparm *thee = VNULL;
00118     thee = (MGparm*)Vmem_malloc(VNULL, 1, sizeof(MGparm));
00119     VASSERT( thee != VNULL);
00120     VASSERT( MGparm_ctor2(thee, type) == VRC_SUCCESS );
00121
00122     return thee;
00123 }
00124
00125 VPUBLIC Vrc_Codes MGparm_ctor2(MGparm *thee, MGparm_CalcType type) {
00126
00127     int i;
00128
00129     if (thee == VNULL) return VRC_FAILURE;
00130
00131     for (i=0; i<3; i++) {
00132         thee->dime[i] = -1;
00133         thee->pdime[i] = 1;
00134     }
00135
00136     thee->parsed = 0;
00137     thee->type = type;
00138
00139     /* *** GENERIC PARAMETERS *** */
00140     thee->setdime = 0;
00141     thee->setchgms = 0;
00142
00143     /* *** TYPE 0 PARAMETERS *** */
00144     thee->nlev = VMGNLEV;
00145     thee->setnlev = 1;
00146     thee->etol = 1.0e-6;
00147     thee->setetol = 0;
00148     thee->setgrid = 0;
00149     thee->setglen = 0;
00150     thee->setgcen = 0;
00151
00152     /* *** TYPE 1 & 2 PARAMETERS *** */
00153     thee->setcglen = 0;
00154     thee->setfglen = 0;
00155     thee->setcgcent = 0;
00156     thee->setfgcent = 0;
00157
00158     /* *** TYPE 2 PARAMETERS *** */
00159     thee->setpdime = 0;
00160     thee->setrank = 0;
00161     thee->setsize = 0;
00162     thee->setfrac = 0;
00163     for (i=0; i<6; i++) thee->partDisjOwnSide[i] = 0;
00164     thee->setasyn = 0;
00165
00166     /* *** Default parameters for TINKER *** */
00167     thee->chgs = VCM_CHARGE;
00168
00169     thee->useAqua = 0;
00170     thee->setUseAqua = 0;
00171
00172     return VRC_SUCCESS;
00173 }
00174
00175 VPUBLIC void MGparm_dtor(MGparm **thee) {
00176     if ((*thee) != VNULL) {
00177         MGparm_dtor2(*thee);
00178         Vmem_free(VNULL, 1, sizeof(MGparm), (void **)thee);

```

```

00179         (*thee) = VNULL;
00180     }
00181 }
00182
00183 VPUBLIC void MGparm_dtor2(MGparm *thee) { ; }
00184
00185 VPUBLIC Vrc_Codes MGparm_check(MGparm *thee) {
00186     Vrc_Codes rc;
00187     int i, tdime[3], ti, tnlev[3], nlev;
00188
00189     rc = VRC_SUCCESS;
00190
00191     Vnm_print(0, "MGparm_check:  checking MGparm object of type %d.\n",
00192             thee->type);
00193
00194     /* Check to see if we were even filled... */
00195     if (!thee->parsed) {
00196         Vnm_print(2, "MGparm_check:  not filled!\n");
00197         return VRC_FAILURE;
00198     }
00199
00200     /* Check generic settings */
00201     if (!thee->setdime) {
00202         Vnm_print(2, "MGparm_check:  DIME not set!\n");
00203         rc = VRC_FAILURE;
00204     }
00205     if (!thee->setchgm) {
00206         Vnm_print(2, "MGparm_check:  CHGM not set!\n");
00207         return VRC_FAILURE;
00208     }
00209
00210     /* Check sequential manual & dummy settings */
00211     if ((thee->type == MCT_MANUAL) || (thee->type == MCT_DUMMY)) {
00212         if ((!thee->setgrid) && (!thee->setglen)) {
00213             Vnm_print(2, "MGparm_check:  Neither GRID nor GLEN set!\n");
00214             rc = VRC_FAILURE;
00215         }
00216         if ((thee->setgrid) && (thee->setglen)) {
00217             Vnm_print(2, "MGparm_check:  Both GRID and GLEN set!\n");
00218             rc = VRC_FAILURE;
00219         }
00220         if (!thee->setgcent) {
00221             Vnm_print(2, "MGparm_check:  GCENT not set!\n");
00222             rc = VRC_FAILURE;
00223         }
00224     }
00225
00226     /* Check sequential and parallel automatic focusing settings */
00227     if ((thee->type == MCT_AUTO) || (thee->type == MCT_PARALLEL)) {
00228         if (!thee->setcglen) {
00229             Vnm_print(2, "MGparm_check:  CGLEN not set!\n");
00230             rc = VRC_FAILURE;
00231         }
00232         if (!thee->setfglen) {
00233             Vnm_print(2, "MGparm_check:  FGLEN not set!\n");
00234             rc = VRC_FAILURE;
00235         }
00236         if (!thee->setcgcent) {
00237             Vnm_print(2, "MGparm_check:  CGCENT not set!\n");
00238             rc = VRC_FAILURE;
00239         }
00240         if (!thee->setfgcent) {
00241             Vnm_print(2, "MGparm_check:  FGCENT not set!\n");
00242             rc = VRC_FAILURE;
00243         }
00244     }
00245
00246     /* Check parallel automatic focusing settings */
00247     if (thee->type == MCT_PARALLEL) {
00248         if (!thee->setpdime) {
00249             Vnm_print(2, "MGparm_check:  PDIME not set!\n");
00250             rc = VRC_FAILURE;
00251         }
00252         if (!thee->setrank) {
00253             Vnm_print(2, "MGparm_check:  PROC_RANK not set!\n");
00254             rc = VRC_FAILURE;
00255         }
00256         if (!thee->setsize) {
00257             Vnm_print(2, "MGparm_check:  PROC_SIZE not set!\n");
00258         }
00259     }

```



```

00260         rc = VRC_FAILURE;
00261     }
00262     if (!thee->setofrac) {
00263         Vnm_print(2, "MGparm_check: OFRAC not set!\n");
00264         rc = VRC_FAILURE;
00265     }
00266 }
00267
00268 /* Perform a sanity check on nlev and dime, resetting values as necessary */
00269 if (rc == 1) {
00270     /* Calculate the actual number of grid points and nlev to satisfy the
00271     * formula:  $n = c * 2^{(l+1)} + 1$ , where  $n$  is the number of grid points,
00272     *  $c$  is an integer, and  $l$  is the number of levels */
00273     if (thee->type != MCT_DUMMY) {
00274         for (i=0; i<3; i++) {
00275             /* See if the user picked a reasonable value, if not then fix it */
00276             ti = thee->dime[i] - 1;
00277             if (ti == VPOW(2, (thee->nlev+1))) {
00278                 tnlev[i] = thee->nlev;
00279                 tdime[i] = thee->dime[i];
00280             } else {
00281                 tdime[i] = thee->dime[i];
00282                 ti = tdime[i] - 1;
00283                 tnlev[i] = 0;
00284                 /* Find the maximum number of times this dimension can be
00285                 * divided by two */
00286                 while (VEVEN(ti)) {
00287                     (tnlev[i])++;
00288                     ti = (int)ceil(0.5*ti);
00289                 }
00290                 (tnlev[i])--;
00291                 /* We'd like to have at least VMGNLEV levels in the multigrid
00292                 * hierarchy. This means that the dimension needs to be
00293                 *  $c*2^{VMGNLEV} + 1$ , where  $c$  is an integer. */
00294                 if ((tdime[i] > 65) && (tnlev[i] < VMGNLEV)) {
00295                     Vnm_print(2, "Nosh: Bad dime[%d] = %d (%d nlev)!\n",
00296                             i, tdime[i], tnlev[i]);
00297                     ti = (int)(tdime[i]/VPOW(2., (VMGNLEV+1)));
00298                     if (ti < 1) ti = 1;
00299                     tdime[i] = ti*(int)(VPOW(2., (VMGNLEV+1))) + 1;
00300                     tnlev[i] = 4;
00301                     Vnm_print(2, "Nosh: Reset dime[%d] to %d and (nlev = %d).\n", i, tdime[i], VMGNLEV);
00302                 }
00303             }
00304         }
00305     } else { /* We are a dummy calculation, but we still need positive numbers of points */
00306         for (i=0; i<3; i++) {
00307             tnlev[i] = thee->nlev;
00308             tdime[i] = thee->dime[i];
00309             if (thee->dime[i] <= 0) {
00310                 Vnm_print(2, "Nosh: Resetting dime[%d] from %d to 3.\n", i, thee->dime[i]);
00311                 thee->dime[i] = 3;
00312             }
00313         }
00314     }
00315
00316     /* The actual number of levels we'll be using is the smallest number of
00317     * possible levels in any dimensions */
00318     nlev = VMIN2(tnlev[0], tnlev[1]);
00319     nlev = VMIN2(nlev, tnlev[2]);
00320     /* Set the number of levels and dimensions */
00321     Vnm_print(0, "Nosh: nlev = %d, dime = (%d, %d, %d)\n", nlev, tdime[0],
00322             tdime[1], tdime[2]);
00323     thee->nlev = nlev;
00324     if (thee->nlev <= 0) {
00325         Vnm_print(2, "MGparm_check: illegal nlev (%d); check your grid dimensions!\n", thee->nlev);
00326         rc = VRC_FAILURE;
00327     }
00328     if (thee->nlev < 2) {
00329         Vnm_print(2, "MGparm_check: you're using a very small nlev (%d) and therefore\n",
00330                 thee->nlev);
00331         Vnm_print(2, "MGparm_check: will not get the optimal performance of the multigrid\n");
00332         Vnm_print(2, "MGparm_check: algorithm. Please check your grid dimensions.\n");
00333     }
00334     for (i=0; i<3; i++) thee->dime[i] = tdime[i];
00335 }
00336 if (!thee->setUseAqua) thee->useAqua = 0;
00337
00338 return rc;
00339 }

```

```

00340
00341 VPUBLIC void MGparm_copy(MGparm *thee, MGparm *parm) {
00342
00343     int i;
00344
00345     VASSERT(thee != VNULL);
00346     VASSERT(parm != VNULL);
00347
00348
00349     thee->type = parm->type;
00350     thee->parsed = parm->parsed;
00351
00352     /* *** GENERIC PARAMETERS *** */
00353     for (i=0; i<3; i++) thee->dime[i] = parm->dime[i];
00354     thee->setdime = parm->setdime;
00355     thee->chgm = parm->chgm;
00356     thee->setchgm = parm->setchgm;
00357     thee->chgs = parm->chgs;
00358
00359     /* *** TYPE 0 PARMS *** */
00360     thee->nlev = parm->nlev;
00361     thee->setnlev = parm->setnlev;
00362     thee->etol = parm->etol;
00363     thee->setetol = parm->setetol;
00364     for (i=0; i<3; i++) thee->grid[i] = parm->grid[i];
00365     thee->setgrid = parm->setgrid;
00366     for (i=0; i<3; i++) thee->glen[i] = parm->glen[i];
00367     thee->setglen = parm->setglen;
00368     thee->cmeth = parm->cmeth;
00369     for (i=0; i<3; i++) thee->center[i] = parm->center[i];
00370     thee->setgcent = parm->setgcent;
00371     thee->centmol = parm->centmol;
00372
00373     /* *** TYPE 1 & 2 PARMS *** */
00374     for (i=0; i<3; i++) thee->cglen[i] = parm->cglen[i];
00375     thee->setcglen = parm->setcglen;
00376     for (i=0; i<3; i++) thee->fglen[i] = parm->fglen[i];
00377     thee->setfglen = parm->setfglen;
00378     thee->ccmeth = parm->ccmeth;
00379     for (i=0; i<3; i++) thee->ccenter[i] = parm->ccenter[i];
00380     thee->setcgcent = parm->setcgcent;
00381     thee->ccentmol = parm->ccentmol;
00382     thee->fcmeth = parm->fcmeth;
00383     for (i=0; i<3; i++) thee->fcenter[i] = parm->fcenter[i];
00384     thee->setfgcent = parm->setfgcent;
00385     thee->fcentmol = parm->fcentmol;
00386
00387     /* *** TYPE 2 PARMS *** */
00388     for (i=0; i<3; i++)
00389         thee->partDisjCenter[i] = parm->partDisjCenter[i];
00390     for (i=0; i<3; i++)
00391         thee->partDisjLength[i] = parm->partDisjLength[i];
00392     for (i=0; i<6; i++)
00393         thee->partDisjOwnSide[i] = parm->partDisjOwnSide[i];
00394     for (i=0; i<3; i++) thee->pdime[i] = parm->pdime[i];
00395     thee->setpdime = parm->setpdime;
00396     thee->proc_rank = parm->proc_rank;
00397     thee->setrank = parm->setrank;
00398     thee->proc_size = parm->proc_size;
00399     thee->setsize = parm->setsize;
00400     thee->ofrac = parm->ofrac;
00401     thee->setofrac = parm->setofrac;
00402     thee->setasync = parm->setasync;
00403     thee->async = parm->async;
00404
00405     thee->nonlotype = parm->nonlotype;
00406     thee->setnonlotype = parm->setnonlotype;
00407
00408     thee->method = parm->method;
00409     thee->method = parm->method;
00410
00411     thee->useAqua = parm->useAqua;
00412     thee->setUseAqua = parm->setUseAqua;
00413 }
00414
00415 VPRIVATE Vrc_Codes MGparm_parseDIME(MGparm *thee, Vio *sock) {
00416
00417     char tok[VMAX_BUFSIZE];
00418     int ti;
00419
00420     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);

```

```

00421     if (sscanf(tok, "%d", &ti) == 0){
00422         Vnm_print(2, "parseMG: Read non-integer (%s) while parsing DIME \
00423 keyword!\n", tok);
00424         return VRC_WARNING;
00425     } else thee->dime[0] = ti;
00426     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00427     if (sscanf(tok, "%d", &ti) == 0) {
00428         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing DIME \
00429 keyword!\n", tok);
00430         return VRC_WARNING;
00431     } else thee->dime[1] = ti;
00432     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00433     if (sscanf(tok, "%d", &ti) == 0) {
00434         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing DIME \
00435 keyword!\n", tok);
00436         return VRC_WARNING;
00437     } else thee->dime[2] = ti;
00438     thee->setdime = 1;
00439     return VRC_SUCCESS;
00440
00441     ERROR1:
00442     Vnm_print(2, "parseMG: ran out of tokens!\n");
00443     return VRC_WARNING;
00444 }
00445
00446 VPRIVATE Vrc_Codes MGparm_parseCHGM(MGparm *thee, Vio *sock) {
00447
00448     char tok[VMAX_BUFSIZE];
00449     Vchrg_Meth ti;
00450
00451     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00452     if (sscanf(tok, "%d", (int*)&ti) == 1) {
00453         thee->chgm = ti;
00454         thee->setchgm = 1;
00455         Vnm_print(2, "Nosh: Warning -- parsed deprecated statment \"chgm %d\".\n", ti);
00456         Vnm_print(2, "Nosh: Please use \"chgm \"");
00457         switch (thee->chgm) {
00458             case VCM_TRIL:
00459                 Vnm_print(2, "spl0");
00460                 break;
00461             case VCM_BSPL2:
00462                 Vnm_print(2, "spl2");
00463                 break;
00464             case VCM_BSPL4:
00465                 Vnm_print(2, "spl4");
00466                 break;
00467             default:
00468                 Vnm_print(2, "UNKNOWN");
00469                 break;
00470         }
00471         Vnm_print(2, "\" instead!\n");
00472         return VRC_SUCCESS;
00473     } else if (Vstring_strcasecmp(tok, "spl0") == 0) {
00474         thee->chgm = VCM_TRIL;
00475         thee->setchgm = 1;
00476         return VRC_SUCCESS;
00477     } else if (Vstring_strcasecmp(tok, "spl2") == 0) {
00478         thee->chgm = VCM_BSPL2;
00479         thee->setchgm = 1;
00480         return VRC_SUCCESS;
00481     } else if (Vstring_strcasecmp(tok, "spl4") == 0) {
00482         thee->chgm = VCM_BSPL4;
00483         thee->setchgm = 1;
00484         return VRC_SUCCESS;
00485     } else {
00486         Vnm_print(2, "Nosh: Unrecognized parameter (%s) when parsing \
00487 chgm!\n", tok);
00488         return VRC_WARNING;
00489     }
00490     return VRC_WARNING;
00491
00492     ERROR1:
00493     Vnm_print(2, "parseMG: ran out of tokens!\n");
00494     return VRC_WARNING;
00495 }
00496
00497 VPRIVATE Vrc_Codes MGparm_parseNLEV(MGparm *thee, Vio *sock) {
00498
00499     char tok[VMAX_BUFSIZE];
00500     int ti;
00501

```

```

00502     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00503     if (sscanf(tok, "%d", &ti) == 0) {
00504         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing NLEV \
00505 keyword!\n", tok);
00506         return VRC_WARNING;
00507     } else thee->nlev = ti;
00508     thee->setnlev = 1;
00509     return VRC_SUCCESS;
00510
00511     ERROR1:
00512     Vnm_print(2, "parseMG: ran out of tokens!\n");
00513     return VRC_WARNING;
00514 }
00515
00516 VPRIVATE Vrc_Codes MGparm_parseETOL(MGparm *thee, Vio *sock) {
00517     char tok[VMAX_BUFSIZE];
00518     double tf;
00519
00520     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00521     if (sscanf(tok, "%lf", &tf) == 0) {
00522         Vnm_print(2, "Nosh: Read non-float (%s) while parsing etol \
00523 keyword!\n", tok);
00524         return VRC_WARNING;
00525     } else if (tf <= 0.0) {
00526         Vnm_print(2, "parseMG: etol must be greater than 0!\n");
00527         return VRC_WARNING;
00528     } else thee->etol = tf;
00529     thee->setetol = 1;
00530     return VRC_SUCCESS;
00531
00532     ERROR1:
00533     Vnm_print(2, "parseMG: ran out of tokens!\n");
00534     return VRC_WARNING;
00535 }
00536
00537
00538 VPRIVATE Vrc_Codes MGparm_parseGRID(MGparm *thee, Vio *sock) {
00539     char tok[VMAX_BUFSIZE];
00540     double tf;
00541
00542     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00543     if (sscanf(tok, "%lf", &tf) == 0) {
00544         Vnm_print(2, "Nosh: Read non-float (%s) while parsing GRID \
00545 keyword!\n", tok);
00546         return VRC_WARNING;
00547     } else thee->grid[0] = tf;
00548     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00549     if (sscanf(tok, "%lf", &tf) == 0) {
00550         Vnm_print(2, "Nosh: Read non-float (%s) while parsing GRID \
00551 keyword!\n", tok);
00552         return VRC_WARNING;
00553     } else thee->grid[1] = tf;
00554     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00555     if (sscanf(tok, "%lf", &tf) == 0) {
00556         Vnm_print(2, "Nosh: Read non-float (%s) while parsing GRID \
00557 keyword!\n", tok);
00558         return VRC_WARNING;
00559     } else thee->grid[2] = tf;
00560     thee->setgrid = 1;
00561     return VRC_SUCCESS;
00562
00563     ERROR1:
00564     Vnm_print(2, "parseMG: ran out of tokens!\n");
00565     return VRC_WARNING;
00566 }
00567
00568
00569 VPRIVATE Vrc_Codes MGparm_parseGLEN(MGparm *thee, Vio *sock) {
00570     char tok[VMAX_BUFSIZE];
00571     double tf;
00572
00573     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00574     if (sscanf(tok, "%lf", &tf) == 0) {
00575         Vnm_print(2, "Nosh: Read non-float (%s) while parsing GLEN \
00576 keyword!\n", tok);
00577         return VRC_WARNING;
00578     } else thee->glen[0] = tf;
00579     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00580     if (sscanf(tok, "%lf", &tf) == 0) {

```

```

00583     Vnm_print(2, "NOsh: Read non-float (%s) while parsing GLEN \
00584 keyword!\n", tok);
00585     return VRC_WARNING;
00586 } else thee->glen[1] = tf;
00587 VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00588 if (sscanf(tok, "%lf", &tf) == 0) {
00589     Vnm_print(2, "NOsh: Read non-float (%s) while parsing GLEN \
00590 keyword!\n", tok);
00591     return VRC_WARNING;
00592 } else thee->glen[2] = tf;
00593 thee->setglen = 1;
00594 return VRC_SUCCESS;
00595
00596 ERROR1:
00597     Vnm_print(2, "parseMG: ran out of tokens!\n");
00598     return VRC_WARNING;
00599 }
00600
00601 VPRIVATE Vrc_Codes MGparm_parseGAMMA(MGparm *thee, Vio *sock) {
00602
00603     char tok[VMAX_BUFSIZE];
00604
00605     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00606     Vnm_print(2, "parseMG: GAMMA keyword deprecated!\n");
00607     Vnm_print(2, "parseMG: If you are using PyMOL or VMD and still seeing this message,\n");
00608     Vnm_print(2, "parseMG: please contact the developers of those programs regarding this message.\n");
00609     return VRC_SUCCESS;
00610
00611 ERROR1:
00612     Vnm_print(2, "parseMG: ran out of tokens!\n");
00613     return VRC_WARNING;
00614 }
00615
00616 VPRIVATE Vrc_Codes MGparm_parseGCENT(MGparm *thee, Vio *sock) {
00617
00618     char tok[VMAX_BUFSIZE];
00619     double tf;
00620     int ti;
00621
00622     /* If the next token isn't a float, it probably means we want to
00623      * center on a molecule */
00624     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00625     if (sscanf(tok, "%lf", &tf) == 0) {
00626         if (Vstring_strcasecmp(tok, "mol") == 0) {
00627             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00628             if (sscanf(tok, "%d", &ti) == 0) {
00629                 Vnm_print(2, "NOsh: Read non-int (%s) while parsing \
00630 GCENT MOL keyword!\n", tok);
00631                 return VRC_WARNING;
00632             } else {
00633                 thee->cmeth = MCM_MOLECULE;
00634                 /* Subtract 1 here to convert user numbering (1, 2, 3, ...) into
00635                  array index */
00636                 thee->centmol = ti - 1;
00637             }
00638         } else {
00639             Vnm_print(2, "NOsh: Unexpected keyword (%s) while parsing \
00640 GCENT!\n", tok);
00641             return VRC_WARNING;
00642         }
00643     } else {
00644         thee->center[0] = tf;
00645         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00646         if (sscanf(tok, "%lf", &tf) == 0) {
00647             Vnm_print(2, "NOsh: Read non-float (%s) while parsing \
00648 GCENT keyword!\n", tok);
00649             return VRC_WARNING;
00650         }
00651         thee->center[1] = tf;
00652         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00653         if (sscanf(tok, "%lf", &tf) == 0) {
00654             Vnm_print(2, "NOsh: Read non-float (%s) while parsing \
00655 GCENT keyword!\n", tok);
00656             return VRC_WARNING;
00657         }
00658         thee->center[2] = tf;
00659     }
00660     thee->setgcent = 1;
00661     return VRC_SUCCESS;
00662
00663 ERROR1:

```

```
00664         Vnm_print(2, "parseMG: ran out of tokens!\n");
00665         return VRC_WARNING;
00666     }
00667
00668     VPRIVATE Vrc_Codes MGparm_parseCGLEN(MGparm *thee, Vio *sock) {
00669
00670         char tok[VMAX_BUFSIZE];
00671         double tf;
00672
00673         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00674         if (sscanf(tok, "%lf", &tf) == 0) {
00675             Vnm_print(2, "NOsh: Read non-float (%s) while parsing CGLEN \
00676 keyword!\n", tok);
00677             return VRC_WARNING;
00678         } else thee->cglen[0] = tf;
00679         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00680         if (sscanf(tok, "%lf", &tf) == 0) {
00681             Vnm_print(2, "NOsh: Read non-float (%s) while parsing CGLEN \
00682 keyword!\n", tok);
00683             return VRC_WARNING;
00684         } else thee->cglen[1] = tf;
00685         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00686         if (sscanf(tok, "%lf", &tf) == 0) {
00687             Vnm_print(2, "NOsh: Read non-float (%s) while parsing CGLEN \
00688 keyword!\n", tok);
00689             return VRC_WARNING;
00690         } else thee->cglen[2] = tf;
00691         thee->setcglen = 1;
00692         return VRC_SUCCESS;
00693
00694     ERROR1:
00695         Vnm_print(2, "parseMG: ran out of tokens!\n");
00696         return VRC_WARNING;
00697 }
00698
00699     VPRIVATE Vrc_Codes MGparm_parseFGLEN(MGparm *thee, Vio *sock) {
00700
00701         char tok[VMAX_BUFSIZE];
00702         double tf;
00703
00704         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00705         if (sscanf(tok, "%lf", &tf) == 0) {
00706             Vnm_print(2, "NOsh: Read non-float (%s) while parsing FGLEN \
00707 keyword!\n", tok);
00708             return VRC_WARNING;
00709         } else thee->fglen[0] = tf;
00710         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00711         if (sscanf(tok, "%lf", &tf) == 0) {
00712             Vnm_print(2, "NOsh: Read non-float (%s) while parsing FGLEN \
00713 keyword!\n", tok);
00714             return VRC_WARNING;
00715         } else thee->fglen[1] = tf;
00716         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00717         if (sscanf(tok, "%lf", &tf) == 0) {
00718             Vnm_print(2, "NOsh: Read non-float (%s) while parsing FGLEN \
00719 keyword!\n", tok);
00720             return VRC_WARNING;
00721         } else thee->fglen[2] = tf;
00722         thee->setfglen = 1;
00723         return VRC_SUCCESS;
00724
00725     ERROR1:
00726         Vnm_print(2, "parseMG: ran out of tokens!\n");
00727         return VRC_WARNING;
00728 }
00729
00730     VPRIVATE Vrc_Codes MGparm_parseCGCENT(MGparm *thee, Vio *sock) {
00731
00732         char tok[VMAX_BUFSIZE];
00733         double tf;
00734         int ti;
00735
00736         /* If the next token isn't a float, it probably means we want to
00737          * center on a molecule */
00738         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00739         if (sscanf(tok, "%lf", &tf) == 0) {
00740             if (Vstring_strcasecmp(tok, "mol") == 0) {
00741                 VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00742                 if (sscanf(tok, "%d", &ti) == 0) {
00743                     Vnm_print(2, "NOsh: Read non-int (%s) while parsing \
00744 CGCENT MOL keyword!\n", tok);
```

```

00745         return VRC_WARNING;
00746     } else {
00747         thee->ccmeth = MCM_MOLECULE;
00748         /* Subtract 1 here to convert user numbering (1, 2, 3, ...) into
00749          array index */
00750         thee->ccentmol = ti - 1;
00751     }
00752 } else {
00753     Vnm_print(2, "Nosh: Unexpected keyword (%s) while parsing \
00754 CGCENT!\n", tok);
00755     return VRC_WARNING;
00756 }
00757 } else {
00758     thee->ccenter[0] = tf;
00759     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00760     if (sscanf(tok, "%lf", &tf) == 0) {
00761         Vnm_print(2, "Nosh: Read non-float (%s) while parsing \
00762 CGCENT keyword!\n", tok);
00763         return VRC_WARNING;
00764     }
00765     thee->ccenter[1] = tf;
00766     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00767     if (sscanf(tok, "%lf", &tf) == 0) {
00768         Vnm_print(2, "Nosh: Read non-float (%s) while parsing \
00769 CGCENT keyword!\n", tok);
00770         return VRC_WARNING;
00771     }
00772     thee->ccenter[2] = tf;
00773 }
00774 thee->setcgcent = 1;
00775 return VRC_SUCCESS;
00776
00777 ERROR1:
00778     Vnm_print(2, "parseMG: ran out of tokens!\n");
00779     return VRC_WARNING;
00780 }
00781
00782 PRIVATE Vrc_Codes MGparm_parseFGCENT(MGparm *thee, Vio *sock) {
00783
00784     char tok[VMAX_BUFSIZE];
00785     double tf;
00786     int ti;
00787
00788     /* If the next token isn't a float, it probably means we want to
00789      * center on a molecule */
00790     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00791     if (sscanf(tok, "%lf", &tf) == 0) {
00792         if (Vstring_strcasecmp(tok, "mol") == 0) {
00793             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00794             if (sscanf(tok, "%d", &ti) == 0) {
00795                 Vnm_print(2, "Nosh: Read non-int (%s) while parsing \
00796 FGCENT MOL keyword!\n", tok);
00797                 return VRC_WARNING;
00798             } else {
00799                 thee->fcmeth = MCM_MOLECULE;
00800                 /* Subtract 1 here to convert user numbering (1, 2, 3, ...) into
00801                  array index */
00802                 thee->fcentmol = ti - 1;
00803             }
00804         } else {
00805             Vnm_print(2, "Nosh: Unexpected keyword (%s) while parsing \
00806 FGCENT!\n", tok);
00807             return VRC_WARNING;
00808         }
00809     } else {
00810         thee->fcenter[0] = tf;
00811         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00812         if (sscanf(tok, "%lf", &tf) == 0) {
00813             Vnm_print(2, "Nosh: Read non-float (%s) while parsing \
00814 FGCENT keyword!\n", tok);
00815             return VRC_WARNING;
00816         }
00817         thee->fcenter[1] = tf;
00818         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00819         if (sscanf(tok, "%lf", &tf) == 0) {
00820             Vnm_print(2, "Nosh: Read non-float (%s) while parsing \
00821 FGCENT keyword!\n", tok);
00822             return VRC_WARNING;
00823         }
00824         thee->fcenter[2] = tf;
00825     }

```

```

00826     thee->setfgcent = 1;
00827     return VRC_SUCCESS;
00828
00829     ERROR1:
00830         Vnm_print(2, "parseMG: ran out of tokens!\n");
00831         return VRC_WARNING;
00832 }
00833
00834 VPRIVATE Vrc_Codes MGparm_parsePDIME(MGparm *thee, Vio *sock) {
00835     char tok[VMAX_BUFSIZE];
00836     int ti;
00837
00838     /* Read the number of grid points */
00839     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00840     if (sscanf(tok, "%d", &ti) == 0) {
00841         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing PDIME \
00842 keyword!\n", tok);
00843         return VRC_WARNING;
00844     } else {
00845         thee->pdime[0] = ti;
00846     }
00847
00848     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00849     if (sscanf(tok, "%d", &ti) == 0) {
00850         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing PDIME \
00851 keyword!\n", tok);
00852         return VRC_WARNING;
00853     } else {
00854         thee->pdime[1] = ti;
00855     }
00856
00857     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00858     if (sscanf(tok, "%d", &ti) == 0) {
00859         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing PDIME \
00859 keyword!\n", tok);
00860         return VRC_WARNING;
00861     } else {
00862         thee->pdime[2] = ti;
00863     }
00864     thee->setpdime = 1;
00865     return VRC_SUCCESS;
00866
00867     ERROR1:
00868         Vnm_print(2, "parseMG: ran out of tokens!\n");
00869         return VRC_WARNING;
00870 }
00871
00872 VPRIVATE Vrc_Codes MGparm_parseOFRAC(MGparm *thee, Vio *sock) {
00873     char tok[VMAX_BUFSIZE];
00874     double tf;
00875
00876     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00877     if (sscanf(tok, "%lf", &tf) == 0) {
00878         Vnm_print(2, "Nosh: Read non-int (%s) while parsing OFRAC \
00879 keyword!\n", tok);
00880         return VRC_WARNING;
00881     }
00882     thee->ofrac = tf;
00883     thee->setofrac = 1;
00884     return VRC_SUCCESS;
00885
00886     ERROR1:
00887         Vnm_print(2, "parseMG: ran out of tokens!\n");
00888         return VRC_WARNING;
00889 }
00890
00891 VPRIVATE Vrc_Codes MGparm_parseASYNC(MGparm *thee, Vio *sock) {
00892     char tok[VMAX_BUFSIZE];
00893     int ti;
00894
00895     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00896     if (sscanf(tok, "%i", &ti) == 0) {
00897         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing ASYNC \
00898 keyword!\n", tok);
00899         return VRC_WARNING;
00900     }
00901     thee->async = ti;
00902     thee->setasync = 1;
00903     return VRC_SUCCESS;
00904
00905     ERROR1:
00906         Vnm_print(2, "parseMG: ran out of tokens!\n");
00907         return VRC_WARNING;
00908 }

```



```

00907     ERROR1:
00908         Vnm_print(2, "parseMG: ran out of tokens!\n");
00909         return VRC_WARNING;
00910 }
00911
00912 VPRIVATE Vrc_Codes MGparm_parseUSEAQUA(MGparm *thee, Vio *sock) {
00913     Vnm_print(0, "Nosh: parsed useaqua\n");
00914     thee->useAqua = 1;
00915     thee->setUseAqua = 1;
00916     return VRC_SUCCESS;
00917 }
00918
00919 VPUBLIC Vrc_Codes MGparm_parseToken(MGparm *thee, char tok[VMAX_BUFSIZE],
00920     Vio *sock) {
00921
00922     if (thee == VNULL) {
00923         Vnm_print(2, "parseMG: got NULL thee!\n");
00924         return VRC_WARNING;
00925     }
00926     if (sock == VNULL) {
00927         Vnm_print(2, "parseMG: got NULL socket!\n");
00928         return VRC_WARNING;
00929     }
00930
00931     Vnm_print(0, "MGparm_parseToken: trying %s...\n", tok);
00932
00933     if (Vstring_strcasecmp(tok, "dime") == 0) {
00934         return MGparm_parseDIME(thee, sock);
00935     } else if (Vstring_strcasecmp(tok, "chgm") == 0) {
00936         return MGparm_parseCHGM(thee, sock);
00937     } else if (Vstring_strcasecmp(tok, "nlev") == 0) {
00938         Vnm_print(2, "Warning: The 'nlev' keyword is now deprecated!\n");
00939         return MGparm_parseNLEV(thee, sock);
00940     } else if (Vstring_strcasecmp(tok, "etol") == 0) {
00941         return MGparm_parseETOL(thee, sock);
00942     } else if (Vstring_strcasecmp(tok, "grid") == 0) {
00943         return MGparm_parseGRID(thee, sock);
00944     } else if (Vstring_strcasecmp(tok, "glen") == 0) {
00945         return MGparm_parseGLEN(thee, sock);
00946     } else if (Vstring_strcasecmp(tok, "gcent") == 0) {
00947         return MGparm_parseGCENT(thee, sock);
00948     } else if (Vstring_strcasecmp(tok, "cglen") == 0) {
00949         return MGparm_parseCGLEN(thee, sock);
00950     } else if (Vstring_strcasecmp(tok, "fglen") == 0) {
00951         return MGparm_parseFGLEN(thee, sock);
00952     } else if (Vstring_strcasecmp(tok, "cgcent") == 0) {
00953         return MGparm_parseCGCENT(thee, sock);
00954     } else if (Vstring_strcasecmp(tok, "fgcent") == 0) {
00955         return MGparm_parseFGCENT(thee, sock);
00956     } else if (Vstring_strcasecmp(tok, "pdime") == 0) {
00957         return MGparm_parsePDIME(thee, sock);
00958     } else if (Vstring_strcasecmp(tok, "ofrac") == 0) {
00959         return MGparm_parseOFRAC(thee, sock);
00960     } else if (Vstring_strcasecmp(tok, "async") == 0) {
00961         return MGparm_parseASYNCH(thee, sock);
00962     } else if (Vstring_strcasecmp(tok, "gamma") == 0) {
00963         return MGparm_parseGAMMA(thee, sock);
00964     } else if (Vstring_strcasecmp(tok, "useaqua") == 0) {
00965         return MGparm_parseUSEAQUA(thee, sock);
00966     } else {
00967         Vnm_print(2, "parseMG: Unrecognized keyword (%s)!\n", tok);
00968         return VRC_WARNING;
00969     }
00970
00971     return VRC_FAILURE;
00972 }
00973
00974 }

```

9.32 src/generic/mgparm.h File Reference

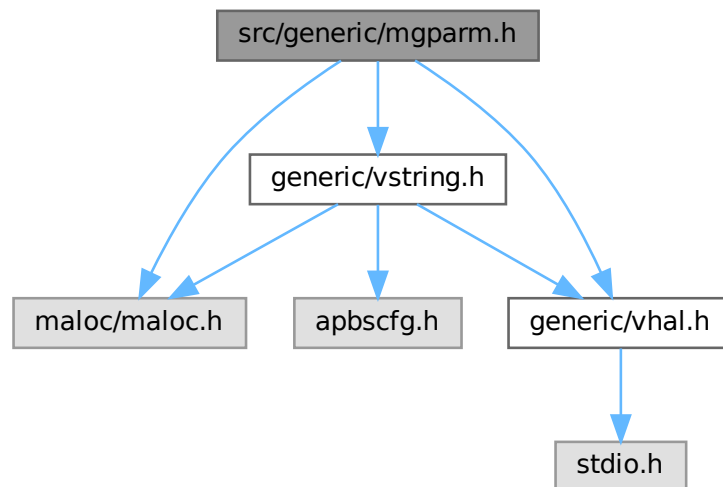
Contains declarations for class MGparm.

```

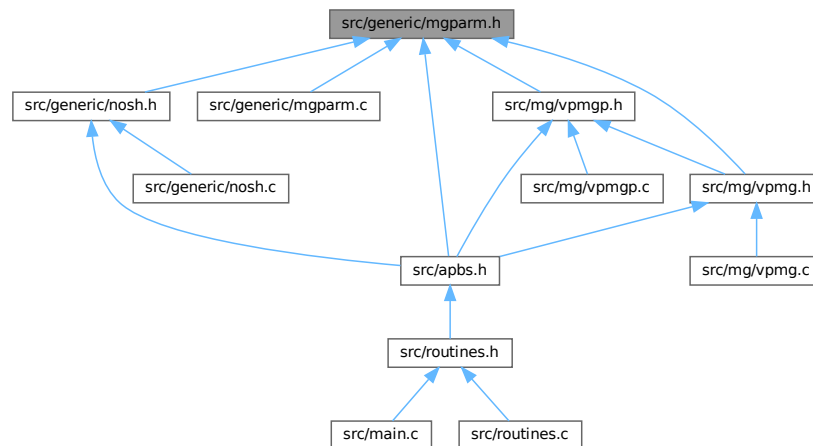
#include "malloc/malloc.h"
#include "generic/vhal.h"
#include "generic/vstring.h"

```

Include dependency graph for mgparm.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sMGparm](#)

Parameter structure for MG-specific variables from input files.

Typedefs

- typedef enum [eMGparm_CalcType](#) [MGparm_CalcType](#)
Declare MGparm_CalcType type.
- typedef enum [eMGparm_CentMeth](#) [MGparm_CentMeth](#)
Declare MGparm_CentMeth type.
- typedef struct [sMGparm](#) [MGparm](#)
Declaration of the MGparm class as the MGparm structure.

Enumerations

- enum [eMGparm_CalcType](#) {
[MCT_MANUAL](#) =0 , [MCT_AUTO](#) =1 , [MCT_PARALLEL](#) =2 , [MCT_DUMMY](#) =3 ,
[MCT_NONE](#) =4 }
Calculation type.
- enum [eMGparm_CentMeth](#) { [MCM_POINT](#) =0 , [MCM_MOLECULE](#) =1 , [MCM_FOCUS](#) =2 }
Centering method.

Functions

- VEXTERNC int [MGparm_getNx](#) ([MGparm](#) *thee)
Get number of grid points in x direction.
- VEXTERNC int [MGparm_getNy](#) ([MGparm](#) *thee)
Get number of grid points in y direction.
- VEXTERNC int [MGparm_getNz](#) ([MGparm](#) *thee)
Get number of grid points in z direction.
- VEXTERNC double [MGparm_getHx](#) ([MGparm](#) *thee)
Get grid spacing in x direction (Å)
- VEXTERNC double [MGparm_getHy](#) ([MGparm](#) *thee)
Get grid spacing in y direction (Å)
- VEXTERNC double [MGparm_getHz](#) ([MGparm](#) *thee)
Get grid spacing in z direction (Å)
- VEXTERNC void [MGparm_setCenterX](#) ([MGparm](#) *thee, double x)
Set center x-coordinate.
- VEXTERNC void [MGparm_setCenterY](#) ([MGparm](#) *thee, double y)
Set center y-coordinate.
- VEXTERNC void [MGparm_setCenterZ](#) ([MGparm](#) *thee, double z)
Set center z-coordinate.
- VEXTERNC double [MGparm_getCenterX](#) ([MGparm](#) *thee)
Get center x-coordinate.
- VEXTERNC double [MGparm_getCenterY](#) ([MGparm](#) *thee)
Get center y-coordinate.
- VEXTERNC double [MGparm_getCenterZ](#) ([MGparm](#) *thee)
Get center z-coordinate.
- VEXTERNC [MGparm](#) * [MGparm_ctor](#) ([MGparm_CalcType](#) type)
Construct MGparm object.
- VEXTERNC [Vrc_Codes](#) [MGparm_ctor2](#) ([MGparm](#) *thee, [MGparm_CalcType](#) type)
FORTTRAN stub to construct MGparm object.
- VEXTERNC void [MGparm_dtor](#) ([MGparm](#) **thee)

Object destructor.

- VEXTERNC void `MGparm_dtor2` (`MGparm *thee`)

FORTTRAN stub for object destructor.

- VEXTERNC Vrc_Codes `MGparm_check` (`MGparm *thee`)

Consistency check for parameter values stored in object.

- VEXTERNC void `MGparm_copy` (`MGparm *thee`, `MGparm *parm`)

Copy MGparm object into thee.

- VEXTERNC Vrc_Codes `MGparm_parseToken` (`MGparm *thee`, char tok[VMAX_BUFSIZE], Vio *sock)

Parse an MG keyword from an input file.

9.32.1 Detailed Description

Contains declarations for class `MGparm`.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
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* Pacific Northwest National Laboratory
*
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*
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```

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* THE POSSIBILITY OF SUCH DAMAGE.
*
*

```

Definition in file [mgparm.h](#).

9.33 mgparm.h

[Go to the documentation of this file.](#)

```

00001
00064 #ifndef _MGPARAM_H_
00065 #define _MGPARAM_H_
00066
00067 /* Generic header files */
00068 #include "malloc/malloc.h"
00069
00070 #include "generic/vhal.h"
00071 #include "generic/vstring.h"
00072
00077 enum eMGparm_CalcType {
00078     MCT_MANUAL=0,
00079     MCT_AUTO=1,
00080     MCT_PARALLEL=2,
00081     MCT_DUMMY=3,
00082     MCT_NONE=4
00083 };
00084
00089 typedef enum eMGparm_CalcType MGparm_CalcType;
00090
00095 enum eMGparm_CentMeth {
00096     MCM_POINT=0,
00097     MCM_MOLECULE=1,
00098     MCM_FOCUS=2
00099 };
00100
00105 typedef enum eMGparm_CentMeth MGparm_CentMeth;
00114 struct sMGparm {
00115
00116     MGparm_CalcType type;
00117     int parsed;
00119     /* *** GENERIC PARAMETERS *** */
00120     int dime[3];
00121     int setdime;
00122     Vchrg_Meth chgm;
00123     int setchgm;
00124     Vchrg_Src chgs;
00127     /* *** TYPE 0 PARAMETERS (SEQUENTIAL MANUAL) *** */
00128     int nlev;
00130     int setnlev;
00131     double etol;
00132     int setetol;
00133     double grid[3];
00134     int setgrid;
00135     double glen[3];
00136     int setglen;
00137     MGparm_CentMeth cmeth;
00138     double center[3];
00146     int centmol;
00149     int setgcent;
00151     /* ***** TYPE 1 & 2 PARAMETERS (SEQUENTIAL & PARALLEL AUTO-FOCUS) *** */
00152     double cglen[3];
00153     int setcglen;
00154     double fglen[3];
00155     int setfglen;
00156     MGparm_CentMeth ccmeth;
00157     double ccenter[3];
00158     int ccentmol;
00161     int setcgcent;
00162     MGparm_CentMeth fcmeth;
00163     double fcenter[3];
00164     int fcentmol;

```

```

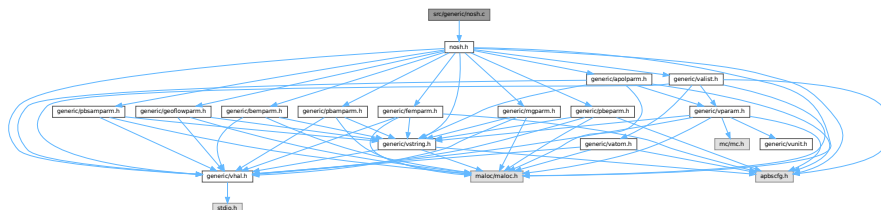
00167     int  setfgcent;
00170     /* ***** TYPE 2 PARAMETERS (PARALLEL AUTO-FOCUS) ***** */
00171     double partDisjCenter[3];
00173     double partDisjLength[3];
00175     int  partDisjOwnSide[6];
00178     int  pdime[3];
00179     int  setpdime;
00180     int  proc_rank;
00181     int  setrank;
00182     int  proc_size;
00183     int  setsize;
00184     double ofrac;
00185     int  setofrac;
00186     int  async;
00187     int  setasync;
00189     int  nonlintype;
00190     int  setnonlintype;
00192     int  method;
00193     int  setmethod;
00195     int  useAqua;
00196     int  setUseAqua;
00197 };
00198
00203 typedef struct sMGparm MGparm;
00204
00211 VEXTERNC int  MGparm_getNx(MGparm *thee);
00212
00219 VEXTERNC int  MGparm_getNy(MGparm *thee);
00220
00227 VEXTERNC int  MGparm_getNz(MGparm *thee);
00228
00235 VEXTERNC double MGparm_getHx(MGparm *thee);
00236
00243 VEXTERNC double MGparm_getHy(MGparm *thee);
00244
00251 VEXTERNC double MGparm_getHz(MGparm *thee);
00252
00259 VEXTERNC void  MGparm_setCenterX(MGparm *thee, double x);
00260
00267 VEXTERNC void  MGparm_setCenterY(MGparm *thee, double y);
00268
00275 VEXTERNC void  MGparm_setCenterZ(MGparm *thee, double z);
00276
00283 VEXTERNC double MGparm_getCenterX(MGparm *thee);
00284
00291 VEXTERNC double MGparm_getCenterY(MGparm *thee);
00292
00299 VEXTERNC double MGparm_getCenterZ(MGparm *thee);
00300
00307 VEXTERNC MGparm*  MGparm_ctor(MGparm_CalcType type);
00308
00316 VEXTERNC Vrc_Codes  MGparm_ctor2(MGparm *thee, MGparm_CalcType type);
00317
00323 VEXTERNC void  MGparm_dtor(MGparm **thee);
00324
00330 VEXTERNC void  MGparm_dtor2(MGparm *thee);
00331
00338 VEXTERNC Vrc_Codes  MGparm_check(MGparm *thee);
00339
00346 VEXTERNC void  MGparm_copy(MGparm *thee, MGparm *parm);
00347
00357 VEXTERNC Vrc_Codes  MGparm_parseToken(MGparm *thee, char tok[VMAX_BUFSIZE],
00358                                         Vio *sock);
00359
00360 #endif
00361

```

9.34 src/generic/nosh.c File Reference

Class NOsh methods.

Include dependency graph for nosh.c:



- VPRIVATE int [Nosh_parseREAD](#) ([Nosh](#) *thee, [Vio](#) *sock)
- VPRIVATE int [Nosh_parsePRINT](#) ([Nosh](#) *thee, [Vio](#) *sock)
- VPRIVATE int [Nosh_parseELEC](#) ([Nosh](#) *thee, [Vio](#) *sock)
- VPRIVATE int [Nosh_parseAPOLAR](#) ([Nosh](#) *thee, [Vio](#) *sock)
- VEXTERNC int [Nosh_parseFEM](#) ([Nosh](#) *thee, [Vio](#) *sock, [Nosh_calc](#) *elec)
- VEXTERNC int [Nosh_parseMG](#) ([Nosh](#) *thee, [Vio](#) *sock, [Nosh_calc](#) *elec)
- VEXTERNC int [Nosh_parseBEM](#) ([Nosh](#) *thee, [Vio](#) *sock, [Nosh_calc](#) *elec)
- VEXTERNC int [Nosh_parseGEOFLOW](#) ([Nosh](#) *thee, [Vio](#) *sock, [Nosh_calc](#) *elec)
- VEXTERNC int [Nosh_parsePBAM](#) ([Nosh](#) *thee, [Vio](#) *sock, [Nosh_calc](#) *elec)
- VEXTERNC int [Nosh_parsePBSAM](#) ([Nosh](#) *thee, [Vio](#) *sock, [Nosh_calc](#) *elec)
- VEXTERNC int [Nosh_parseAPOL](#) ([Nosh](#) *thee, [Vio](#) *sock, [Nosh_calc](#) *elec)
- VPRIVATE int [Nosh_setupCalcMG](#) ([Nosh](#) *thee, [Nosh_calc](#) *elec)
- VPRIVATE int [Nosh_setupCalcMGAUTO](#) ([Nosh](#) *thee, [Nosh_calc](#) *elec)
- VPRIVATE int [Nosh_setupCalcMGMANUAL](#) ([Nosh](#) *thee, [Nosh_calc](#) *elec)
- VPRIVATE int [Nosh_setupCalcMGPARA](#) ([Nosh](#) *thee, [Nosh_calc](#) *elec)
- VPRIVATE int [Nosh_setupCalcFEM](#) ([Nosh](#) *thee, [Nosh_calc](#) *elec)
- VPRIVATE int [Nosh_setupCalcFEMANUAL](#) ([Nosh](#) *thee, [Nosh_calc](#) *elec)
- VPRIVATE int [Nosh_setupCalcGEOFLOW](#) ([Nosh](#) *thee, [Nosh_calc](#) *elec)
- VPRIVATE int [Nosh_setupCalcPBAM](#) ([Nosh](#) *thee, [Nosh_calc](#) *elec)
- VPRIVATE int [Nosh_setupCalcPBSAM](#) ([Nosh](#) *thee, [Nosh_calc](#) *elec)
- VPRIVATE int [Nosh_setupCalcBEMMANUAL](#) ([Nosh](#) *thee, [Nosh_calc](#) *elec)
- VPRIVATE int [Nosh_setupCalcGEOFLOWMANUAL](#) ([Nosh](#) *thee, [Nosh_calc](#) *elec)
- VPRIVATE int [Nosh_setupCalcPBAMAUTO](#) ([Nosh](#) *thee, [Nosh_calc](#) *elec)
- VPRIVATE int [Nosh_setupCalcPBSAMAUTO](#) ([Nosh](#) *thee, [Nosh_calc](#) *elec)
- VPRIVATE int [Nosh_setupCalcAPOL](#) ([Nosh](#) *thee, [Nosh_calc](#) *elec)
- VPUBLIC char * [Nosh_getMolpath](#) ([Nosh](#) *thee, int imol)
Returns path to specified molecule.
- VPUBLIC char * [Nosh_getDielXpath](#) ([Nosh](#) *thee, int imol)
Returns path to specified x-shifted dielectric map.
- VPUBLIC char * [Nosh_getDielYpath](#) ([Nosh](#) *thee, int imol)
Returns path to specified y-shifted dielectric map.
- VPUBLIC char * [Nosh_getDielZpath](#) ([Nosh](#) *thee, int imol)
Returns path to specified z-shifted dielectric map.
- VPUBLIC char * [Nosh_getKappapath](#) ([Nosh](#) *thee, int imol)
Returns path to specified kappa map.

- VPUBLIC char * [NOsh_getPotpath](#) (NOsh *thee, int imol)
Returns path to specified potential map.
- VPUBLIC char * [NOsh_getChargepath](#) (NOsh *thee, int imol)
Returns path to specified charge distribution map.
- VPUBLIC [NOsh_calc](#) * [NOsh_getCalc](#) (NOsh *thee, int icalc)
Returns specified calculation object.
- VPUBLIC int [NOsh_getDielfmt](#) (NOsh *thee, int i)
Returns format of specified dielectric map.
- VPUBLIC int [NOsh_getKappafmt](#) (NOsh *thee, int i)
Returns format of specified kappa map.
- VPUBLIC int [NOsh_getPotfmt](#) (NOsh *thee, int i)
Returns format of specified potential map.
- VPUBLIC int [NOsh_getChargefmt](#) (NOsh *thee, int i)
Returns format of specified charge map.
- VPUBLIC [NOsh_PrintType](#) [NOsh_printWhat](#) (NOsh *thee, int iprint)
Return an integer ID of the observable to print (.
- VPUBLIC int [NOsh_printNarg](#) (NOsh *thee, int iprint)
Return number of arguments to PRINT statement (.
- VPUBLIC int [NOsh_elec2calc](#) (NOsh *thee, int icalc)
Return the name of an elec statement.
- VPUBLIC int [NOsh_apol2calc](#) (NOsh *thee, int icalc)
Return the name of an apol statement.
- VPUBLIC char * [NOsh_elecname](#) (NOsh *thee, int ielec)
Return an integer mapping of an ELEC statement to a calculation ID (.
- VPUBLIC int [NOsh_printOp](#) (NOsh *thee, int iprint, int iarg)
Return integer ID for specified operation (.
- VPUBLIC int [NOsh_printCalc](#) (NOsh *thee, int iprint, int iarg)
Return calculation ID for specified PRINT statement (.
- VPUBLIC [NOsh](#) * [NOsh_ctor](#) (int rank, int size)
Construct NOsh.
- VPUBLIC int [NOsh_ctor2](#) (NOsh *thee, int rank, int size)
FORTTRAN stub to construct NOsh.
- VPUBLIC void [NOsh_dtor](#) (NOsh **thee)
Object destructor.
- VPUBLIC void [NOsh_dtor2](#) (NOsh *thee)
FORTTRAN stub for object destructor.
- VPUBLIC [NOsh_calc](#) * [NOsh_calc_ctor](#) (NOsh_CalcType calctype)
Construct NOsh_calc.
- VPUBLIC void [NOsh_calc_dtor](#) (NOsh_calc **thee)
Object destructor.
- VPUBLIC int [NOsh_calc_copy](#) (NOsh_calc *thee, NOsh_calc *source)
Copy NOsh_calc object into thee.
- VPUBLIC int [NOsh_parseInputFile](#) (NOsh *thee, char *filename)
Parse an input file only from a file.
- VPUBLIC int [NOsh_parseInput](#) (NOsh *thee, Vio *sock)
Parse an input file from a socket.
- VPRIVATE int [NOsh_parseREAD_MOL](#) (NOsh *thee, Vio *sock)

- VPRIVATE int `NOsh_parseREAD_PARM` (`NOsh *thee`, `Vio *sock`)
- VPRIVATE int `NOsh_parseREAD_DIEL` (`NOsh *thee`, `Vio *sock`)
- VPRIVATE int `NOsh_parseREAD_KAPPA` (`NOsh *thee`, `Vio *sock`)
- VPRIVATE int `NOsh_parseREAD_POTENTIAL` (`NOsh *thee`, `Vio *sock`)
- VPRIVATE int `NOsh_parseREAD_CHARGE` (`NOsh *thee`, `Vio *sock`)
- VPRIVATE int `NOsh_parseREAD_MESH` (`NOsh *thee`, `Vio *sock`)
- VPUBLIC int `NOsh_setupElecCalc` (`NOsh *thee`, `Valist *alist[NOSH_MAXMOL]`)
Setup the series of electrostatics calculations.
- VPUBLIC int `NOsh_setupApolCalc` (`NOsh *thee`, `Valist *alist[NOSH_MAXMOL]`)
Setup the series of non-polar calculations.

9.34.1 Detailed Description

Class NOsh methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
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*
*

```

Definition in file [nosh.c](#).

9.34.2 Function Documentation

9.34.2.1 NOsh_parseAPOL()

```

VPUBLIC int NOsh_parseAPOL (
    NOsh * thee,
    Vio * sock,
    NOsh_calc * elec )

```

Definition at line [2508](#) of file [nosh.c](#).

9.34.2.2 NOsh_parseAPOLAR()

```

VPRIVATE int NOsh_parseAPOLAR (
    NOsh * thee,
    Vio * sock )

```

Definition at line [1313](#) of file [nosh.c](#).

9.34.2.3 NOsh_parseBEM()

```

VPUBLIC int NOsh_parseBEM (
    NOsh * thee,
    Vio * sock,
    NOsh_calc * elec )

```

Definition at line [2845](#) of file [nosh.c](#).

9.34.2.4 NOsh_parseELEC()

```

VPRIVATE int NOsh_parseELEC (
    NOsh * thee,
    Vio * sock )

```

Definition at line [1187](#) of file [nosh.c](#).

9.34.2.5 NOsh_parseFEM()

```

VPUBLIC int NOsh_parseFEM (
    NOsh * thee,
    Vio * sock,
    NOsh_calc * elec )

```

Definition at line [2385](#) of file [nosh.c](#).

9.34.2.6 NOsh_parseGEOFLOW()

```
VPUBLIC int NOsh_parseGEOFLOW (
    NOsh * thee,
    Vio * sock,
    NOsh_calc * elec )
```

Definition at line 2934 of file [nosh.c](#).

9.34.2.7 NOsh_parseMG()

```
VPUBLIC int NOsh_parseMG (
    NOsh * thee,
    Vio * sock,
    NOsh_calc * elec )
```

Definition at line 1510 of file [nosh.c](#).

9.34.2.8 NOsh_parsePBAM()

```
VPUBLIC int NOsh_parsePBAM (
    NOsh * thee,
    Vio * sock,
    NOsh_calc * elec )
```

Definition at line 3048 of file [nosh.c](#).

9.34.2.9 NOsh_parsePBSAM()

```
VPUBLIC int NOsh_parsePBSAM (
    NOsh * thee,
    Vio * sock,
    NOsh_calc * elec )
```

Definition at line 3166 of file [nosh.c](#).

9.34.2.10 NOsh_parsePRINT()

```
VPRIVATE int NOsh_parsePRINT (
    NOsh * thee,
    Vio * sock )
```

Definition at line 1021 of file [nosh.c](#).

9.34.2.11 NOsh_parseREAD()

```
VPRIVATE int NOsh_parseREAD (
    NOsh * thee,
    Vio * sock )
```

Definition at line 970 of file [nosh.c](#).

9.34.2.12 NOsh_parseREAD_CHARGE()

```
VPRIVATE int NOsh_parseREAD_CHARGE (  
    NOsh * thee,  
    Vio * sock )
```

Definition at line 884 of file [nosh.c](#).

9.34.2.13 NOsh_parseREAD_DIEL()

```
VPRIVATE int NOsh_parseREAD_DIEL (  
    NOsh * thee,  
    Vio * sock )
```

Definition at line 739 of file [nosh.c](#).

9.34.2.14 NOsh_parseREAD_KAPPA()

```
VPRIVATE int NOsh_parseREAD_KAPPA (  
    NOsh * thee,  
    Vio * sock )
```

Definition at line 793 of file [nosh.c](#).

9.34.2.15 NOsh_parseREAD_MESH()

```
VPRIVATE int NOsh_parseREAD_MESH (  
    NOsh * thee,  
    Vio * sock )
```

Definition at line 930 of file [nosh.c](#).

9.34.2.16 NOsh_parseREAD_MOL()

```
VPRIVATE int NOsh_parseREAD_MOL (  
    NOsh * thee,  
    Vio * sock )
```

Definition at line 598 of file [nosh.c](#).

9.34.2.17 NOsh_parseREAD_PARM()

```
VPRIVATE int NOsh_parseREAD_PARM (  
    NOsh * thee,  
    Vio * sock )
```

Definition at line 675 of file [nosh.c](#).

9.34.2.18 NOsh_parseREAD_POTENTIAL()

```
VPRIVATE int NOsh_parseREAD_POTENTIAL (  
    NOsh * thee,  
    Vio * sock )
```

Definition at line 839 of file [nosh.c](#).

9.34.2.19 NOsh_setupCalcAPOL()

```
VPRIVATE int NOsh_setupCalcAPOL (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 2581 of file [nosh.c](#).

9.34.2.20 NOsh_setupCalcBEM()

```
VPRIVATE int NOsh_setupCalcBEM (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 1638 of file [nosh.c](#).

9.34.2.21 NOsh_setupCalcBEMMANUAL()

```
VPRIVATE int NOsh_setupCalcBEMMANUAL (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 2612 of file [nosh.c](#).

9.34.2.22 NOsh_setupCalcFEM()

```
VPRIVATE int NOsh_setupCalcFEM (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 1722 of file [nosh.c](#).

9.34.2.23 NOsh_setupCalcFEMANUAL()

```
VPRIVATE int NOsh_setupCalcFEMANUAL (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 2471 of file [nosh.c](#).

9.34.2.24 NOsh_setupCalcGEOFLOW()

```
VPRIVATE int NOsh_setupCalcGEOFLOW (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 1666 of file [nosh.c](#).

9.34.2.25 NOsh_setupCalcGEOFLOWMANUAL()

```
VPRIVATE int NOsh_setupCalcGEOFLOWMANUAL (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 2677 of file [nosh.c](#).

9.34.2.26 NOsh_setupCalcMG()

```
VPRIVATE int NOsh_setupCalcMG (  
    NOsh * thee,  
    NOsh_calc * elec )
```

Definition at line 1603 of file [nosh.c](#).

9.34.2.27 NOsh_setupCalcMGAUTO()

```
VPUBLIC int NOsh_setupCalcMGAUTO (  
    NOsh * thee,  
    NOsh_calc * elec )
```

Definition at line 1815 of file [nosh.c](#).

9.34.2.28 NOsh_setupCalcMGMANUAL()

```
VPRIVATE int NOsh_setupCalcMGMANUAL (  
    NOsh * thee,  
    NOsh_calc * elec )
```

Definition at line 1747 of file [nosh.c](#).

9.34.2.29 NOsh_setupCalcMGPARA()

```
VPUBLIC int NOsh_setupCalcMGPARA (  
    NOsh * thee,  
    NOsh_calc * elec )
```

Definition at line 2090 of file [nosh.c](#).

9.34.2.30 NOsh_setupCalcPBAM()

```
VPRIVATE int NOsh_setupCalcPBAM (  
    NOsh * thee,  
    NOsh_calc * elec )
```

Definition at line 1686 of file [nosh.c](#).

9.34.2.31 NOsh_setupCalcPBAMAUTO()

```
VPRIVATE int NOsh_setupCalcPBAMAUTO (  
    NOsh * thee,  
    NOsh_calc * elec )
```

Definition at line 2735 of file [nosh.c](#).

9.34.2.32 NOsh_setupCalcPBSAM()

```
VPRIVATE int NOsh_setupCalcPBSAM (  
    NOsh * thee,  
    NOsh_calc * elec )
```

Definition at line 1704 of file [nosh.c](#).

9.34.2.33 NOsh_setupCalcPBSAMAUTO()

```
VPRIVATE int NOsh_setupCalcPBSAMAUTO (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 2786 of file [nosh.c](#).

9.35 nosh.c

[Go to the documentation of this file.](#)

```
00001
00057 #include "nosh.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061
00062 VPRIVATE int NOsh_parseREAD(
00063     NOsh *thee,
00064     Vio *sock);
00065
00066 VPRIVATE int NOsh_parsePRINT(
00067     NOsh *thee,
00068     Vio *sock);
00069
00070 VPRIVATE int NOsh_parseELEC(
00071     NOsh *thee,
00072     Vio *sock
00073 );
00074
00075 VPRIVATE int NOsh_parseAPOLAR(
00076     NOsh *thee,
00077     Vio *sock
00078 );
00079
00080 VEXTERNC int NOsh_parseFEM(
00081     NOsh *thee,
00082     Vio *sock,
00083     NOsh_calc *elec
00084 );
00085
00086 VEXTERNC int NOsh_parseMG(
00087     NOsh *thee,
00088     Vio *sock,
00089     NOsh_calc *elec
00090 );
00091
00092 VEXTERNC int NOsh_parseBEM(
00093     NOsh *thee,
00094     Vio *sock,
00095     NOsh_calc *elec
00096 );
00097
00098 VEXTERNC int NOsh_parseGEOFLOW(
00099     NOsh *thee,
00100     Vio *sock,
00101     NOsh_calc *elec
00102 );
00103
00104 VEXTERNC int NOsh_parsePBAM(
00105     NOsh *thee,
00106     Vio *sock,
00107     NOsh_calc *elec
00108 );
00109
00110 VEXTERNC int NOsh_parsePBSAM(
00111     NOsh *thee,
00112     Vio *sock,
00113     NOsh_calc *elec
00114 );
00115
00116 VEXTERNC int NOsh_parseAPOL(
00117     NOsh *thee,
00118     Vio *sock,
00119     NOsh_calc *elec
00120 );
00121
```

```
00122 VPRIVATE int NOsh_setupCalcMG(  
00123     NOsh *thee,  
00124     NOsh_calc *elec  
00125 );  
00126  
00127  
00128 VPRIVATE int NOsh_setupCalcMGAUTO(  
00129     NOsh *thee,  
00130     NOsh_calc *elec  
00131 );  
00132  
00133 VPRIVATE int NOsh_setupCalcMGMANUAL(  
00134     NOsh *thee,  
00135     NOsh_calc *elec  
00136 );  
00137  
00138 VPRIVATE int NOsh_setupCalcMGPARA(  
00139     NOsh *thee,  
00140     NOsh_calc *elec  
00141 );  
00142  
00143 VPRIVATE int NOsh_setupCalcFEM(  
00144     NOsh *thee,  
00145     NOsh_calc *elec  
00146 );  
00147  
00148 VPRIVATE int NOsh_setupCalcFEMANUAL(  
00149     NOsh *thee,  
00150     NOsh_calc *elec  
00151 );  
00152  
00153 VPRIVATE int NOsh_setupCalcBEM(  
00154     NOsh *thee,  
00155     NOsh_calc *elec  
00156 );  
00157  
00158 VPRIVATE int NOsh_setupCalcGEOFLOW(  
00159     NOsh *thee,  
00160     NOsh_calc *elec  
00161 );  
00162  
00163 VPRIVATE int NOsh_setupCalcPBAM(  
00164     NOsh *thee,  
00165     NOsh_calc *elec  
00166 );  
00167  
00168 VPRIVATE int NOsh_setupCalcPBSAM(  
00169     NOsh *thee,  
00170     NOsh_calc *elec  
00171 );  
00172  
00173 VPRIVATE int NOsh_setupCalcBEMMANUAL(  
00174     NOsh *thee,  
00175     NOsh_calc *elec  
00176 );  
00177  
00178 VPRIVATE int NOsh_setupCalcGEOFLOWMANUAL(  
00179     NOsh *thee,  
00180     NOsh_calc *elec  
00181 );  
00182  
00183 VPRIVATE int NOsh_setupCalcPBAMAUTO(  
00184     NOsh *thee,  
00185     NOsh_calc *elec  
00186 );  
00187  
00188 VPRIVATE int NOsh_setupCalcPBSAMAUTO(  
00189     NOsh *thee,  
00190     NOsh_calc *elec  
00191 );  
00192  
00193 VPRIVATE int NOsh_setupCalcAPOL(  
00194     NOsh *thee,  
00195     NOsh_calc *elec  
00196 );  
00197  
00198 #if !defined(VINLINE_NOSH)  
00199  
00200 VPUBLIC char* NOsh_getMolpath(NOsh *thee, int imol) {  
00201     VASSERT(thee != VNULL);  
00202     VASSERT(imol < thee->nmol);
```



```

00203     return thee->molpath[imol];
00204 }
00205 VPUBLIC char* NOsh_getDielXpath(NOsh *thee, int imol) {
00206     VASSERT(thee != VNULL);
00207     VASSERT(imol < thee->nmol);
00208     return thee->dielXpath[imol];
00209 }
00210 VPUBLIC char* NOsh_getDielYpath(NOsh *thee, int imol) {
00211     VASSERT(thee != VNULL);
00212     VASSERT(imol < thee->nmol);
00213     return thee->dielYpath[imol];
00214 }
00215 VPUBLIC char* NOsh_getDielZpath(NOsh *thee, int imol) {
00216     VASSERT(thee != VNULL);
00217     VASSERT(imol < thee->nmol);
00218     return thee->dielZpath[imol];
00219 }
00220 VPUBLIC char* NOsh_getKappapath(NOsh *thee, int imol) {
00221     VASSERT(thee != VNULL);
00222     VASSERT(imol < thee->nmol);
00223     return thee->kappapath[imol];
00224 }
00225 VPUBLIC char* NOsh_getPotpath(NOsh *thee, int imol) {
00226     VASSERT(thee != VNULL);
00227     VASSERT(imol < thee->nmol);
00228     return thee->potpath[imol];
00229 }
00230 VPUBLIC char* NOsh_getChargepath(NOsh *thee, int imol) {
00231     VASSERT(thee != VNULL);
00232     VASSERT(imol < thee->nmol);
00233     return thee->chargepath[imol];
00234 }
00235 VPUBLIC NOsh_calc* NOsh_getCalc(NOsh *thee, int icalc) {
00236     VASSERT(thee != VNULL);
00237     VASSERT(icalc < thee->ncalc);
00238     return thee->calc[icalc];
00239 }
00240 VPUBLIC int NOsh_getDielfmt(NOsh *thee, int i) {
00241     VASSERT(thee != VNULL);
00242     VASSERT(i < thee->ndiel);
00243     return (thee->dielfmt[i]);
00244 }
00245 VPUBLIC int NOsh_getKappafmt(NOsh *thee, int i) {
00246     VASSERT(thee != VNULL);
00247     VASSERT(i < thee->nkappa);
00248     return (thee->kappafmt[i]);
00249 }
00250 VPUBLIC int NOsh_getPotfmt(NOsh *thee, int i) {
00251     VASSERT(thee != VNULL);
00252     VASSERT(i < thee->npot);
00253     return (thee->potfmt[i]);
00254 }
00255 VPUBLIC int NOsh_getChargefmt(NOsh *thee, int i) {
00256     VASSERT(thee != VNULL);
00257     VASSERT(i < thee->ncharge);
00258     return (thee->chargefmt[i]);
00259 }
00260
00261
00262 #endif /* if !defined(VINLINE_NOSH) */
00263
00264 VPUBLIC NOsh_PrintType NOsh_printWhat(NOsh *thee, int iprint) {
00265     VASSERT(thee != VNULL);
00266     VASSERT(iprint < thee->nprint);
00267     return thee->printwhat[iprint];
00268 }
00269
00270 VPUBLIC int NOsh_printNarg(NOsh *thee, int iprint) {
00271     VASSERT(thee != VNULL);
00272     VASSERT(iprint < thee->nprint);
00273     return thee->printnarg[iprint];
00274 }
00275
00276 VPUBLIC int NOsh_elec2calc(NOsh *thee, int icalc) {
00277     VASSERT(thee != VNULL);
00278     VASSERT(icalc < thee->ncalc);
00279     return thee->elec2calc[icalc];
00280 }
00281
00282 VPUBLIC int NOsh_apol2calc(NOsh *thee, int icalc) {
00283     VASSERT(thee != VNULL);

```

```

00284     VASSERT(icalc < thee->ncalc);
00285     return thee->apol2calc[icalc];
00286 }
00287
00288 VPUBLIC char* NOsh_elecname(NOsh *thee, int ielec) {
00289     VASSERT(thee != VNULL);
00290     VASSERT(ielec < thee->nelec + 1);
00291     return thee->elecname[ielec];
00292 }
00293
00294 VPUBLIC int NOsh_printOp(NOsh *thee, int iprint, int iarg) {
00295     VASSERT(thee != VNULL);
00296     VASSERT(iprint < thee->nprint);
00297     VASSERT(iarg < thee->printnarg[iprint]);
00298     return thee->printop[iprint][iarg];
00299 }
00300
00301 VPUBLIC int NOsh_printCalc(NOsh *thee, int iprint, int iarg) {
00302     VASSERT(thee != VNULL);
00303     VASSERT(iprint < thee->nprint);
00304     VASSERT(iarg < thee->printnarg[iprint]);
00305     return thee->printcalc[iprint][iarg];
00306 }
00307
00308 VPUBLIC NOsh* NOsh_ctor(int rank, int size) {
00309     /* Set up the structure */
00310     NOsh *thee = VNULL;
00311     thee = (NOsh*)Vmem_malloc(VNULL, 1, sizeof(NOsh) );
00312     VASSERT( thee != VNULL);
00313     VASSERT( NOsh_ctor2(thee, rank, size) );
00314     return thee;
00315 }
00316
00317 }
00318
00319 VPUBLIC int NOsh_ctor2(NOsh *thee, int rank, int size) {
00320     int i;
00321
00322     if (thee == VNULL) return 0;
00323
00324     thee->proc_rank = rank;
00325     thee->proc_size = size;
00326
00327     thee->ispara = 0;
00328     thee->parsed = 0;
00329
00330     thee->nmol = 0;
00331     thee->gotparm = 0;
00332     thee->ncharge = 0;
00333     thee->ndiel = 0;
00334     thee->nkappa = 0;
00335     thee->npot = 0;
00336     thee->nprint = 0;
00337
00338     for (i=0; i<NOSH_MAXCALC; i++) {
00339         thee->calc[i] = VNULL;
00340         thee->elec[i] = VNULL;
00341         thee->apol[i] = VNULL;
00342     }
00343     for (i=0; i<NOSH_MAXMOL; i++) {
00344         thee->alist[i] = VNULL;
00345     }
00346     thee->ncalc = 0;
00347     thee->nelec = 0;
00348     thee->napol = 0;
00349
00350     return 1;
00351 }
00352
00353
00354 VPUBLIC void NOsh_dtor(NOsh **thee) {
00355     if ((*thee) != VNULL) {
00356         NOsh_dtor2(*thee);
00357         Vmem_free(VNULL, 1, sizeof(NOsh), (void **)thee);
00358         (*thee) = VNULL;
00359     }
00360 }
00361
00362 VPUBLIC void NOsh_dtor2(NOsh *thee) {
00363     int i;

```

```

00365
00366     if (thee != VNULL) {
00367         for (i=0; i<(thee->ncalc); i++) NOsh_calc_dtor(&(thee->calc[i]));
00368         for (i=0; i<(thee->nelec); i++) NOsh_calc_dtor(&(thee->elec[i]));
00369         for (i=0; i<(thee->napol); i++) NOsh_calc_dtor(&(thee->apol[i]));
00370     }
00371
00372 }
00373
00374 VPUBLIC NOsh_calc* NOsh_calc_ctor(
00375     NOsh_CalcType calctype
00376 ) {
00377     NOsh_calc *thee;
00378     thee = (NOsh_calc *)Vmem_malloc(VNULL, 1, sizeof(NOsh_calc));
00379     thee->calctype = calctype;
00380
00381     thee->mgparm = VNULL;
00382     thee->femparm = VNULL;
00383     thee->apolparm = VNULL;
00384     thee->bemparm = VNULL;
00385     thee->geoflowparm = VNULL;
00386     thee->pbamparm = VNULL;
00387     thee->pbsamparm = VNULL;
00388
00389     switch (calctype) {
00390     case NCT_MG:
00391         thee->mgparm = MGparm_ctor(MCT_NONE);
00392         break;
00393     case NCT_FEM:
00394         thee->femparm = FEMparm_ctor(FCT_NONE);
00395         break;
00396     case NCT_APOL:
00397         thee->apolparm = APOLparm_ctor();
00398         break;
00399     case NCT_BEM:
00400         thee->bemparm = BEMparm_ctor(BCT_MANUAL);
00401         break;
00402     case NCT_GEOFLOW:
00403         thee->geoflowparm = GEOFLOWparm_ctor(GFCT_AUTO);
00404         thee->apolparm = APOLparm_ctor();
00405         break;
00406     case NCT_PBAM:
00407         thee->pbamparm = PBAMparm_ctor(PBAMCT_AUTO);
00408         break;
00409     case NCT_PBSAM:
00410         thee->pbamparm = PBAMparm_ctor(PBAMCT_AUTO);
00411         thee->pbsamparm = PBSAMparm_ctor(PBSAMCT_AUTO);
00412         break;
00413     default:
00414         Vnm_print(2, "NOsh_calc_ctor: unknown calculation type (%d)!\n",
00415             calctype);
00416         VASSERT(0);
00417     }
00418     thee->pbeparm = PBEParm_ctor();
00419
00420     return thee;
00421 }
00422
00423 VPUBLIC void NOsh_calc_dtor(
00424     NOsh_calc **thee
00425 ) {
00426
00427     NOsh_calc *calc = VNULL;
00428     calc = *thee;
00429     if (calc == VNULL) return;
00430
00431     switch (calc->calctype) {
00432     case NCT_MG:
00433         MGparm_dtor(&(calc->mgparm));
00434         break;
00435     case NCT_FEM:
00436         FEMparm_dtor(&(calc->femparm));
00437         break;
00438     case NCT_APOL:
00439         APOLparm_dtor(&(calc->apolparm));
00440         break;
00441     case NCT_BEM:
00442         BEMparm_dtor(&(calc->bemparm));
00443         break;
00444     case NCT_GEOFLOW:
00445         GEOFLOWparm_dtor(&(calc->geoflowparm));

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```

00446         APOLparam_dtor(&(calc->apolparam));
00447         break;
00448     case NCT_PBAM:
00449         PBAMparam_dtor(&(calc->pbamparm));
00450         break;
00451     case NCT_PBSAM:
00452         PBAMparam_dtor(&(calc->pbamparm));
00453         PBSAMparam_dtor(&(calc->pbsamparm));
00454         break;
00455     default:
00456         Vnm_print(2, "Nosh_calc_ctor: unknown calculation type (%d)!\n",
00457                 calc->calctype);
00458         VASSERT(0);
00459     }
00460     PBEparam_dtor(&(calc->pbeparm));
00461
00462     Vmem_free(VNULL, 1, sizeof(Nosh_calc), (void **)thee);
00463     calc = VNULL;
00464 }
00465 }
00466
00467 VPUBLIC int Nosh_calc_copy(
00468     Nosh_calc *thee,
00469     Nosh_calc *source
00470 ) {
00471
00472     VASSERT(thee != VNULL);
00473     VASSERT(source != VNULL);
00474     VASSERT(thee->calctype == source->calctype);
00475     if (source->mgparam != VNULL)
00476         MGparam_copy(thee->mgparam, source->mgparam);
00477     if (source->femparm != VNULL)
00478         FEMparam_copy(thee->femparm, source->femparm);
00479     if (source->bemparm != VNULL)
00480         BEMparam_copy(thee->bemparm, source->bemparm);
00481     if (source->pbeparm != VNULL)
00482         PBEparam_copy(thee->pbeparm, source->pbeparm);
00483     if (source->apolparam != VNULL)
00484         APOLparam_copy(thee->apolparam, source->apolparam);
00485     /*I think here is where the the geoflow changes get lost*/
00486     if (source->geoflowparam != VNULL)
00487         GEOFLOWparam_copy(thee->geoflowparam, source->geoflowparam);
00488     if (source->pbamparm != VNULL)
00489         PBAMparam_copy(thee->pbamparm, source->pbamparm);
00490     if (source->pbsamparm != VNULL)
00491         PBSAMparam_copy(thee->pbsamparm, source->pbsamparm);
00492
00493     return 1;
00494 }
00495 }
00496 }
00497
00498 VPUBLIC int Nosh_parseInputFile(
00499     Nosh *thee,
00500     char *filename
00501 ) {
00502
00503     Vio *sock;
00504     int rc;
00505
00506     sock = Vio_ctor("FILE", "ASC", VNULL, filename, "r");
00507     rc = Nosh_parseInput(thee, sock);
00508     Vio_dtor(&sock);
00509
00510     return rc;
00511 }
00512
00513 VPUBLIC int Nosh_parseInput(
00514     Nosh *thee,
00515     Vio *sock
00516 ) {
00517
00518     char *MCwhiteChars = " =,;\t\r\n";
00519     char *MCcommChars = "#%";
00520     char tok[VMAX_BUFSIZE];
00521
00522     if (thee == VNULL) {
00523         Vnm_print(2, "Nosh_parseInput: Got NULL thee!\n");
00524         return 0;
00525     }
00526

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```

00527     if (sock == VNULL) {
00528         Vnm_print(2, "Nosh_parseInput: Got pointer to NULL socket!\n");
00529         Vnm_print(2, "Nosh_parseInput: The specified input file was not found!\n");
00530         return 0;
00531     }
00532
00533     if (thee->parsed) {
00534         Vnm_print(2, "Nosh_parseInput: Already parsed an input file!\n");
00535         return 0;
00536     }
00537
00538     if (Vio_accept(sock, 0) < 0) {
00539         Vnm_print(2, "Nosh_parseInput: Problem reading from socket!\n");
00540         return 0;
00541     }
00542
00543     /* Set up the whitespace and comment character definitions */
00544     Vio_setWhiteChars(sock, MCwhiteChars);
00545     Vio_setCommChars(sock, MCcommChars);
00546
00547     /* We parse the file until we run out of tokens */
00548     Vnm_print(0, "Nosh_parseInput: Starting file parsing...\n");
00549     while (Vio_scanf(sock, "%s", tok) == 1) {
00550         /* At the highest level, we look for keywords that indicate functions like:
00551
00552         read => Read in a molecule file
00553         elec => Do an electrostatics calculation
00554         print => Print some results
00555         apolar => do a non-polar calculation
00556         quit => Quit
00557
00558         These cause the code to go to a lower-level parser routine which
00559         handles keywords specific to the particular function. Each
00560         lower-level parser routine then returns when it hits the "end"
00561         keyword. Due to this simple layout, no nesting of these "function"
00562         sections is allowed.
00563         */
00564         if (Vstring_strcasecmp(tok, "read") == 0) {
00565             /* printf("read\n");
00566             Vnm_print(0, "Nosh: Parsing READ section\n");
00567             if (!Nosh_parseREAD(thee, sock)) return 0;
00568             Vnm_print(0, "Nosh: Done parsing READ section \
00569 (nmol=%d, ndiel=%d, nkappa=%d, ncharge=%d, npot=%d)\n", thee->nmol, thee->ndiel,
00570             thee->nkappa, thee->ncharge, thee->npot);
00571             } else if (Vstring_strcasecmp(tok, "print") == 0) {
00572             Vnm_print(0, "Nosh: Parsing PRINT section\n");
00573             if (!Nosh_parsePRINT(thee, sock)) return 0;
00574             Vnm_print(0, "Nosh: Done parsing PRINT section\n");
00575             } else if (Vstring_strcasecmp(tok, "elec") == 0) {
00576             Vnm_print(0, "Nosh: Parsing ELEC section\n");
00577             if (!Nosh_parseELEC(thee, sock)) return 0;
00578             Vnm_print(0, "Nosh: Done parsing ELEC section (nelec = %d)\n",
00579             thee->nelec);
00580             } else if (Vstring_strcasecmp(tok, "apolar") == 0) {
00581             Vnm_print(0, "Nosh: Parsing APOLAR section\n");
00582             if (!Nosh_parseAPOLAR(thee, sock)) return 0;
00583             Vnm_print(0, "Nosh: Done parsing APOLAR section (nelec = %d)\n",
00584             thee->nelec);
00585             } else if (Vstring_strcasecmp(tok, "quit") == 0) {
00586             Vnm_print(0, "Nosh: Done parsing file (got QUIT)\n");
00587             break;
00588             } else {
00589             Vnm_print(2, "Nosh_parseInput: Ignoring undefined keyword %s!\n", tok);
00590             }
00591         }
00592
00593         thee->parsed = 1;
00594         return 1;
00595     }
00596 }
00597
00598 VPRIVATE int Nosh_parseREAD_MOL(Nosh *thee, Vio *sock) {
00599
00600     char tok[VMAX_BUFSIZE], str[VMAX_BUFSIZE]="", strnew[VMAX_BUFSIZE]="";
00601     Nosh_MolFormat molfmt;
00602
00603     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00604     if (Vstring_strcasecmp(tok, "pqr") == 0) {
00605         molfmt = NMF_PQR;
00606         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00607         if (tok[0]=='"') {

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```

00608         strcpy(strnew, "");
00609         while (tok[strlen(tok)-1] != '"') {
00610             strcat(str, tok);
00611             strcat(str, " ");
00612             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00613         }
00614         strcat(str, tok);
00615         strncpy(strnew, str+1, strlen(str)-2);
00616         strcpy(tok, strnew);
00617     }
00618     Vnm_print(0, "Nosh: Storing molecule %d path %s\n",
00619             thee->nmol, tok);
00620     thee->molfmt[thee->nmol] = molfmt;
00621     strncpy(thee->molpath[thee->nmol], tok, VMAX_ARGLEN);
00622     (thee->nmol)++;
00623 } else if (Vstring_strcasecmp(tok, "pdb") == 0) {
00624     molfmt = NMF_PDB;
00625     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00626     if (tok[0]=='"') {
00627         strcpy(strnew, "");
00628         while (tok[strlen(tok)-1] != '"') {
00629             strcat(str, tok);
00630             strcat(str, " ");
00631             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00632         }
00633         strcat(str, tok);
00634         strncpy(strnew, str+1, strlen(str)-2);
00635         strcpy(tok, strnew);
00636     }
00637     Vnm_print(0, "Nosh: Storing molecule %d path %s\n",
00638             thee->nmol, tok);
00639     thee->molfmt[thee->nmol] = molfmt;
00640     strncpy(thee->molpath[thee->nmol], tok, VMAX_ARGLEN);
00641     (thee->nmol)++;
00642 } else if (Vstring_strcasecmp(tok, "xml") == 0) {
00643     molfmt = NMF_XML;
00644     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00645     if (tok[0]=='"') {
00646         strcpy(strnew, "");
00647         while (tok[strlen(tok)-1] != '"') {
00648             strcat(str, tok);
00649             strcat(str, " ");
00650             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00651         }
00652         strcat(str, tok);
00653         strncpy(strnew, str+1, strlen(str)-2);
00654         strcpy(tok, strnew);
00655     }
00656     Vnm_print(0, "Nosh: Storing molecule %d path %s\n",
00657             thee->nmol, tok);
00658     thee->molfmt[thee->nmol] = molfmt;
00659     strncpy(thee->molpath[thee->nmol], tok, VMAX_ARGLEN);
00660     (thee->nmol)++;
00661 } else {
00662     Vnm_print(2, "Nosh_parseREAD: Ignoring undefined mol format \
00663 %s!\n", tok);
00664 }
00665 return 1;
00666
00667
00668
00669 VERROR1:
00670     Vnm_print(2, "Nosh_parseREAD_MOL: Ran out of tokens while parsing READ section!\n");
00671     return 0;
00672 }
00673 }
00674
00675 VPRIVATE int Nosh_parseREAD_PARM(NOsh *thee, Vio *sock) {
00676
00677     char tok[VMAX_BUFSIZE], str[VMAX_BUFSIZE]="", strnew[VMAX_BUFSIZE]="";
00678     NOsh_ParmFormat parmfmt;
00679
00680     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00681     if (Vstring_strcasecmp(tok, "flat") == 0) {
00682         parmfmt = NPF_FLAT;
00683         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00684         if (tok[0]=='"') {
00685             strcpy(strnew, "");
00686             while (tok[strlen(tok)-1] != '"') {
00687                 strcat(str, tok);
00688                 strcat(str, " ");

```

```

00689         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00690     }
00691     strcat(str, tok);
00692     strncpy(strnew, str+1, strlen(str)-2);
00693     strcpy(tok, strnew);
00694 }
00695 if (thee->gotparm) {
00696     Vnm_print(2, "Nosh: Hey! You already specified a parameterfile (%s)!\n", thee->parmpath);
00697     Vnm_print(2, "Nosh: I'm going to ignore this one (%s)!\n", tok);
00698 } else {
00699     thee->parmfmt = parmfmt;
00700     thee->gotparm = 1;
00701     strncpy(thee->parmpath, tok, VMAX_ARGLEN);
00702 }
00703 } else if(Vstring_strcasecmp(tok, "xml") == 0) {
00704     parmfmt = NPF_XML;
00705     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00706     if (tok[0]=='\"') {
00707         strcpy(strnew, "");
00708         while (tok[strlen(tok)-1] != '\"') {
00709             strcat(str, tok);
00710             strcat(str, " ");
00711             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00712         }
00713         strcat(str, tok);
00714         strncpy(strnew, str+1, strlen(str)-2);
00715         strcpy(tok, strnew);
00716     }
00717     if (thee->gotparm) {
00718         Vnm_print(2, "Nosh: Hey! You already specified a parameterfile (%s)!\n", thee->parmpath);
00719         Vnm_print(2, "Nosh: I'm going to ignore this one (%s)!\n", tok);
00720     } else {
00721         thee->parmfmt = parmfmt;
00722         thee->gotparm = 1;
00723         strncpy(thee->parmpath, tok, VMAX_ARGLEN);
00724     }
00725 } else {
00726     Vnm_print(2, "Nosh_parseREAD: Ignoring undefined parm format \
00727 %s!\n", tok);
00728 }
00729 }
00730 return 1;
00731 }
00732
00733 VERROR1:
00734     Vnm_print(2, "Nosh_parseREAD_PARM: Ran out of tokens while parsing READ section!\n");
00735     return 0;
00736 }
00737 }
00738
00739 VPRIVATE int Nosh_parseREAD_DIEL(Nosh *thee, Vio *sock) {
00740
00741     char tok[VMAX_BUFSIZE], str[VMAX_BUFSIZE]="", strnew[VMAX_BUFSIZE]="";
00742     Vdata_Format dielfmt;
00743
00744     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00745     if (Vstring_strcasecmp(tok, "dx") == 0) {
00746         dielfmt = VDF_DX;
00747         //added VDF_BIN to take binary files.
00748     } else if (Vstring_strcasecmp(tok, "dxbin") == 0){
00749         dielfmt = VDF_DXBIN;
00750     } else if (Vstring_strcasecmp(tok, "gz") == 0) {
00751         dielfmt = VDF_GZ;
00752     } else {
00753         Vnm_print(2, "Nosh_parseREAD: Ignoring undefined format \
00754 %s!\n", tok);
00755         return VRC_FAILURE;
00756     }
00757
00758     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00759     if (tok[0]=='\"') {
00760         strcpy(strnew, "");
00761         while (tok[strlen(tok)-1] != '\"') {
00762             strcat(str, tok);
00763             strcat(str, " ");
00764             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00765         }
00766         strcat(str, tok);
00767         strncpy(strnew, str+1, strlen(str)-2);
00768         strcpy(tok, strnew);
00769     }

```

```

00770     Vnm_print(0, "Nosh: Storing x-shifted dielectric map %d path \
00771               %s\n", thee->ndiel, tok);
00772     strncpy(thee->dielXpath[thee->ndiel], tok, VMAX_ARGLEN);
00773     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00774     Vnm_print(0, "Nosh: Storing y-shifted dielectric map %d path \
00775               %s\n", thee->ndiel, tok);
00776     strncpy(thee->dielYpath[thee->ndiel], tok, VMAX_ARGLEN);
00777     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00778     Vnm_print(0, "Nosh: Storing z-shifted dielectric map %d path \
00779               %s\n", thee->ndiel, tok);
00780     strncpy(thee->dielZpath[thee->ndiel], tok, VMAX_ARGLEN);
00781     thee->dielfmt[thee->ndiel] = dielfmt;
00782     (thee->ndiel)++;
00783
00784     return 1;
00785
00786 ERROR1:
00787     Vnm_print(2, "Nosh_parseREAD_DIEL: Ran out of tokens while parsing READ \
00788 section!\n");
00789     return 0;
00790
00791 }
00792
00793 PRIVATE int Nosh_parseREAD_KAPPA(Nosh *thee, Vio *sock) {
00794
00795     char tok[VMAX_BUFSIZE], str[VMAX_BUFSIZE]="", strnew[VMAX_BUFSIZE]="";
00796     Vdata_Format kappafmt;
00797
00798     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00799     if (Vstring_strcasecmp(tok, "dx") == 0) {
00800         kappafmt = VDF_DX;
00801     } else if (Vstring_strcasecmp(tok, "gz") == 0) {
00802         kappafmt = VDF_GZ;
00803     } else if (Vstring_strcasecmp(tok, "dxbin") == 0) {
00804         kappafmt = VDF_DXBIN;
00805     } else {
00806
00807         Vnm_print(2, "Nosh_parseREAD: Ignoring undefined format \
00808               %s!\n", tok);
00809         return VRC_FAILURE;
00810     }
00811
00812     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00813     if (tok[0]!='"') {
00814         strcpy(strnew, "");
00815         while (tok[strlen(tok)-1] != '"') {
00816             strcat(str, tok);
00817             strcat(str, " ");
00818             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00819         }
00820         strcat(str, tok);
00821         strncpy(strnew, str+1, strlen(str)-2);
00822         strcpy(tok, strnew);
00823     }
00824     Vnm_print(0, "Nosh: Storing kappa map %d path %s\n",
00825               thee->nkappa, tok);
00826     thee->kappafmt[thee->nkappa] = kappafmt;
00827     strncpy(thee->kappapath[thee->nkappa], tok, VMAX_ARGLEN);
00828     (thee->nkappa)++;
00829
00830     return 1;
00831
00832 ERROR1:
00833     Vnm_print(2, "Nosh_parseREAD: Ran out of tokens while parsing READ \
00834 section!\n");
00835     return 0;
00836
00837 }
00838
00839 PRIVATE int Nosh_parseREAD_POTENTIAL(Nosh *thee, Vio *sock) {
00840
00841     char tok[VMAX_BUFSIZE], str[VMAX_BUFSIZE]="", strnew[VMAX_BUFSIZE]="";
00842     Vdata_Format potfmt;
00843
00844     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00845     if (Vstring_strcasecmp(tok, "dx") == 0) {
00846         potfmt = VDF_DX;
00847     } else if (Vstring_strcasecmp(tok, "gz") == 0) {
00848         potfmt = VDF_GZ;
00849     } else if (Vstring_strcasecmp(tok, "dxbin") == 0) {
00850         potfmt = VDF_DXBIN;

```



```

00851     } else {
00852         Vnm_print(2, "Nosh_parseREAD: Ignoring undefined format \
00853             %s!\n", tok);
00854         return VRC_FAILURE;
00855     }
00856
00857     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00858     if (tok[0]=='"') {
00859         strcpy(strnew, "");
00860         while (tok[strlen(tok)-1] != '"') {
00861             strcat(str, tok);
00862             strcat(str, " ");
00863             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00864         }
00865         strcat(str, tok);
00866         strncpy(strnew, str+1, strlen(str)-2);
00867         strcpy(tok, strnew);
00868     }
00869     Vnm_print(0, "Nosh: Storing potential map %d path %s\n",
00870         thee->npot, tok);
00871     thee->potfmt[thee->npot] = potfmt;
00872     strncpy(thee->potpath[thee->npot], tok, VMAX_ARGLEN);
00873     (thee->npot)++;
00874
00875     return 1;
00876
00877 ERROR1:
00878     Vnm_print(2, "Nosh_parseREAD: Ran out of tokens while parsing READ \
00879         section!\n");
00880     return 0;
00881 }
00882
00883 VPRIVATE int Nosh_parseREAD_CHARGE(Nosh *thee, Vio *sock) {
00884     char tok[VMAX_BUFSIZE], str[VMAX_BUFSIZE]="", strnew[VMAX_BUFSIZE]="";
00885     Vdata_Format chargefmt;
00886
00887     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00888     if (Vstring_strcasecmp(tok, "dx") == 0) {
00889         chargefmt = VDF_DX;
00890     }
00891     else if (Vstring_strcasecmp(tok, "dxbin") == 0) {
00892         chargefmt = VDF_DXBIN;
00893     }
00894     else if (Vstring_strcasecmp(tok, "gz") == 0) {
00895         chargefmt = VDF_GZ;
00896     }
00897     else {
00898         Vnm_print(2, "Nosh_parseREAD: Ignoring undefined format \
00899             %s!\n", tok);
00900         return VRC_FAILURE;
00901     }
00902
00903     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00904     if (tok[0]=='"') {
00905         strcpy(strnew, "");
00906         while (tok[strlen(tok)-1] != '"') {
00907             strcat(str, tok);
00908             strcat(str, " ");
00909             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00910         }
00911         strcat(str, tok);
00912         strncpy(strnew, str+1, strlen(str)-2);
00913         strcpy(tok, strnew);
00914     }
00915     Vnm_print(0, "Nosh: Storing charge map %d path %s\n",
00916         thee->ncharge, tok);
00917     thee->chargefmt[thee->ncharge] = chargefmt;
00918     strncpy(thee->chargepath[thee->ncharge], tok, VMAX_ARGLEN);
00919     (thee->ncharge)++;
00920
00921     return 1;
00922
00923 ERROR1:
00924     Vnm_print(2, "Nosh_parseREAD: Ran out of tokens while parsing READ \
00925         section!\n");
00926     return 0;
00927 }
00928
00929 VPRIVATE int Nosh_parseREAD_MESH(Nosh *thee, Vio *sock) {
00930
00931

```

```

00932     char tok[VMAX_BUF_SIZE], str[VMAX_BUF_SIZE]="", strnew[VMAX_BUF_SIZE]="";
00933     Vdata_Format meshfmt;
00934
00935     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00936     if (Vstring_strcasecmp(tok, "mcsf") == 0) {
00937         meshfmt = VDF_MCSF;
00938         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00939         if (tok[0]!='\n') {
00940             strcpy(strnew, "");
00941             while (tok[strlen(tok)-1] != '\n') {
00942                 strcat(str, tok);
00943                 strcat(str, " ");
00944                 VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00945             }
00946             strcat(str, tok);
00947             strncpy(strnew, str+1, strlen(str)-2);
00948             strcpy(tok, strnew);
00949         }
00950         Vnm_print(0, "Nosh: Storing mesh %d path %s\n",
00951             thee->nmesh, tok);
00952         thee->meshfmt[thee->nmesh] = meshfmt;
00953         strncpy(thee->meshpath[thee->nmesh], tok, VMAX_ARGLEN);
00954         (thee->nmesh)++;
00955     } else {
00956         Vnm_print(2, "Nosh_parseREAD: Ignoring undefined mesh format \
00957             %s!\n", tok);
00958     }
00959     return 1;
00960
00961 ERROR1:
00962     Vnm_print(2, "Nosh_parseREAD: Ran out of tokens while parsing READ \
00963         section!\n");
00964     return 0;
00965 }
00966
00967 }
00968
00969 VPRIVATE int NOsh_parseREAD(NOsh *thee, Vio *sock) {
00970     char tok[VMAX_BUF_SIZE];
00971
00972     if (thee == VNULL) {
00973         Vnm_print(2, "Nosh_parseREAD: Got NULL thee!\n");
00974         return 0;
00975     }
00976
00977     if (sock == VNULL) {
00978         Vnm_print(2, "Nosh_parseREAD: Got pointer to NULL socket!\n");
00979         return 0;
00980     }
00981
00982     if (thee->parsed) {
00983         Vnm_print(2, "Nosh_parseREAD: Already parsed an input file!\n");
00984         return 0;
00985     }
00986
00987     /* Read until we run out of tokens (bad) or hit the "END" keyword (good) */
00988     while (Vio_scanf(sock, "%s", tok) == 1) {
00989         if (Vstring_strcasecmp(tok, "end") == 0) {
00990             Vnm_print(0, "Nosh: Done parsing READ section\n");
00991             return 1;
00992         } else if (Vstring_strcasecmp(tok, "mol") == 0) {
00993             NOsh_parseREAD_MOL(thee, sock);
00994         } else if (Vstring_strcasecmp(tok, "parm") == 0) {
00995             NOsh_parseREAD_PARM(thee, sock);
00996         } else if (Vstring_strcasecmp(tok, "diel") == 0) {
00997             NOsh_parseREAD_DIEL(thee, sock);
00998         } else if (Vstring_strcasecmp(tok, "kappa") == 0) {
00999             NOsh_parseREAD_KAPPA(thee, sock);
01000         } else if (Vstring_strcasecmp(tok, "pot") == 0) {
01001             NOsh_parseREAD_POTENTIAL(thee, sock);
01002         } else if (Vstring_strcasecmp(tok, "charge") == 0) {
01003             NOsh_parseREAD_CHARGE(thee, sock);
01004         } else if (Vstring_strcasecmp(tok, "mesh") == 0) {
01005             NOsh_parseREAD_MESH(thee, sock);
01006         } else {
01007             Vnm_print(2, "Nosh_parseREAD: Ignoring undefined keyword %s!\n",
01008                 tok);
01009         }
01010     }
01011 }
01012

```

```

01013
01014     /* We ran out of tokens! */
01015     Vnm_print(2, "Nosh_parseREAD: Ran out of tokens while parsing READ \
01016 section!\n");
01017     return 0;
01018
01019 }
01020
01021 VPRIVATE int Nosh_parsePRINT(NOsh *thee, Vio *sock) {
01022     char tok[VMAX_BUFSIZE];
01023     char name[VMAX_BUFSIZE];
01024     int ti, idx, expect, ielec, iapol;
01025
01026     if (thee == VNULL) {
01027         Vnm_print(2, "Nosh_parsePRINT: Got NULL thee!\n");
01028         return 0;
01029     }
01030
01031     if (sock == VNULL) {
01032         Vnm_print(2, "Nosh_parsePRINT: Got pointer to NULL socket!\n");
01033         return 0;
01034     }
01035
01036     if (thee->parsed) {
01037         Vnm_print(2, "Nosh_parsePRINT: Already parsed an input file!\n");
01038         return 0;
01039     }
01040
01041     idx = thee->nprint;
01042     if (thee->nprint >= NOSH_MAXPRINT) {
01043         Vnm_print(2, "Nosh_parsePRINT: Exceeded max number (%d) of PRINT \
01044 sections\n",
01045                 NOSH_MAXPRINT);
01046         return 0;
01047     }
01048
01049     /* The first thing we read is the thing we want to print */
01050     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01051     if (Vstring_strcasecmp(tok, "energy") == 0) {
01052         thee->printwhat[idx] = NPT_ENERGY;
01053         thee->printnarg[idx] = 0;
01054     } else if (Vstring_strcasecmp(tok, "force") == 0) {
01055         thee->printwhat[idx] = NPT_FORCE;
01056         thee->printnarg[idx] = 0;
01057     } else if (Vstring_strcasecmp(tok, "elecEnergy") == 0) {
01058         thee->printwhat[idx] = NPT_ELECENERGY;
01059         thee->printnarg[idx] = 0;
01060     } else if (Vstring_strcasecmp(tok, "elecForce") == 0) {
01061         thee->printwhat[idx] = NPT_ELECFORCE;
01062         thee->printnarg[idx] = 0;
01063     } else if (Vstring_strcasecmp(tok, "apolEnergy") == 0) {
01064         thee->printwhat[idx] = NPT_APOLENERGY;
01065         thee->printnarg[idx] = 0;
01066     } else if (Vstring_strcasecmp(tok, "apolForce") == 0) {
01067         thee->printwhat[idx] = NPT_APOLFORCE;
01068         thee->printnarg[idx] = 0;
01069     } else {
01070         Vnm_print(2, "Nosh_parsePRINT: Undefined keyword %s while parsing \
01071 PRINT section!\n", tok);
01072         return 0;
01073     }
01074
01075     expect = 0; /* We first expect a calculation ID (0) then an op (1) */
01076
01077     /* Read until we run out of tokens (bad) or hit the "END" keyword (good) */
01078     while (Vio_scanf(sock, "%s", tok) == 1) {
01079         /* The next thing we read is either END or an ARG OP ARG statement */
01080         if (Vstring_strcasecmp(tok, "end") == 0) {
01081             if (expect != 0) {
01082                 (thee->nprint)++;
01083                 (thee->printnarg[idx])++;
01084                 Vnm_print(0, "Nosh: Done parsing PRINT section\n");
01085                 return 1;
01086             } else {
01087                 Vnm_print(2, "Nosh_parsePRINT: Got premature END to PRINT!\n");
01088                 return 0;
01089             }
01090         } else {
01091             }
01092         } else {
01093

```

```

01094
01095     /* Grab a calculation ID */
01096     if ((sscanf(tok, "%d", &ti) == 1) &&
01097         (Vstring_isdigit(tok) == 1)) {
01098         if (expect == 0) {
01099             thee->printcalc[idx][thee->printnarg[idx]] = ti-1;
01100             expect = 1;
01101         } else {
01102             Vnm_print(2, "Nosh_parsePRINT: Syntax error in PRINT \
01103 section while reading %s!\n", tok);
01104             return 0;
01105         }
01106     /* Grab addition operation */
01107     } else if (Vstring_strcasecmp(tok, "+") == 0) {
01108         if (expect == 1) {
01109             thee->printop[idx][thee->printnarg[idx]] = 0;
01110             (thee->printnarg[idx])++;
01111             expect = 0;
01112             if (thee->printnarg[idx] >= NOSH_MAXPOP) {
01113                 Vnm_print(2, "Nosh_parsePRINT: Exceeded max number \
01114 (%d) of arguments for PRINT section!\n",
01115                     NOSH_MAXPOP);
01116                 return 0;
01117             }
01118         } else {
01119             Vnm_print(2, "Nosh_parsePRINT: Syntax error in PRINT \
01120 section while reading %s!\n", tok);
01121             return 0;
01122         }
01123     /* Grab subtraction operation */
01124     } else if (Vstring_strcasecmp(tok, "-") == 0) {
01125         if (expect == 1) {
01126             thee->printop[idx][thee->printnarg[idx]] = 1;
01127             (thee->printnarg[idx])++;
01128             expect = 0;
01129             if (thee->printnarg[idx] >= NOSH_MAXPOP) {
01130                 Vnm_print(2, "Nosh_parseREAD: Exceeded max number \
01131 (%d) of arguments for PRINT section!\n",
01132                     NOSH_MAXPOP);
01133                 return 0;
01134             }
01135         } else {
01136             Vnm_print(2, "Nosh_parsePRINT: Syntax error in PRINT \
01137 section while reading %s!\n", tok);
01138             return 0;
01139         }
01140     /* Grab a calculation name from elec ID */
01141     } else if (sscanf(tok, "%s", name) == 1) {
01142         if (expect == 0) {
01143             for (ielec=0; ielec<thee->nelec; ielec++) {
01144                 if (Vstring_strcasecmp(thee->elecname[ielec], name) == 0) {
01145                     thee->printcalc[idx][thee->printnarg[idx]] = ielec;
01146                     expect = 1;
01147                     break;
01148                 }
01149             }
01150             for (iapol=0; iapol<thee->napol; iapol++) {
01151                 if (Vstring_strcasecmp(thee->apolname[iapol], name) == 0) {
01152                     thee->printcalc[idx][thee->printnarg[idx]] = iapol;
01153                     expect = 1;
01154                     break;
01155                 }
01156             }
01157             if (expect == 0) {
01158                 Vnm_print(2, "No ELEC or APOL statement has been named %s!\n",
01159                     name);
01160                 return 0;
01161             }
01162         } else {
01163             Vnm_print(2, "Nosh_parsePRINT: Syntax error in PRINT \
01164 section while reading %s!\n", tok);
01165             return 0;
01166         }
01167     /* Got bad operation */
01168     } else {
01169         Vnm_print(2, "Nosh_parsePRINT: Undefined keyword %s while \
01170 parsing PRINT section!\n", tok);
01171         return 0;
01172     }
01173     } /* end parse token */
01174

```

```

01175     } /* end while */
01176
01177     VJMPERR1(0);
01178
01179     /* We ran out of tokens! */
01180 VERROR1:
01181     Vnm_print(2, "Nosh_parsePRINT: Ran out of tokens while parsing PRINT \
01182 section!\n");
01183     return 0;
01184 }
01185 }
01186
01187 VPRIVATE int Nosh_parseELEC(Nosh *thee, Vio *sock) {
01188
01189     Nosh_calc *calc = VNULL;
01190
01191     char tok[VMAX_BUFSIZE];
01192
01193     if (thee == VNULL) {
01194         Vnm_print(2, "Nosh_parseELEC: Got NULL thee!\n");
01195         return 0;
01196     }
01197
01198     if (sock == VNULL) {
01199         Vnm_print(2, "Nosh_parseELEC: Got pointer to NULL socket!\n");
01200         return 0;
01201     }
01202
01203     if (thee->parsed) {
01204         Vnm_print(2, "Nosh_parseELEC: Already parsed an input file!\n");
01205         return 0;
01206     }
01207
01208     /* Get a pointer to the latest ELEC calc object and update the ELEC
01209        statement number */
01210     if (thee->nelec >= NOSH_MAXCALC) {
01211         Vnm_print(2, "Nosh: Too many electrostatics calculations in this \
01212 run!\n");
01213         Vnm_print(2, "Nosh: Current max is %d; ignoring this calculation\n",
01214                 NOSH_MAXCALC);
01215         return 1;
01216     }
01217
01218     /* The next token HAS to be the method OR "name" */
01219     if (Vio_scanf(sock, "%s", tok) == 1) {
01220         if (Vstring_strcasecmp(tok, "name") == 0) {
01221             Vio_scanf(sock, "%s", tok);
01222             strncpy(thee->elecname[thee->nelec], tok, VMAX_ARGLEN);
01223             if (Vio_scanf(sock, "%s", tok) != 1) {
01224                 Vnm_print(2, "Nosh_parseELEC: Ran out of tokens while reading \
01225 ELEC section!\n");
01226                 return 0;
01227             }
01228         }
01229         if (Vstring_strcasecmp(tok, "mg-manual") == 0) {
01230             thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_MG);
01231             calc = thee->elec[thee->nelec];
01232             (thee->nelec)++;
01233             calc->mgparm->type = MCT_MANUAL;
01234             return Nosh_parseMG(thee, sock, calc);
01235         } else if (Vstring_strcasecmp(tok, "mg-auto") == 0) {
01236             thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_MG);
01237             calc = thee->elec[thee->nelec];
01238             (thee->nelec)++;
01239             calc->mgparm->type = MCT_AUTO;
01240             return Nosh_parseMG(thee, sock, calc);
01241         } else if (Vstring_strcasecmp(tok, "mg-para") == 0) {
01242             thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_MG);
01243             calc = thee->elec[thee->nelec];
01244             (thee->nelec)++;
01245             calc->mgparm->type = MCT_PARALLEL;
01246             return Nosh_parseMG(thee, sock, calc);
01247         } else if (Vstring_strcasecmp(tok, "mg-dummy") == 0) {
01248             thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_MG);
01249             calc = thee->elec[thee->nelec];
01250             (thee->nelec)++;
01251             calc->mgparm->type = MCT_DUMMY;
01252             return Nosh_parseMG(thee, sock, calc);
01253         } else if (Vstring_strcasecmp(tok, "fe-manual") == 0) {
01254             thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_FEM);
01255             calc = thee->elec[thee->nelec];

```

```

01256         (thee->nelec)++;
01257         calc->femparm->type = FCT_MANUAL;
01258         return Nosh_parseFEM(thee, sock, calc);
01259     } else if (Vstring_strcasecmp(tok, "tabi") == 0) {
01260         thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_BEM);
01261         calc = thee->elec[thee->nelec];
01262         (thee->nelec)++;
01263         calc->bemparm->type = BCT_MANUAL;
01264         return Nosh_parseBEM(thee, sock, calc);
01265     } else if (Vstring_strcasecmp(tok, "bem") == 0) {
01266         thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_BEM);
01267         calc = thee->elec[thee->nelec];
01268         (thee->nelec)++;
01269         calc->bemparm->type = BCT_MANUAL;
01270         return Nosh_parseBEM(thee, sock, calc);
01271     } else if (Vstring_strcasecmp(tok, "bem-manual") == 0) {
01272         thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_BEM);
01273         calc = thee->elec[thee->nelec];
01274         (thee->nelec)++;
01275         calc->bemparm->type = BCT_MANUAL;
01276         return Nosh_parseBEM(thee, sock, calc);
01277     } else if (Vstring_strcasecmp(tok, "geoflow-manual") == 0) {
01278         Vnm_print(2, "Geoflow currently does not support geoflow-manual please use geoflow instead!\n");
01279         return 0;
01280     } else if (Vstring_strcasecmp(tok, "geoflow-none") == 0) {
01281         Vnm_print(2, "Geoflow currently does not support geoflow-none please use geoflow instead!\n");
01282         return 0;
01283     } else if (Vstring_strcasecmp(tok, "geoflow") == 0) {
01284         thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_GEOFLOW);
01285         calc = thee->elec[thee->nelec];
01286         (thee->nelec)++;
01287         calc->geoflowparm->type = GFCT_AUTO;
01288         return Nosh_parseGEOFLOW(thee, sock, calc);
01289     } else if (Vstring_strcasecmp(tok, "pbam") == 0) {
01290         thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_PBAM);
01291         calc = thee->elec[thee->nelec];
01292         (thee->nelec)++;
01293         calc->pbamparm->type = PBAMCT_AUTO;
01294         return Nosh_parsePBAM(thee, sock, calc);
01295     } else if (Vstring_strcasecmp(tok, "pbsam") == 0) {
01296         thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_PBSAM);
01297         calc = thee->elec[thee->nelec];
01298         (thee->nelec)++;
01299         calc->pbsamparm->type = PBSAMCT_AUTO;
01300         return Nosh_parsePBSAM(thee, sock, calc);
01301     } else {
01302         Vnm_print(2, "Nosh_parseELEC: The method (\\"mg\\", \\"fem\\", \\"bem\\", \\"geoflow\\", \\"pbam\\",
01303         \\"pbsam\\") or \\"name\\" must be the first keyword in the ELEC section\n");
01304         return 0;
01305     }
01306 }
01307
01308 Vnm_print(2, "Nosh_parseELEC: Ran out of tokens while reading ELEC section!\n");
01309 return 0;
01310
01311 }
01312
01313 VPRIVATE int Nosh_parseAPOLAR(Nosh *thee, Vio *sock) {
01314
01315     Nosh_calc *calc = VNULL;
01316
01317     char tok[VMAX_BUFSIZE];
01318
01319     if (thee == VNULL) {
01320         Vnm_print(2, "Nosh_parseAPOLAR: Got NULL thee!\n");
01321         return 0;
01322     }
01323
01324     if (sock == VNULL) {
01325         Vnm_print(2, "Nosh_parseAPOLAR: Got pointer to NULL socket!\n");
01326         return 0;
01327     }
01328
01329     if (thee->parsed) {
01330         Vnm_print(2, "Nosh_parseAPOLAR: Already parsed an input file!\n");
01331         return 0;
01332     }
01333
01334     /* Get a pointer to the latest ELEC calc object and update the ELEC
01335     statement number */

```

```

01336     if (thee->napol >= NOSH_MAXCALC) {
01337         Vnm_print(2, "Nosh: Too many non-polar calculations in this \
01338 run!\n");
01339         Vnm_print(2, "Nosh: Current max is %d; ignoring this calculation\n",
01340                 NOSH_MAXCALC);
01341         return 1;
01342     }
01343
01344     /* The next token HAS to be the method OR "name" */
01345     if (Vio_scanf(sock, "%s", tok) == 1) {
01346         if (Vstring_strcasecmp(tok, "name") == 0) {
01347             Vio_scanf(sock, "%s", tok);
01348             strncpy(thee->apolname[thee->napol], tok, VMAX_ARGLEN);
01349
01350             /* Parse the non-polar parameters */
01351             thee->apol[thee->napol] = Nosh_calc_ctor(NCT_APOL);
01352             calc = thee->apol[thee->napol];
01353             (thee->napol)++;
01354             return Nosh_parseAPOL(thee, sock, calc);
01355         } else if (Vstring_strcasecmp(tok, "geoflow-manual") == 0) {
01356             thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_GEOFLOW);
01357             calc = thee->elec[thee->nelec];
01358             (thee->nelec)++;
01359             calc->geoflowparm->type = GFCT_MANUAL;
01360             return Nosh_parseGEOFLOW(thee, sock, calc);
01361         } else if (Vstring_strcasecmp(tok, "geoflow-auto") == 0) {
01362             thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_GEOFLOW);
01363             calc = thee->elec[thee->nelec];
01364             (thee->nelec)++;
01365             calc->geoflowparm->type = GFCT_AUTO;
01366             return Nosh_parseGEOFLOW(thee, sock, calc);
01367         }
01368     }
01369
01370     return 1;
01371 }
01372 }
01373
01374 VPUBLIC int Nosh_setupElecCalc(
01375     Nosh *thee,
01376     Valist *alist[NOSH_MAXMOL]
01377 ) {
01378     int ielec, imol, i;
01379     Nosh_calc *elec = VNULL;
01380     MGparm *mgparm = VNULL;
01381     Valist *mymol = VNULL;
01382
01383     VASSERT(thee != VNULL);
01384     for (imol=0; imol<thee->nmol; imol++) {
01385         thee->alist[imol] = alist[imol];
01386     }
01387
01388     for (ielec=0; ielec<(thee->nelec); ielec++) {
01389         /* Unload the calculation object containing the ELEC information */
01390         elec = thee->elec[ielec];
01391
01392         if (((thee->ndiel != 0) || (thee->nkappa != 0) ||
01393             (thee->ncharge != 0) || (thee->npot != 0)) &&
01394             (elec->pbeparm->calcforce != PCF_NO)) {
01395             Vnm_print(2, "Nosh_setupElecCalc: Calculation of forces disabled because surface \
01396 map is used!\n");
01397             elec->pbeparm->calcforce = PCF_NO;
01398         }
01399     }
01400
01401     /* Setup the calculation */
01402     switch (elec->calctype) {
01403     case NCT_MG:
01404         /* Center on the molecules, if requested */
01405         mgparm = elec->mgparm;
01406         VASSERT(mgparm != VNULL);
01407         if (elec->mgparm->cmeth == MCM_MOLECULE) {
01408             VASSERT(mgparm->centmol >= 0);
01409             VASSERT(mgparm->centmol < thee->nmol);
01410             mymol = thee->alist[mgparm->centmol];
01411             VASSERT(mymol != VNULL);
01412             for (i=0; i<3; i++) {
01413                 mgparm->center[i] = mymol->center[i];
01414             }
01415         }
01416         if (elec->mgparm->fcmeth == MCM_MOLECULE) {

```

```

01417         VASSERT(mgparm->fcentmol >= 0);
01418         VASSERT(mgparm->fcentmol < thee->nmol);
01419         mymol = thee->alist[mgparm->fcentmol];
01420         VASSERT(mymol != VNULL);
01421         for (i=0; i<3; i++) {
01422             mgparm->fcenter[i] = mymol->center[i];
01423         }
01424     }
01425     if (elec->mgparm->ccmeth == MCM_MOLECULE) {
01426         VASSERT(mgparm->ccentmol >= 0);
01427         VASSERT(mgparm->ccentmol < thee->nmol);
01428         mymol = thee->alist[mgparm->ccentmol];
01429         VASSERT(mymol != VNULL);
01430         for (i=0; i<3; i++) {
01431             mgparm->ccenter[i] = mymol->center[i];
01432         }
01433     }
01434     Nosh_setupCalcMG(thee, elec);
01435     break;
01436 case NCT_FEM:
01437     Nosh_setupCalcFEM(thee, elec);
01438     break;
01439 case NCT_PBAM:
01440     Nosh_setupCalcPBAM(thee, elec);
01441     break;
01442 case NCT_PBSAM:
01443     Nosh_setupCalcPBSAM(thee, elec);
01444     break;
01445 case NCT_BEM:
01446     Nosh_setupCalcBEM(thee, elec);
01447     break;
01448 case NCT_GEOFLOW:
01449     Nosh_setupCalcGEOFLOW(thee, elec);
01450     break;
01451 default:
01452     Vnm_print(2, "Nosh_setupCalc: Invalid calculation type (%d)!\n",
01453             elec->calctype);
01454     return 0;
01455 }
01456
01457 /* At this point, the most recently-created Nosh_calc object should be the
01458    one we use for results for this ELEC statement. Assign it. */
01459 /* Associate ELEC statement with the calculation */
01460 thee->elec2calc[ielec] = thee->ncalc-1;
01461 Vnm_print(0, "Nosh_setupCalc: Mapping ELEC statement %d (%d) to \
01462 calculation %d (%d)\n", ielec, ielec+1, thee->elec2calc[ielec],
01463             thee->elec2calc[ielec]+1);
01464 }
01465
01466 return 1;
01467 }
01468
01469 VPUBLIC int Nosh_setupApolCalc(
01470     Nosh *thee,
01471     Valist *alist[NOSH_MAXMOL]
01472 ) {
01473     int iapol, imol;
01474     int doCalc = ACD_NO;
01475     Nosh_calc *calc = VNULL;
01476
01477     VASSERT(thee != VNULL);
01478     for (imol=0; imol<thee->nmol; imol++) {
01479         thee->alist[imol] = alist[imol];
01480     }
01481
01482     for (iapol=0; iapol<(thee->napol); iapol++) {
01483         /* Unload the calculation object containing the APOL information */
01484         calc = thee->apol[iapol];
01485
01486         /* Setup the calculation */
01487         switch (calc->calctype) {
01488             case NCT_APOL:
01489                 Nosh_setupCalcAPOL(thee, calc);
01490                 doCalc = ACD_YES;
01491                 break;
01492             default:
01493                 Vnm_print(2, "Nosh_setupCalc: Invalid calculation type (%d)!\n", calc->calctype);
01494                 return ACD_ERROR;
01495         }
01496
01497         /* At this point, the most recently-created Nosh_calc object should be the
01498            one we use for results for this APOL statement. Assign it. */

```



```

01498     /* Associate APOL statement with the calculation */
01499     thee->apol2calc[iapol] = thee->ncalc-1;
01500     Vnm_print(0, "Nosh_setupCalc: Mapping APOL statement %d (%d) to calculation %d (%d)\n", iapol,
iapol+1, thee->apol2calc[iapol], thee->apol2calc[iapol]+1);
01501 }
01502
01503     if(doCalc == ACD_YES){
01504         return ACD_YES;
01505     }else{
01506         return ACD_NO;
01507     }
01508 }
01509
01510 VPUBLIC int Nosh_parseMG(
01511     NOsh *thee,
01512     Vio *sock,
01513     NOsh_calc *elec
01514 ) {
01515
01516     char tok[VMAX_BUFSIZE];
01517     MGparm *mgparm = VNULL;
01518     PBEparm *pbeparm = VNULL;
01519     int rc;
01520
01521     /* Check the arguments */
01522     if (thee == VNULL) {
01523         Vnm_print(2, "Nosh: Got NULL thee!\n");
01524         return 0;
01525     }
01526     if (sock == VNULL) {
01527         Vnm_print(2, "Nosh: Got pointer to NULL socket!\n");
01528         return 0;
01529     }
01530     if (elec == VNULL) {
01531         Vnm_print(2, "Nosh: Got pointer to NULL elec object!\n");
01532         return 0;
01533     }
01534     mgparm = elec->mgparm;
01535     if (mgparm == VNULL) {
01536         Vnm_print(2, "Nosh: Got pointer to NULL mgparm object!\n");
01537         return 0;
01538     }
01539     pbeparm = elec->pbeparm;
01540     if (pbeparm == VNULL) {
01541         Vnm_print(2, "Nosh: Got pointer to NULL pbeparm object!\n");
01542         return 0;
01543     }
01544
01545     Vnm_print(0, "Nosh_parseMG: Parsing parameters for MG calculation\n");
01546
01547     /* Parallel stuff */
01548     if (mgparm->type == MCT_PARALLEL) {
01549         mgparm->proc_rank = thee->proc_rank;
01550         mgparm->proc_size = thee->proc_size;
01551         mgparm->setrank = 1;
01552         mgparm->setsize = 1;
01553     }
01554
01555     /* Start snarfing tokens from the input stream */
01556     rc = 1;
01557     while (Vio_scanf(sock, "%s", tok) == 1) {
01558
01559         Vnm_print(0, "Nosh_parseMG: Parsing %s...\n", tok);
01560
01561         /* See if it's an END token */
01562         if (Vstring_strcasecmp(tok, "end") == 0) {
01563             mgparm->parsed = 1;
01564             pbeparm->parsed = 1;
01565             rc = 1;
01566             break;
01567         }
01568     }
01569
01570     /* Pass the token through a series of parsers */
01571     rc = PBEparm_parseToken(pbeparm, tok, sock);
01572     if (rc == -1) {
01573         Vnm_print(0, "Nosh_parseMG: parsePBE error!\n");
01574         break;
01575     } else if (rc == 0) {
01576         /* Pass the token to the generic MG parser */
01577         rc = MGparm_parseToken(mgparm, tok, sock);

```

```

01578         if (rc == -1) {
01579             Vnm_print(0, "Nosh_parseMG: parseMG error!\n");
01580             break;
01581         } else if (rc == 0) {
01582             /* We ran out of parsers! */
01583             Vnm_print(2, "Nosh: Unrecognized keyword: %s\n", tok);
01584             break;
01585         }
01586     }
01587 }
01588
01589 /* Handle various errors arising in the token-snarfing loop -- these all
01590    just result in simple returns right now */
01591 if (rc == -1) return 0;
01592 if (rc == 0) return 0;
01593
01594 /* Check the status of the parameter objects */
01595 if ((MGparm_check(mgparm) == VRC_FAILURE) || (!PBEParm_check(pbeparm))) {
01596     Vnm_print(2, "Nosh: MG parameters not set correctly!\n");
01597     return 0;
01598 }
01599
01600 return 1;
01601 }
01602
01603 VPRIVATE int Nosh_setupCalcMG(
01604     Nosh *thee,
01605     Nosh_calc *calc
01606 ) {
01607
01608     MGparm *mgparm = VNULL;
01609
01610     VASSERT(thee != VNULL);
01611     VASSERT(calc != VNULL);
01612     mgparm = calc->mgparm;
01613     VASSERT(mgparm != VNULL);
01614
01615     /* Now we're ready to whatever sorts of post-processing operations that are
01616        necessary for the various types of calculations */
01617     switch (mgparm->type) {
01618     case MCT_MANUAL:
01619         return Nosh_setupCalcMGMANUAL(thee, calc);
01620     case MCT_DUMMY:
01621         return Nosh_setupCalcMGMANUAL(thee, calc);
01622     case MCT_AUTO:
01623         return Nosh_setupCalcMGAUTO(thee, calc);
01624     case MCT_PARALLEL:
01625         return Nosh_setupCalcMGPARA(thee, calc);
01626     default:
01627         Vnm_print(2, "Nosh_setupCalcMG: undefined MG calculation type (%d)!\n",
01628             mgparm->type);
01629         return 0;
01630     }
01631 }
01632
01633 /* Shouldn't get here */
01634 return 0;
01635 }
01636
01637 VPRIVATE int Nosh_setupCalcBEM(
01638     Nosh *thee,
01639     Nosh_calc *calc
01640 ) {
01641
01642     BEMparm *bemparm = VNULL;
01643
01644     VASSERT(thee != VNULL);
01645     VASSERT(calc != VNULL);
01646     bemparm = calc->bemparm;
01647     VASSERT(bemparm != VNULL);
01648
01649     /* Now we're ready to whatever sorts of post-processing operations that are
01650        necessary for the various types of calculations */
01651     switch (bemparm->type) {
01652     case BCT_MANUAL:
01653         return Nosh_setupCalcBEMMANUAL(thee, calc);
01654     default:
01655         Vnm_print(2, "Nosh_setupCalcBEM: undefined BEM calculation type (%d)!\n",
01656             bemparm->type);
01657     }
01658 }

```

```

01659         return 0;
01660     }
01661
01662     /* Shouldn't get here */
01663     return 0;
01664 }
01665
01666 VPRIVATE int Nosh_setupCalcGEOFLOW(NOsh *thee, NOsh_calc *calc) {
01667     GEOFLOWparm *parm = VNULL;
01668
01669     VASSERT(thee != VNULL);
01670     VASSERT(calc != VNULL);
01671     parm = calc->geoflowparm;
01672     VASSERT(parm != VNULL);
01673
01674
01675
01676     /* Now we're ready to whatever sorts of post-processing operations that are
01677      * necessary for the various types of calculations */
01678     if ((*parm->type == GFCT_MANUAL || *parm->type == GFCT_AUTO) {
01679         return Nosh_setupCalcGEOFLOWMANUAL(thee, calc);
01680     } else {
01681         Vnm_print(2, "Nosh_setupCalcGEOFLOW: undefined GEOFLOW calculation type (%d)!\n", parm->type);
01682         return 0;
01683     }
01684 }
01685
01686 VPRIVATE int Nosh_setupCalcPBAM(NOsh *thee, NOsh_calc *calc) {
01687     PBAMparm *parm = VNULL;
01688
01689     VASSERT(thee != VNULL);
01690     VASSERT(calc != VNULL);
01691     parm = calc->pbamparm;
01692     VASSERT(parm != VNULL);
01693
01694
01695     if (parm->type == PBAMCT_AUTO) {
01696         return Nosh_setupCalcPBAM_AUTO(thee, calc);
01697     } else {
01698         Vnm_print(2, "Nosh_setupCalcPBAM: undefined PBAM calculation type (%d)!\n", parm->type);
01699         return 0;
01700     }
01701 }
01702
01703
01704 VPRIVATE int Nosh_setupCalcPBSAM(NOsh *thee, NOsh_calc *calc) {
01705     PBSAMparm *parm = VNULL;
01706
01707     VASSERT(thee != VNULL);
01708     VASSERT(calc != VNULL);
01709     parm = calc->pbsamparm;
01710     VASSERT(parm != VNULL);
01711
01712
01713     if (parm->type == PBSAMCT_AUTO) {
01714         return Nosh_setupCalcPBSAM_AUTO(thee, calc);
01715     } else {
01716         Vnm_print(2, "Nosh_setupCalcPBSAM: undefined PBSAM calculation type (%d)!\n", parm->type);
01717         return 0;
01718     }
01719 }
01720
01721
01722 VPRIVATE int Nosh_setupCalcFEM(
01723     NOsh *thee,
01724     NOsh_calc *calc
01725 ) {
01726
01727     VASSERT(thee != VNULL);
01728     VASSERT(calc != VNULL);
01729     VASSERT(calc->femparm != VNULL);
01730
01731
01732     /* Now we're ready to whatever sorts of post-processing operations that are
01733      * necessary for the various types of calculations */
01734     switch (calc->femparm->type) {
01735     case FCT_MANUAL:
01736         return Nosh_setupCalcFEMANUAL(thee, calc);
01737     default:
01738         Vnm_print(2, "Nosh_parseFEM: unknown calculation type (%d)!\n",
01739             calc->femparm->type);
01740         return 0;
01741     }
01742 }

```

```

01740     }
01741
01742     /* Shouldn't get here */
01743     return 0;
01744 }
01745
01746
01747 VPRIVATE int NOsh_setupCalcMGMANUAL(
01748     NOsh *thee,
01749     NOsh_calc *elec
01750 ) {
01751
01752     MGparm *mgparm = VNULL;
01753     PBEParm *pbeparm = VNULL;
01754     NOsh_calc *calc = VNULL;
01755
01756     if (thee == VNULL) {
01757         Vnm_print(2, "NOsh_setupCalcMGMANUAL: Got NULL thee!\n");
01758         return 0;
01759     }
01760     if (elec == VNULL) {
01761         Vnm_print(2, "NOsh_setupCalcMGMANUAL: Got NULL calc!\n");
01762         return 0;
01763     }
01764     mgparm = elec->mgparm;
01765     if (mgparm == VNULL) {
01766         Vnm_print(2, "NOsh_setupCalcMGMANUAL: Got NULL mgparm -- was this calculation \
01767 set up?\n");
01768         return 0;
01769     }
01770     pbeparm = elec->pbeparm;
01771     if (pbeparm == VNULL) {
01772         Vnm_print(2, "NOsh_setupCalcMGMANUAL: Got NULL pbeparm -- was this calculation \
01773 set up?\n");
01774         return 0;
01775     }
01776
01777     /* Set up missing MG parameters */
01778     if (mgparm->setgrid == 0) {
01779         VASSERT(mgparm->setglen);
01780         mgparm->grid[0] = mgparm->glen[0]/((double) (mgparm->dime[0]-1));
01781         mgparm->grid[1] = mgparm->glen[1]/((double) (mgparm->dime[1]-1));
01782         mgparm->grid[2] = mgparm->glen[2]/((double) (mgparm->dime[2]-1));
01783     }
01784     if (mgparm->setglen == 0) {
01785         VASSERT(mgparm->setgrid);
01786         mgparm->glen[0] = mgparm->grid[0]*((double) (mgparm->dime[0]-1));
01787         mgparm->glen[1] = mgparm->grid[1]*((double) (mgparm->dime[1]-1));
01788         mgparm->glen[2] = mgparm->grid[2]*((double) (mgparm->dime[2]-1));
01789     }
01790
01791     /* Check to see if he have any room left for this type of calculation, if
01792        so: set the calculation type, update the number of calculations of this type,
01793        and parse the rest of the section */
01794     if (thee->ncalc >= NOSH_MAXCALC) {
01795         Vnm_print(2, "NOsh: Too many calculations in this run!\n");
01796         Vnm_print(2, "NOsh: Current max is %d; ignoring this calculation\n",
01797             NOSH_MAXCALC);
01798         return 0;
01799     }
01800
01801     /* Get the next calculation object and increment the number of calculations */
01802     thee->calc[thee->ncalc] = NOsh_calc_ctor(NCT_MG);
01803     calc = thee->calc[thee->ncalc];
01804     (thee->ncalc)++;
01805
01806
01807     /* Copy over contents of ELEC */
01808     NOsh_calc_copy(calc, elec);
01809
01810
01811     return 1;
01812 }
01813
01814
01815 VPUBLIC int NOsh_setupCalcMGAUTO(
01816     NOsh *thee,
01817     NOsh_calc *elec
01818 ) {
01819
01820     NOsh_calc *calcf = VNULL;

```

```

01821     NOsh_calc *calcc = VNULL;
01822     double fgrid[3], cgrid[3];
01823     double d[3], minf[3], maxf[3], minc[3], maxc[3];
01824     double redfrac, redrat[3], td;
01825     int ifocus, nfocus, tnfocus[3];
01826     int j;
01827     int icalc;
01828     int dofif;
01829
01830     /* A comment about the coding style in this function. I use lots and lots
01831        and lots of pointer deferencing. I could (and probably should) save
01832        these in temporary variables. However, since there are so many MGparm,
01833        etc. and NOsh_calc, etc. objects running around in this function, the
01834        current scheme is easiest to debug. */
01835
01836
01837     if (thee == VNULL) {
01838         Vnm_print(2, "NOsh_setupCalcMGAUTO: Got NULL thee!\n");
01839         return 0;
01840     }
01841     if (elec == VNULL) {
01842         Vnm_print(2, "NOsh_setupCalcMGAUTO: Got NULL elec!\n");
01843         return 0;
01844     }
01845     if (elec->mgparm == VNULL) {
01846         Vnm_print(2, "NOsh_setupCalcMGAUTO: Got NULL mgparm!\n");
01847         return 0;
01848     }
01849     if (elec->pbeparm == VNULL) {
01850         Vnm_print(2, "NOsh_setupCalcMGAUTO: Got NULL pbeparm!\n");
01851         return 0;
01852     }
01853
01854     Vnm_print(0, "NOsh_setupCalcMGAUTO(%s, %d): coarse grid center = %g %g %g\n",
01855         __FILE__, __LINE__,
01856         elec->mgparm->ccenter[0],
01857         elec->mgparm->ccenter[1],
01858         elec->mgparm->ccenter[2]);
01859     Vnm_print(0, "NOsh_setupCalcMGAUTO(%s, %d): fine grid center = %g %g %g\n",
01860         __FILE__, __LINE__,
01861         elec->mgparm->fcenter[0],
01862         elec->mgparm->fcenter[1],
01863         elec->mgparm->fcenter[2]);
01864
01865     /* Calculate the grid spacing on the coarse and fine levels */
01866     for (j=0; j<3; j++) {
01867         cgrid[j] = (elec->mgparm->cglen[j])/((double)(elec->mgparm->dime[j]-1));
01868         fgrid[j] = (elec->mgparm->fglen[j])/((double)(elec->mgparm->dime[j]-1));
01869         d[j] = elec->mgparm->fcenter[j] - elec->mgparm->ccenter[j];
01870     }
01871     Vnm_print(0, "NOsh_setupCalcMGAUTO (%s, %d): Coarse grid spacing = %g, %g, %g\n",
01872         __FILE__, __LINE__, cgrid[0], cgrid[1], cgrid[2]);
01873     Vnm_print(0, "NOsh_setupCalcMGAUTO (%s, %d): Fine grid spacing = %g, %g, %g\n",
01874         __FILE__, __LINE__, fgrid[0], fgrid[1], fgrid[2]);
01875     Vnm_print(0, "NOsh_setupCalcMGAUTO (%s, %d): Displacement between fine and \
01876 coarse grids = %g, %g, %g\n", __FILE__, __LINE__, d[0], d[1], d[2]);
01877
01878     /* Now calculate the number of focusing levels, never reducing the grid
01879        spacing by more than redfrac at each level */
01880     for (j=0; j<3; j++) {
01881         if (fgrid[j]/cgrid[j] < VREDFRAC) {
01882             redfrac = fgrid[j]/cgrid[j];
01883             td = log(redfrac)/log(VREDFRAC);
01884             tnfocus[j] = (int)ceil(td) + 1;
01885         } else tnfocus[j] = 2;
01886     }
01887     nfocus = VMAX2(VMAX2(tnfocus[0], tnfocus[1]), tnfocus[2]);
01888
01889     /* Now set redrat to the actual value by which the grid spacing is reduced
01890        at each level of focusing */
01891     for (j=0; j<3; j++) {
01892         redrat[j] = VPOW((fgrid[j]/cgrid[j]), 1.0/((double)nfocus-1.0));
01893     }
01894     Vnm_print(0, "NOsh: %d levels of focusing with %g, %g, %g reductions\n",
01895         nfocus, redrat[0], redrat[1], redrat[2]);
01896
01897     /* Now that we know how many focusing levels to use, we're ready to set up
01898        the parameter objects */
01899     if (nfocus > (NOSH_MAXCALC-(thee->ncalc))) {
01900         Vnm_print(2, "NOsh: Require more calculations than max (%d)!\n",
01901             NOSH_MAXCALC);
01902     }

```

```

01902     return 0;
01903 }
01904
01905 for (ifocus=0; ifocus<nfocus; ifocus++) {
01906
01907     /* Generate the new calc object */
01908     icalc = thee->ncalc;
01909     thee->calc[icalc] = NOsh_calc_ctor(NCT_MG);
01910     (thee->ncalc)++;
01911
01912     /* This is the _current_ NOsh_calc object */
01913     calcf = thee->calc[icalc];
01914     /* This is the _previous_ Nosh_calc object */
01915     if (ifocus != 0) {
01916         calcc = thee->calc[icalc-1];
01917     } else {
01918         calcc = VNULL;
01919     }
01920
01921     /* Copy over most of the parameters from the ELEC object */
01922     NOsh_calc_copy(calcf, elec);
01923
01924     /* Set up the grid lengths and spacings */
01925     if (ifocus == 0) {
01926         for (j=0; j<3; j++) {
01927             calcf->mgparm->grid[j] = cgrid[j];
01928             calcf->mgparm->glen[j] = elec->mgparm->cglen[j];
01929         }
01930     } else {
01931         for (j=0; j<3; j++) {
01932             calcf->mgparm->grid[j] = reidrat[j]*(calcc->mgparm->grid[j]);
01933             calcf->mgparm->glen[j] = reidrat[j]*(calcc->mgparm->glen[j]);
01934         }
01935     }
01936     calcf->mgparm->setgrid = 1;
01937     calcf->mgparm->setglen = 1;
01938
01939     /* Get centers and centering method from coarse and fine meshes */
01940     if (ifocus == 0) {
01941         calcf->mgparm->cmeth = elec->mgparm->ccmeth;
01942         calcf->mgparm->centmol = elec->mgparm->ccentmol;
01943         for (j=0; j<3; j++) {
01944             calcf->mgparm->center[j] = elec->mgparm->ccenter[j];
01945         }
01946     } else if (ifocus == (nfocus-1)) {
01947         calcf->mgparm->cmeth = elec->mgparm->fcmeth;
01948         calcf->mgparm->centmol = elec->mgparm->fcentmol;
01949         for (j=0; j<3; j++) {
01950             calcf->mgparm->center[j] = elec->mgparm->fcenter[j];
01951         }
01952     } else {
01953         calcf->mgparm->cmeth = MCM_FOCUS;
01954         /* TEMPORARILY move the current grid center
01955         to the fine grid center. In general, this will move portions of
01956         the current mesh off the immediately-coarser mesh. We'll fix that
01957         in the next step. */
01958         for (j=0; j<3; j++) {
01959             calcf->mgparm->center[j] = elec->mgparm->fcenter[j];
01960         }
01961     }
01962
01963     /* As mentioned above, it is highly likely that the previous "jump"
01964     to the fine grid center put portions of the current mesh off the
01965     previous (coarser) mesh. Fix this by displacing the current mesh
01966     back onto the previous coarser mesh. */
01967     if (ifocus != 0) {
01968         Vnm_print(0, "NOsh_setupCalcMGAUTO (%s, %d): starting mesh \
01969 repositioning.\n", __FILE__, __LINE__);
01970         Vnm_print(0, "NOsh_setupCalcMGAUTO (%s, %d): coarse mesh center = \
01971 %g %g %g\n", __FILE__, __LINE__,
01972             calcc->mgparm->center[0],
01973             calcc->mgparm->center[1],
01974             calcc->mgparm->center[2]);
01975         Vnm_print(0, "NOsh_setupCalcMGAUTO (%s, %d): coarse mesh upper corner = \
01976 %g %g %g\n", __FILE__, __LINE__,
01977             calcc->mgparm->center[0]+0.5*(calcc->mgparm->glen[0]),
01978             calcc->mgparm->center[1]+0.5*(calcc->mgparm->glen[1]),
01979             calcc->mgparm->center[2]+0.5*(calcc->mgparm->glen[2]));
01980         Vnm_print(0, "NOsh_setupCalcMGAUTO (%s, %d): coarse mesh lower corner = \
01981 %g %g %g\n", __FILE__, __LINE__,

```

```

01983         calcc->mgparm->center[0]-0.5*(calcc->mgparm->glen[0]),
01984         calcc->mgparm->center[1]-0.5*(calcc->mgparm->glen[1]),
01985         calcc->mgparm->center[2]-0.5*(calcc->mgparm->glen[2]));
01986     Vnm_print(0, "Nosh_setupCalcMGAUTO (%s, %d):  initial fine mesh upper corner = \
01987 %g %g %g\n", __FILE__, __LINE__,
01988         calcf->mgparm->center[0]+0.5*(calcf->mgparm->glen[0]),
01989         calcf->mgparm->center[1]+0.5*(calcf->mgparm->glen[1]),
01990         calcf->mgparm->center[2]+0.5*(calcf->mgparm->glen[2]));
01991     Vnm_print(0, "Nosh_setupCalcMGAUTO (%s, %d):  initial fine mesh lower corner = \
01992 %g %g %g\n", __FILE__, __LINE__,
01993         calcf->mgparm->center[0]-0.5*(calcf->mgparm->glen[0]),
01994         calcf->mgparm->center[1]-0.5*(calcf->mgparm->glen[1]),
01995         calcf->mgparm->center[2]-0.5*(calcf->mgparm->glen[2]));
01996     for (j=0; j<3; j++) {
01997         /* Check if we've fallen off of the lower end of the mesh */
01998         dofix = 0;
01999         minf[j] = calcf->mgparm->center[j]
02000             - 0.5*(calcf->mgparm->glen[j]);
02001         minc[j] = calcc->mgparm->center[j]
02002             - 0.5*(calcc->mgparm->glen[j]);
02003         d[j] = minc[j] - minf[j];
02004         if (d[j] >= VSMALL) {
02005             if (ifocus == (nfocus-1)) {
02006                 Vnm_print(2, "Nosh_setupCalcMGAUTO:  Error!  Finest \
02007 mesh has fallen off the coarser meshes!\n");
02008                 Vnm_print(2, "Nosh_setupCalcMGAUTO:  difference in min %d-\
02009 direction = %g\n", j, d[j]);
02010                 Vnm_print(2, "Nosh_setupCalcMGAUTO:  min fine = %g %g %g\n",
02011                     minf[0], minf[1], minf[2]);
02012                 Vnm_print(2, "Nosh_setupCalcMGAUTO:  min coarse = %g %g %g\n",
02013                     minc[0], minc[1], minc[2]);
02014                 VASSERT(0);
02015             } else {
02016                 Vnm_print(0, "Nosh_setupCalcMGAUTO (%s, %d):  ifocus = %d, \
02017 fixing mesh min violation (%g in %d-direction).\n", __FILE__, __LINE__, ifocus,
02018                     d[j], j);
02019                 calcf->mgparm->center[j] += d[j];
02020                 dofix = 1;
02021             }
02022         }
02023         /* Check if we've fallen off of the upper end of the mesh */
02024         maxf[j] = calcf->mgparm->center[j] \
02025             + 0.5*(calcf->mgparm->glen[j]);
02026         maxc[j] = calcc->mgparm->center[j] \
02027             + 0.5*(calcc->mgparm->glen[j]);
02028         d[j] = maxf[j] - maxc[j];
02029         if (d[j] >= VSMALL) {
02030             if (ifocus == (nfocus-1)) {
02031                 Vnm_print(2, "Nosh_setupCalcMGAUTO:  Error!  Finest \
02032 mesh has fallen off the coarser meshes!\n");
02033                 Vnm_print(2, "Nosh_setupCalcMGAUTO:  difference in %d-\
02034 direction = %g\n", j, d[j]);
02035                 VASSERT(0);
02036             } else {
02037                 /* If we already fixed the lower boundary and we now need
02038 to fix the upper boundary, we have a serious problem. */
02039                 if (dofix) {
02040                     Vnm_print(2, "Nosh_setupCalcMGAUTO:  Error!  Both \
02041 ends of the finer mesh do not fit in the bigger mesh!\n");
02042                     VASSERT(0);
02043                 }
02044                 Vnm_print(0, "Nosh_setupCalcMGAUTO(%s, %d):  ifocus = %d, \
02045 fixing mesh max violation (%g in %d-direction).\n", __FILE__, __LINE__, ifocus,
02046                     d[j], j);
02047                 calcf->mgparm->center[j] -= d[j];
02048                 dofix = 1;
02049             }
02050         }
02051     }
02052     Vnm_print(0, "Nosh_setupCalcMGAUTO (%s, %d):  final fine mesh upper corner = \
02053 %g %g %g\n", __FILE__, __LINE__,
02054         calcf->mgparm->center[0]+0.5*(calcf->mgparm->glen[0]),
02055         calcf->mgparm->center[1]+0.5*(calcf->mgparm->glen[1]),
02056         calcf->mgparm->center[2]+0.5*(calcf->mgparm->glen[2]));
02057     Vnm_print(0, "Nosh_setupCalcMGAUTO (%s, %d):  final fine mesh lower corner = \
02058 %g %g %g\n", __FILE__, __LINE__,
02059         calcf->mgparm->center[0]-0.5*(calcf->mgparm->glen[0]),
02060         calcf->mgparm->center[1]-0.5*(calcf->mgparm->glen[1]),
02061         calcf->mgparm->center[2]-0.5*(calcf->mgparm->glen[2]));
02062 }
02063

```

```

02064      /* finer levels have focusing boundary conditions */
02065      if (ifocus != 0) calcf->pbeparm->bcfl = BCFL_FOCUS;
02066
02067      /* Only the finest level handles I/O and needs to worry about disjoint
02068         partitioning */
02069      if (ifocus != (nfocus-1)) calcf->pbeparm->numwrite = 0;
02070
02071      /* Reset boundary flags for everything except parallel focusing */
02072      if (calcf->mgparm->type != MCT_PARALLEL) {
02073          Vnm_print(0, "Nosh_setupMGAUTO: Resetting boundary flags\n");
02074          for (j=0; j<6; j++) calcf->mgparm->partDisjOwnSide[j] = 0;
02075          for (j=0; j<3; j++) {
02076              calcf->mgparm->partDisjCenter[j] = 0;
02077              calcf->mgparm->partDisjLength[j] = calcf->mgparm->glen[j];
02078          }
02079      }
02080
02081
02082      calcf->mgparm->parsed = 1;
02083  }
02084
02085
02086      return 1;
02087 }
02088
02089 /* Author:  Nathan Baker and Todd Dolinsky */
02090 VPUBLIC int Nosh_setupCalcMGPARA(
02091     Nosh *thee,
02092     Nosh_calc *elec
02093 ) {
02094
02095     /* NEW (25-Jul-2006): This code should produce modify the ELEC statement
02096        and pass it on to MGAUTO for further processing. */
02097
02098     MGparm *mgparm = VNULL;
02099     double ofrac;
02100     double hx, hy, hzed;
02101     double xofrac, yofrac, zofrac;
02102     int rank, size, npx, npy, npz, nproc, ip, jp, kp;
02103     int xeffGlob, yeffGlob, zeffGlob, xDisj, yDisj, zDisj;
02104     int xigminDisj, xigmaxDisj, yigminDisj, yigmaxDisj, zigminDisj, zigmaxDisj;
02105     int xigminOlap, xigmaxOlap, yigminOlap, yigmaxOlap, zigminOlap, zigmaxOlap;
02106     int xOlapReg, yOlapReg, zOlapReg;
02107     double xlenDisj, ylenDisj, zlenDisj;
02108     double xcentDisj, ycentDisj, zcentDisj;
02109     double xcentOlap, ycentOlap, zcentOlap;
02110     double xlenOlap, ylenOlap, zlenOlap;
02111     double xminOlap, xmaxOlap, yminOlap, ymaxOlap, zminOlap, zmaxOlap;
02112     double xminDisj, xmaxDisj, yminDisj, ymaxDisj, zminDisj, zmaxDisj;
02113     double xcent, ycent, zcent;
02114
02115     /* Grab some useful variables */
02116     VASSERT(thee != VNULL);
02117     VASSERT(elec != VNULL);
02118     mgparm = elec->mgparm;
02119     VASSERT(mgparm != VNULL);
02120
02121     /* Grab some useful variables */
02122     ofrac = mgparm->ofrac;
02123     npx = mgparm->pdime[0];
02124     npy = mgparm->pdime[1];
02125     npz = mgparm->pdime[2];
02126     nproc = npx*npy*npz;
02127
02128     /* If this is not an asynchronous calculation, then we need to make sure we
02129        have all the necessary MPI information */
02130     if (mgparm->setasync == 0) {
02131
02132 #ifndef HAVE_MPI_H
02133
02134         Vnm_tprint(2, "Nosh_setupCalcMGPARA: Oops! You're trying to perform \
02135 an 'mg-para' (parallel) calculation\n");
02136         Vnm_tprint(2, "Nosh_setupCalcMGPARA: with a version of APBS that wasn't \
02137 compiled with MPI!\n");
02138         Vnm_tprint(2, "Nosh_setupCalcMGPARA: Perhaps you meant to use the \
02139 'async' flag?\n");
02140         Vnm_tprint(2, "Nosh_setupCalcMGPARA: Bailing out!\n");
02141
02142         return 0;
02143     }
02144 #endif

```



```

02145
02146     rank = thee->proc_rank;
02147     size = thee->proc_size;
02148     Vnm_print(0, "Nosh_setupCalcMGPARA: Hello from processor %d of %d\n", rank,
02149             size);
02150
02151     /* Check to see if we have too many processors. If so, then simply set
02152        this processor to duplicating the work of processor 0. */
02153     if (rank > (nproc-1)) {
02154         Vnm_print(2, "Nosh_setupMGPARA: There are more processors available than\
02155 the %d you requested.\n", nproc);
02156         Vnm_print(2, "Nosh_setupMGPARA: Eliminating processor %d\n", rank);
02157         thee->bogus = 1;
02158         rank = 0;
02159     }
02160
02161     /* Check to see if we have too few processors. If so, this is a fatal
02162        error. */
02163     if (size < nproc) {
02164         Vnm_print(2, "Nosh_setupMGPARA: There are too few processors (%d) to \
02165 satisfy requirements (%d)\n", size, nproc);
02166         return 0;
02167     }
02168
02169     Vnm_print(0, "Nosh_setupMGPARA: Hello (again) from processor %d of %d\n",
02170             rank, size);
02171
02172     } else { /* Setting up for an asynchronous calculation. */
02173
02174         rank = mgparm->async;
02175
02176         thee->ispara = 1;
02177         thee->proc_rank = rank;
02178
02179         /* Check to see if the async id is greater than the number of
02180            processors. If so, this is a fatal error. */
02181         if (rank > (nproc-1)) {
02182             Vnm_print(2, "Nosh_setupMGPARA: The processor id you requested (%d) \
02183 is not within the range of processors available (0-%d)\n", rank, (nproc-1));
02184             return 0;
02185         }
02186     }
02187
02188     /* Calculate the processor's coordinates in the processor grid */
02189     kp = (int)floor(rank/(npx*ncpy));
02190     jp = (int)floor((rank-kp*npx*ncpy)/npx);
02191     ip = rank - kp*npx*ncpy - jp*npx;
02192     Vnm_print(0, "Nosh_setupMGPARA: Hello world from PE (%d, %d, %d)\n",
02193             ip, jp, kp);
02194
02195     /* Calculate effective overlap fractions for uneven processor distributions */
02196     if (npx == 1) xofrac = 0.0;
02197     else xofrac = ofrac;
02198     if (ncpy == 1) yofrac = 0.0;
02199     else yofrac = ofrac;
02200     if (npz == 1) zofrac = 0.0;
02201     else zofrac = ofrac;
02202
02203     /* Calculate the global grid size and spacing */
02204     xDisj = (int)VFFLOOR(mgparm->dime[0]/(1 + 2*xofrac) + 0.5);
02205     xeffGlob = npx*xDisj;
02206     hx = mgparm->fglen[0]/(double)(xeffGlob-1);
02207     yDisj = (int)VFFLOOR(mgparm->dime[1]/(1 + 2*yofrac) + 0.5);
02208     yeffGlob = npy*yDisj;
02209     hy = mgparm->fglen[1]/(double)(yeffGlob-1);
02210     zDisj = (int)VFFLOOR(mgparm->dime[2]/(1 + 2*zofrac) + 0.5);
02211     zeffGlob = npz*zDisj;
02212     hzed = mgparm->fglen[2]/(double)(zeffGlob-1);
02213     Vnm_print(0, "Nosh_setupMGPARA: Global Grid size = (%d, %d, %d)\n",
02214             xeffGlob, yeffGlob, zeffGlob);
02215     Vnm_print(0, "Nosh_setupMGPARA: Global Grid Spacing = (%.3f, %.3f, %.3f)\n",
02216             hx, hy, hzed);
02217     Vnm_print(0, "Nosh_setupMGPARA: Processor Grid Size = (%d, %d, %d)\n",
02218             xDisj, yDisj, zDisj);
02219
02220     /* Calculate the maximum and minimum processor grid points */
02221     xigminDisj = ip*xDisj;
02222     xigmaxDisj = xigminDisj + xDisj - 1;
02223     yigminDisj = jp*yDisj;
02224     yigmaxDisj = yigminDisj + yDisj - 1;
02225     zigminDisj = kp*zDisj;

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02226     zigmaxDisj = zigminDisj + zDisj - 1;
02227     Vnm_print(0, "Nosh_setupMGPARA: Min Grid Points for this proc. (%d, %d, %d)\n",
02228               xigminDisj, yigminDisj, zigminDisj);
02229     Vnm_print(0, "Nosh_setupMGPARA: Max Grid Points for this proc. (%d, %d, %d)\n",
02230               xigmaxDisj, yigmaxDisj, zigmaxDisj);
02231
02232
02233     /* Calculate the disjoint partition length and center displacement */
02234     xminDisj = VMAX2(hx*(xigminDisj-0.5), 0.0);
02235     xmaxDisj = VMIN2(hx*(xigmaxDisj+0.5), mgparm->fglen[0]);
02236     xlenDisj = xmaxDisj - xminDisj;
02237     yminDisj = VMAX2(hy*(yigminDisj-0.5), 0.0);
02238     ymaxDisj = VMIN2(hy*(yigmaxDisj+0.5), mgparm->fglen[1]);
02239     ylenDisj = ymaxDisj - yminDisj;
02240     zminDisj = VMAX2(hzed*(zigminDisj-0.5), 0.0);
02241     zmaxDisj = VMIN2(hzed*(zigmaxDisj+0.5), mgparm->fglen[2]);
02242     zlenDisj = zmaxDisj - zminDisj;
02243
02244     xcent = 0.5*mgparm->fglen[0];
02245     ycent = 0.5*mgparm->fglen[1];
02246     zcent = 0.5*mgparm->fglen[2];
02247
02248     xcentDisj = xminDisj + 0.5*xlenDisj - xcent;
02249     ycentDisj = yminDisj + 0.5*ylenDisj - ycent;
02250     zcentDisj = zminDisj + 0.5*zlenDisj - zcent;
02251     if (VABS(xcentDisj) < VSMALL) xcentDisj = 0.0;
02252     if (VABS(ycentDisj) < VSMALL) ycentDisj = 0.0;
02253     if (VABS(zcentDisj) < VSMALL) zcentDisj = 0.0;
02254
02255     Vnm_print(0, "Nosh_setupMGPARA: Disj part length = (%g, %g, %g)\n",
02256               xlenDisj, ylenDisj, zlenDisj);
02257     Vnm_print(0, "Nosh_setupMGPARA: Disj part center displacement = (%g, %g, %g)\n",
02258               xcentDisj, ycentDisj, zcentDisj);
02259
02260     /* Calculate the overlapping partition length and center displacement */
02261     xOlapReg = 0;
02262     yOlapReg = 0;
02263     zOlapReg = 0;
02264     if (npx != 1) xOlapReg = (int)VFFLOOR(xofrac*mgparm->fglen[0]/npx/hx + 0.5) + 1;
02265     if (npv != 1) yOlapReg = (int)VFFLOOR(yofrac*mgparm->fglen[1]/npv/hy + 0.5) + 1;
02266     if (npz != 1) zOlapReg = (int)VFFLOOR(zofrac*mgparm->fglen[2]/npz/hzed + 0.5) + 1;
02267
02268     Vnm_print(0, "Nosh_setupMGPARA: No. of Grid Points in Overlap (%d, %d, %d)\n",
02269               xOlapReg, yOlapReg, zOlapReg);
02270
02271     if (ip == 0) xigminOlap = 0;
02272     else if (ip == (npx - 1)) xigminOlap = xeffGlob - mgparm->dime[0];
02273     else xigminOlap = xigminDisj - xOlapReg;
02274     xigmaxOlap = xigminOlap + mgparm->dime[0] - 1;
02275
02276     if (jp == 0) yigminOlap = 0;
02277     else if (jp == (npv - 1)) yigminOlap = yeffGlob - mgparm->dime[1];
02278     else yigminOlap = yigminDisj - yOlapReg;
02279     yigmaxOlap = yigminOlap + mgparm->dime[1] - 1;
02280
02281     if (kp == 0) zigminOlap = 0;
02282     else if (kp == (npz - 1)) zigminOlap = zeffGlob - mgparm->dime[2];
02283     else zigminOlap = zigminDisj - zOlapReg;
02284     zigmaxOlap = zigminOlap + mgparm->dime[2] - 1;
02285
02286     Vnm_print(0, "Nosh_setupMGPARA: Min Grid Points with Overlap (%d, %d, %d)\n",
02287               xigminOlap, yigminOlap, zigminOlap);
02288     Vnm_print(0, "Nosh_setupMGPARA: Max Grid Points with Overlap (%d, %d, %d)\n",
02289               xigmaxOlap, yigmaxOlap, zigmaxOlap);
02290
02291     xminOlap = hx * xigminOlap;
02292     xmaxOlap = hx * xigmaxOlap;
02293     yminOlap = hy * yigminOlap;
02294     ymaxOlap = hy * yigmaxOlap;
02295     zminOlap = hzed * zigminOlap;
02296     zmaxOlap = hzed * zigmaxOlap;
02297
02298     xlenOlap = xmaxOlap - xminOlap;
02299     ylenOlap = ymaxOlap - yminOlap;
02300     zlenOlap = zmaxOlap - zminOlap;
02301
02302     xcentOlap = (xminOlap + 0.5*xlenOlap) - xcent;
02303     ycentOlap = (yminOlap + 0.5*ylenOlap) - ycent;
02304     zcentOlap = (zminOlap + 0.5*zlenOlap) - zcent;
02305     if (VABS(xcentOlap) < VSMALL) xcentOlap = 0.0;
02306     if (VABS(ycentOlap) < VSMALL) ycentOlap = 0.0;

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02307     if (VABS(zcentOlap) < VSMALL) zcentOlap = 0.0;
02308
02309     Vnm_print(0, "Nosh_setupMGPARA: Olap part length = (%g, %g, %g)\n",
02310             xlenOlap, ylenOlap, zlenOlap);
02311     Vnm_print(0, "Nosh_setupMGPARA: Olap part center displacement = (%g, %g, %g)\n",
02312             xcentOlap, ycentOlap, zcentOlap);
02313
02314
02315     /* Calculate the boundary flags:
02316        Flags are set to 1 when another processor is present along the boundary
02317        Flags are otherwise set to 0. */
02318
02319     if (ip == 0) mgparm->partDisjOwnSide[VAPBS_LEFT] = 0;
02320     else mgparm->partDisjOwnSide[VAPBS_LEFT] = 1;
02321     if (ip == (npx-1)) mgparm->partDisjOwnSide[VAPBS_RIGHT] = 0;
02322     else mgparm->partDisjOwnSide[VAPBS_RIGHT] = 1;
02323     if (jp == 0) mgparm->partDisjOwnSide[VAPBS_BACK] = 0;
02324     else mgparm->partDisjOwnSide[VAPBS_BACK] = 1;
02325     if (jp == (npy-1)) mgparm->partDisjOwnSide[VAPBS_FRONT] = 0;
02326     else mgparm->partDisjOwnSide[VAPBS_FRONT] = 1;
02327     if (kp == 0) mgparm->partDisjOwnSide[VAPBS_DOWN] = 0;
02328     else mgparm->partDisjOwnSide[VAPBS_DOWN] = 1;
02329     if (kp == (npz-1)) mgparm->partDisjOwnSide[VAPBS_UP] = 0;
02330     else mgparm->partDisjOwnSide[VAPBS_UP] = 1;
02331
02332     Vnm_print(0, "Nosh_setupMGPARA: partDisjOwnSide[LEFT] = %d\n",
02333             mgparm->partDisjOwnSide[VAPBS_LEFT]);
02334     Vnm_print(0, "Nosh_setupMGPARA: partDisjOwnSide[RIGHT] = %d\n",
02335             mgparm->partDisjOwnSide[VAPBS_RIGHT]);
02336     Vnm_print(0, "Nosh_setupMGPARA: partDisjOwnSide[FRONT] = %d\n",
02337             mgparm->partDisjOwnSide[VAPBS_FRONT]);
02338     Vnm_print(0, "Nosh_setupMGPARA: partDisjOwnSide[BACK] = %d\n",
02339             mgparm->partDisjOwnSide[VAPBS_BACK]);
02340     Vnm_print(0, "Nosh_setupMGPARA: partDisjOwnSide[UP] = %d\n",
02341             mgparm->partDisjOwnSide[VAPBS_UP]);
02342     Vnm_print(0, "Nosh_setupMGPARA: partDisjOwnSide[DOWN] = %d\n",
02343             mgparm->partDisjOwnSide[VAPBS_DOWN]);
02344
02345     /* Set the mesh parameters */
02346     mgparm->fglen[0] = xlenOlap;
02347     mgparm->fglen[1] = ylenOlap;
02348     mgparm->fglen[2] = zlenOlap;
02349     mgparm->partDisjLength[0] = xlenDisj;
02350     mgparm->partDisjLength[1] = ylenDisj;
02351     mgparm->partDisjLength[2] = zlenDisj;
02352     mgparm->partDisjCenter[0] = mgparm->fcenter[0] + xcentDisj;
02353     mgparm->partDisjCenter[1] = mgparm->fcenter[1] + ycentDisj;
02354     mgparm->partDisjCenter[2] = mgparm->fcenter[2] + zcentDisj;
02355     mgparm->fcenter[0] += xcentOlap;
02356     mgparm->fcenter[1] += ycentOlap;
02357     mgparm->fcenter[2] += zcentOlap;
02358
02359     Vnm_print(0, "Nosh_setupCalcMGPARA (%s, %d): Set up *relative* partition \
02360 centers...\n", __FILE__, __LINE__);
02361     Vnm_print(0, "Nosh_setupCalcMGPARA (%s, %d): Absolute centers will be set \
02362 in Nosh_setupMGAUTO\n", __FILE__, __LINE__);
02363     Vnm_print(0, "Nosh_setupCalcMGPARA (%s, %d): partDisjCenter = %g %g %g\n",
02364             __FILE__, __LINE__,
02365             mgparm->partDisjCenter[0],
02366             mgparm->partDisjCenter[1],
02367             mgparm->partDisjCenter[2]);
02368     Vnm_print(0, "Nosh_setupCalcMGPARA (%s, %d): ccenter = %g %g %g\n",
02369             __FILE__, __LINE__,
02370             mgparm->ccenter[0],
02371             mgparm->ccenter[1],
02372             mgparm->ccenter[2]);
02373     Vnm_print(0, "Nosh_setupCalcMGPARA (%s, %d): fcenter = %g %g %g\n",
02374             __FILE__, __LINE__,
02375             mgparm->fcenter[0],
02376             mgparm->fcenter[1],
02377             mgparm->fcenter[2]);
02378
02379
02380     /* Setup the automatic focusing calculations associated with this processor */
02381     return Nosh_setupCalcMGAUTO(thee, elec);
02382 }
02383
02384
02385 VPUBLIC int Nosh_parseFEM(
02386     NOSH *thee,
02387     Vio *sock,

```

```

02388             NOsh_calc *elec
02389         ) {
02390
02391     char tok[VMAX_BUFSIZE];
02392     FEMparm *feparm = VNULL;
02393     PBEparm *pbeparm = VNULL;
02394     int rc;
02395     Vrc_Codes vrc;
02396
02397     /* Check the arguments */
02398     if (thee == VNULL) {
02399         Vnm_print(2, "NOsh_parseFEM: Got NULL thee!\n");
02400         return 0;
02401     }
02402     if (sock == VNULL) {
02403         Vnm_print(2, "NOsh_parseFEM: Got pointer to NULL socket!\n");
02404         return 0;
02405     }
02406     if (elec == VNULL) {
02407         Vnm_print(2, "NOsh_parseFEM: Got pointer to NULL elec object!\n");
02408         return 0;
02409     }
02410     feparm = elec->feparm;
02411     if (feparm == VNULL) {
02412         Vnm_print(2, "NOsh_parseFEM: Got pointer to NULL feparm object!\n");
02413         return 0;
02414     }
02415     pbeparm = elec->pbeparm;
02416     if (pbeparm == VNULL) {
02417         Vnm_print(2, "NOsh_parseFEM: Got pointer to NULL pbeparm object!\n");
02418         return 0;
02419     }
02420
02421     Vnm_print(0, "NOsh_parseFEM: Parsing parameters for FEM calculation\n");
02422
02423     /* Start snarfing tokens from the input stream */
02424     rc = 1;
02425     while (Vio_scanf(sock, "%s", tok) == 1) {
02426
02427         Vnm_print(0, "NOsh_parseFEM: Parsing %s...\n", tok);
02428
02429         /* See if it's an END token */
02430         if (Vstring_strcasecmp(tok, "end") == 0) {
02431             feparm->parsed = 1;
02432             pbeparm->parsed = 1;
02433             rc = 1;
02434             break;
02435         }
02436
02437         /* Pass the token through a series of parsers */
02438         rc = PBEparm_parseToken(pbeparm, tok, sock);
02439         if (rc == -1) {
02440             Vnm_print(0, "NOsh_parseFEM: parsePBE error!\n");
02441             break;
02442         } else if (rc == 0) {
02443             /* Pass the token to the generic MG parser */
02444             vrc = FEMparm_parseToken(feparm, tok, sock);
02445             if (vrc == VRC_FAILURE) {
02446                 Vnm_print(0, "NOsh_parseFEM: parseMG error!\n");
02447                 break;
02448             } else if (vrc == VRC_WARNING) {
02449                 /* We ran out of parsers! */
02450                 Vnm_print(2, "NOsh: Unrecognized keyword: %s\n", tok);
02451                 break;
02452             }
02453         }
02454     }
02455
02456     /* Handle various errors arising in the token-snarfing loop -- these all
02457      * just result in simple returns right now */
02458     if (rc == -1) return 0;
02459     if (rc == 0) return 0;
02460
02461     /* Check the status of the parameter objects */
02462     if ((!FEMparm_check(feparm)) || (!PBEparm_check(pbeparm))) {
02463         Vnm_print(2, "NOsh: FEM parameters not set correctly!\n");
02464         return 0;
02465     }
02466
02467     return 1;
02468

```

```

02469 }
02470
02471 VPRIVATE int NOsh_setupCalcFEMANUAL(
02472     NOsh *thee,
02473     NOsh_calc *elec
02474 ) {
02475
02476     FEMparm *feparm = VNULL;
02477     PBEParm *pbeparm = VNULL;
02478     NOsh_calc *calc = VNULL;
02479
02480     VASSERT(thee != VNULL);
02481     VASSERT(elec != VNULL);
02482     feparm = elec->feparm;
02483     VASSERT(feparm != VNULL);
02484     pbeparm = elec->pbeparm;
02485     VASSERT(pbeparm);
02486
02487     /* Check to see if he have any room left for this type of
02488      * calculation, if so: set the calculation type, update the number
02489      * of calculations of this type, and parse the rest of the section
02490      */
02491     if (thee->ncalc >= NOSH_MAXCALC) {
02492         Vnm_print(2, "NOsh: Too many calculations in this run!\n");
02493         Vnm_print(2, "NOsh: Current max is %d; ignoring this calculation\n",
02494                 NOSH_MAXCALC);
02495         return 0;
02496     }
02497     thee->calc[thee->ncalc] = NOsh_calc_ctor(NCT_FEM);
02498     calc = thee->calc[thee->ncalc];
02499     (thee->ncalc)++;
02500
02501     /* Copy over contents of ELEC */
02502     NOsh_calc_copy(calc, elec);
02503
02504
02505     return 1;
02506 }
02507
02508 VPUBLIC int NOsh_parseAPOL(
02509     NOsh *thee,
02510     Vio *sock,
02511     NOsh_calc *elec
02512 ) {
02513
02514     char tok[VMAX_BUFSIZE];
02515     APOLparm *apolparm = VNULL;
02516     int rc;
02517
02518     /* Check the arguments */
02519     if (thee == VNULL) {
02520         Vnm_print(2, "NOsh_parseAPOL: Got NULL thee!\n");
02521         return 0;
02522     }
02523     if (sock == VNULL) {
02524         Vnm_print(2, "NOsh_parseAPOL: Got pointer to NULL socket!\n");
02525         return 0;
02526     }
02527     if (elec == VNULL) {
02528         Vnm_print(2, "NOsh_parseAPOL: Got pointer to NULL elec object!\n");
02529         return 0;
02530     }
02531     apolparm = elec->apolparm;
02532     if (apolparm == VNULL) {
02533         Vnm_print(2, "NOsh_parseAPOL: Got pointer to NULL apolparm object!\n");
02534         return 0;
02535     }
02536
02537     Vnm_print(0, "NOsh_parseAPOL: Parsing parameters for APOL calculation\n");
02538
02539     /* Start snarfing tokens from the input stream */
02540     rc = 1;
02541     while (Vio_scanf(sock, "%s", tok) == 1) {
02542
02543         Vnm_print(0, "NOsh_parseAPOL: Parsing %s...\n", tok);
02544         /* See if it's an END token */
02545         if (Vstring_strcasecmp(tok, "end") == 0) {
02546             apolparm->parsed = 1;
02547             rc = 1;
02548             break;
02549         }
02550     }

```

```

02550
02551     /* Pass the token through a series of parsers */
02552     /* Pass the token to the generic non-polar parser */
02553     rc = APOLparam_parseToken(apolparam, tok, sock);
02554     if (rc == -1) {
02555         Vnm_print(0, "Nosh_parseFEM: parseMG error!\n");
02556         break;
02557     } else if (rc == 0) {
02558         /* We ran out of parsers! */
02559         Vnm_print(2, "Nosh: Unrecognized keyword: %s\n", tok);
02560         break;
02561     }
02562 }
02563
02564
02565 /* Handle various errors arising in the token-snarfing loop -- these all
02566    * just result in simple returns right now */
02567 if (rc == -1) return 0;
02568 if (rc == 0) return 0;
02569
02570 /* Check the status of the parameter objects */
02571 if (!APOLparam_check(apolparam)) {
02572     Vnm_print(2, "Nosh: APOL parameters not set correctly!\n");
02573     return 0;
02574 }
02575
02576 return 1;
02577 }
02578 }
02579
02580
02581 VPRIVATE int Nosh_setupCalcAPOL(
02582     Nosh *thee,
02583     Nosh_calc *apol
02584 ) {
02585
02586     Nosh_calc *calc = VNULL;
02587
02588     VASSERT(thee != VNULL);
02589     VASSERT(apol != VNULL);
02590
02591     /* Check to see if he have any room left for this type of
02592        * calculation, if so: set the calculation type, update the number
02593        * of calculations of this type, and parse the rest of the section
02594        */
02595     if (thee->ncalc >= NOSH_MAXCALC) {
02596         Vnm_print(2, "Nosh: Too many calculations in this run!\n");
02597         Vnm_print(2, "Nosh: Current max is %d; ignoring this calculation\n",
02598             NOSH_MAXCALC);
02599         return 0;
02600     }
02601     thee->calc[thee->ncalc] = Nosh_calc_ctor(NCT_APOL);
02602     calc = thee->calc[thee->ncalc];
02603     (thee->ncalc)++;
02604
02605     /* Copy over contents of APOL */
02606     Nosh_calc_copy(calc, apol);
02607
02608     return 1;
02609 }
02610
02611
02612 VPRIVATE int Nosh_setupCalcBEMMANUAL(
02613     Nosh *thee,
02614     Nosh_calc *elec
02615 ) {
02616
02617     BEMparam *bemparm = VNULL;
02618     PBEparam *pbeparm = VNULL;
02619     Nosh_calc *calc = VNULL;
02620
02621     if (thee == VNULL) {
02622         Vnm_print(2, "Nosh_setupCalcBEMMANUAL: Got NULL thee!\n");
02623         return 0;
02624     }
02625     if (elec == VNULL) {
02626         Vnm_print(2, "Nosh_setupCalcBEMMANUAL: Got NULL calc!\n");
02627         return 0;
02628     }
02629     bemparm = elec->bemparm;
02630     if (bemparm == VNULL) {

```

```

02631     Vnm_print(2, "Nosh_setupCalcBEMMANUAL: Got NULL bemparm -- was this calculation \
02632 set up?\n");
02633     return 0;
02634 }
02635 pbeparm = elec->pbeparm;
02636 if (pbeparm == VNULL) {
02637     Vnm_print(2, "Nosh_setupCalcBEMMANUAL: Got NULL pbeparm -- was this calculation \
02638 set up?\n");
02639     return 0;
02640 }
02641
02642 /* Set up missing BEM parameters */
02643 if (bemparm->settree_order == 0) {
02644     bemparm->tree_order=1;
02645 }
02646
02647 if (bemparm->settree_n0 == 0) {
02648     bemparm->tree_n0=500;
02649 }
02650
02651 if (bemparm->setmac == 0) {
02652     bemparm->mac=0.8;
02653 }
02654
02655 /* Check to see if he have any room left for this type of calculation, if
02656 so: set the calculation type, update the number of calculations of this type,
02657 and parse the rest of the section */
02658 if (thee->ncalc >= NOSH_MAXCALC) {
02659     Vnm_print(2, "Nosh: Too many calculations in this run!\n");
02660     Vnm_print(2, "Nosh: Current max is %d; ignoring this calculation\n",
02661         NOSH_MAXCALC);
02662     return 0;
02663 }
02664
02665 /* Get the next calculation object and increment the number of calculations */
02666 thee->calc[thee->ncalc] = Nosh_calc_ctor(NCT_BEM);
02667 calc = thee->calc[thee->ncalc];
02668 (thee->ncalc)++;
02669
02670 /* Copy over contents of ELEC */
02671 Nosh_calc_copy(calc, elec);
02672
02673
02674     return 1;
02675 }
02676
02677 VPRIVATE int Nosh_setupCalcGEOFLOWMANUAL(
02678     Nosh *thee,
02679     Nosh_calc *elec
02680 ) {
02681
02682     GEOFLOWparm *parm = VNULL;
02683     APOLparm *apolparm = VNULL;
02684     PBEParm *pbeparm = VNULL;
02685     Nosh_calc *calc = VNULL;
02686
02687     if (thee == VNULL) {
02688         Vnm_print(2, "Nosh_setupCalcGEOFLOWMANUAL: Got NULL thee!\n");
02689         return 0;
02690     }
02691     if (elec == VNULL) {
02692         Vnm_print(2, "Nosh_setupCalcGEOFLOWMANUAL: Got NULL calc!\n");
02693         return 0;
02694     }
02695     parm = elec->geoflowparm;
02696     if (parm == VNULL) {
02697         Vnm_print(2, "Nosh_setupCalcGEOFLOWMANUAL: Got NULL geoflowparm -- was this calculation \
02698 set up?\n");
02699         return 0;
02700     }
02701     apolparm = elec->apolparm;
02702     if (parm == VNULL) {
02703         Vnm_print(2, "Nosh_setupCalcGEOFLOWMANUAL: Got NULL apolparm -- was this calculation \
02704 set up?\n");
02705         return 0;
02706     }
02707     pbeparm = elec->pbeparm;
02708     if (pbeparm == VNULL) {
02709         Vnm_print(2, "Nosh_setupCalcGEOFLOWMANUAL: Got NULL pbeparm -- was this calculation \
02710 set up?\n");
02711         return 0;

```

```

02712     }
02713
02714     /* Check to see if he have any room left for this type of calculation, if
02715        so: set the calculation type, update the number of calculations of this type,
02716        and parse the rest of the section */
02717     if (thee->ncalc >= NOSH_MAXCALC) {
02718         Vnm_print(2, "Nosh: Too many calculations in this run!\n");
02719         Vnm_print(2, "Nosh: Current max is %d; ignoring this calculation\n",
02720                 NOSH_MAXCALC);
02721         return 0;
02722     }
02723
02724     /* Get the next calculation object and increment the number of calculations */
02725     thee->calc[thee->ncalc] = NOsh_calc_ctor(NCT_GEOFLOW);
02726     calc = thee->calc[thee->ncalc];
02727     (thee->ncalc)++;
02728
02729     /* Copy over contents of ELEC */
02730     NOsh_calc_copy(calc, elec);
02731
02732     return 1;
02733 }
02734
02735 VPRIVATE int NOsh_setupCalcPBAMAUTO(
02736         NOsh *thee,
02737         NOsh_calc *elec
02738     ) {
02739
02740     PBAMparm *parm = VNULL;
02741     PBEParm *pbeparm = VNULL;
02742     NOsh_calc *calc = VNULL;
02743
02744     if (thee == VNULL) {
02745         Vnm_print(2, "NOsh_setupCalcPBAMAUTO: Got NULL thee!\n");
02746         return 0;
02747     }
02748     if (elec == VNULL) {
02749         Vnm_print(2, "NOsh_setupCalcPBAMAUTO: Got NULL calc!\n");
02750         return 0;
02751     }
02752     parm = elec->pbamparm;
02753     if (parm == VNULL) {
02754         Vnm_print(2, "NOsh_setupCalcPBAMAUTO: Got NULL pbamparm -- was this calculation \
02755 set up?\n");
02756         return 0;
02757     }
02758     pbeparm = elec->pbeparm;
02759     if (pbeparm == VNULL) {
02760         Vnm_print(2, "NOsh_setupCalcPBAMAUTO: Got NULL pbeparm -- was this calculation \
02761 set up?\n");
02762         return 0;
02763     }
02764
02765     /* Check to see if he have any room left for this type of calculation, if
02766        so: set the calculation type, update the number of calculations of this type,
02767        and parse the rest of the section */
02768     if (thee->ncalc >= NOSH_MAXCALC) {
02769         Vnm_print(2, "Nosh: Too many calculations in this run!\n");
02770         Vnm_print(2, "Nosh: Current max is %d; ignoring this calculation\n",
02771                 NOSH_MAXCALC);
02772         return 0;
02773     }
02774
02775     /* Get the next calculation object and increment the number of calculations */
02776     thee->calc[thee->ncalc] = NOsh_calc_ctor(NCT_PBAM);
02777     calc = thee->calc[thee->ncalc];
02778     (thee->ncalc)++;
02779
02780     /* Copy over contents of ELEC */
02781     NOsh_calc_copy(calc, elec);
02782
02783     return 1;
02784 }
02785
02786 VPRIVATE int NOsh_setupCalcPBSAMAUTO(
02787         NOsh *thee,
02788         NOsh_calc *elec
02789     ) {
02790
02791     PBAMparm *parm = VNULL;
02792     PBSAMparm *sampparm = VNULL;

```



```

02793     PBEParm *pbeparm = VNULL;
02794     NOsh_calc *calc = VNULL;
02795
02796     if (thee == VNULL) {
02797         Vnm_print(2, "NOsh_setupCalcPBSAMAUTO: Got NULL thee!\n");
02798         return 0;
02799     }
02800     if (elec == VNULL) {
02801         Vnm_print(2, "NOsh_setupCalcPBSAMAUTO: Got NULL calc!\n");
02802         return 0;
02803     }
02804     parm = elec->pbamparm;
02805     if (parm == VNULL) {
02806         Vnm_print(2, "NOsh_setupCalcPBSAMAUTO: Got NULL pbamparm -- was this calculation \
02807 set up?\n");
02808         return 0;
02809     }
02810     samparm = elec->pbsamparm;
02811     if (samparm == VNULL) {
02812         Vnm_print(2, "NOsh_setupCalcPBSAMAUTO: Got NULL pbsamparm -- was this calculation \
02813 set up?\n");
02814         return 0;
02815     }
02816     pbeparm = elec->pbeparm;
02817     if (pbeparm == VNULL) {
02818         Vnm_print(2, "NOsh_setupCalcPBAMAUTO: Got NULL pbeparm -- was this calculation \
02819 set up?\n");
02820         return 0;
02821     }
02822
02823     /* Check to see if he have any room left for this type of calculation, if
02824        so: set the calculation type, update the number of calculations of this type,
02825        and parse the rest of the section */
02826     if (thee->ncalc >= NOSH_MAXCALC) {
02827         Vnm_print(2, "NOsh: Too many calculations in this run!\n");
02828         Vnm_print(2, "NOsh: Current max is %d; ignoring this calculation\n",
02829                 NOSH_MAXCALC);
02830         return 0;
02831     }
02832
02833     /* Get the next calculation object and increment the number of calculations */
02834     thee->calc[thee->ncalc] = NOsh_calc_ctor(NCT_PBSAM);
02835     calc = thee->calc[thee->ncalc];
02836     (thee->ncalc)++;
02837
02838     /* Copy over contents of ELEC */
02839     NOsh_calc_copy(calc, elec);
02840
02841     return 1;
02842 }
02843
02844
02845 VPUBLIC int NOsh_parseBEM(
02846     NOsh *thee,
02847     Vio *sock,
02848     NOsh_calc *elec
02849 ) {
02850
02851     char tok[VMAX_BUFSIZE];
02852     BEMParm *bemparm = VNULL;
02853     PBEParm *pbeparm = VNULL;
02854     int rc;
02855
02856     /* Check the arguments */
02857     if (thee == VNULL) {
02858         Vnm_print(2, "NOsh: Got NULL thee!\n");
02859         return 0;
02860     }
02861     if (sock == VNULL) {
02862         Vnm_print(2, "NOsh: Got pointer to NULL socket!\n");
02863         return 0;
02864     }
02865     if (elec == VNULL) {
02866         Vnm_print(2, "NOsh: Got pointer to NULL elec object!\n");
02867         return 0;
02868     }
02869     bemparm = elec->bemparm;
02870     if (bemparm == VNULL) {
02871         Vnm_print(2, "NOsh: Got pointer to NULL bemparm object!\n");
02872         return 0;
02873     }

```

```

02874     pbeparm = elec->pbeparm;
02875     if (pbeparm == VNULL) {
02876         Vnm_print(2, "Nosh: Got pointer to NULL pbeparm object!\n");
02877         return 0;
02878     }
02879
02880     Vnm_print(0, "Nosh_parseBEM: Parsing parameters for BEM calculation\n");
02881
02882
02883     /* Start snarfing tokens from the input stream */
02884     rc = 1;
02885     while (Vio_scanf(sock, "%s", tok) == 1) {
02886
02887         Vnm_print(0, "Nosh_parseBEM: Parsing %s...\n", tok);
02888
02889         /* See if it's an END token */
02890         if (Vstring_strcasecmp(tok, "end") == 0) {
02891             beparm->parsed = 1;
02892             pbeparm->parsed = 1;
02893             rc = 1;
02894             break;
02895         }
02896
02897         /* Pass the token through a series of parsers */
02898         rc = PBeparm_parseToken(pbeparm, tok, sock);
02899         if (rc == -1) {
02900             Vnm_print(0, "Nosh_parseBEM: parsePBE error!\n");
02901             break;
02902         } else if (rc == 0) {
02903             /* Pass the token to the generic BEM parser */
02904             rc = BEMparm_parseToken(beparm, tok, sock);
02905             if (rc == -1) {
02906                 Vnm_print(0, "Nosh_parseBEM: parseBEM error!\n");
02907                 break;
02908             } else if (rc == 0) {
02909                 /* We ran out of parsers! */
02910                 Vnm_print(2, "Nosh: Unrecognized keyword: %s\n", tok);
02911                 break;
02912             }
02913         }
02914     }
02915
02916     pbeparm->setsrfm=1;      // unneeded srfm
02917     pbeparm->setpbe_type=1;  // unneeded pbe type
02918     pbeparm->setbcfl=1;      // unneeded bcfl
02919
02920     /* Handle various errors arising in the token-snarfing loop -- these all
02921        just result in simple returns right now */
02922     if (rc == -1) return 0;
02923     if (rc == 0) return 0;
02924
02925     /* Check the status of the parameter objects */
02926     if ((BEMparm_check(beparm) == VRC_FAILURE) || (!PBeparm_check(pbeparm))) {
02927         Vnm_print(2, "Nosh: BEM parameters not set correctly!\n");
02928         return 0;
02929     }
02930
02931     return 1;
02932 }
02933
02934 VPUBLIC int Nosh_parseGEOFLOW(
02935     Nosh *thee,
02936     Vio *sock,
02937     Nosh_calc *elec
02938 ) {
02939
02940     char tok[VMAX_BUFSIZE];
02941     GEOFLOWparm *parm = VNULL;
02942     APOLparm *apolparm = VNULL;
02943     PBeparm *pbeparm = VNULL;
02944     int rc;
02945
02946     /* Check the arguments */
02947     if (thee == VNULL) {
02948         Vnm_print(2, "Nosh: Got NULL thee!\n");
02949         return 0;
02950     }
02951     if (sock == VNULL) {
02952         Vnm_print(2, "Nosh: Got pointer to NULL socket!\n");
02953         return 0;
02954     }

```

```

02955     if (elec == VNULL) {
02956         Vnm_print(2, "Nosh: Got pointer to NULL elec object!\n");
02957         return 0;
02958     }
02959     parm = elec->geoflowparm;
02960     if (parm == VNULL) {
02961         Vnm_print(2, "Nosh: Got pointer to NULL geoflowparm object!\n");
02962         return 0;
02963     }
02964     apolparm = elec->apolparm;
02965     if (parm == VNULL) {
02966         Vnm_print(2, "Nosh: Got pointer to NULL apolparm object!\n");
02967         return 0;
02968     }
02969     pbeparm = elec->pbeparm;
02970     if (pbeparm == VNULL) {
02971         Vnm_print(2, "Nosh: Got pointer to NULL pbeparm object!\n");
02972         return 0;
02973     }
02974
02975     Vnm_print(0, "Nosh_parseGEOFLOW: Parsing parameters for GEOFLOW calculation\n");
02976
02977     /* Start snarfing tokens from the input stream */
02978     rc = 1;
02979     while (Vio_scanf(sock, "%s", tok) == 1) {
02980
02981         Vnm_print(0, "Nosh_parseGEOFLOW: Parsing %s...\n", tok);
02982
02983         /* See if it's an END token */
02984         if (Vstring_strcasecmp(tok, "end") == 0) {
02985             parm->parsed = 1;
02986             pbeparm->parsed = 1;
02987             apolparm->parsed = 1;
02988             rc = 1;
02989             break;
02990         }
02991
02992         if (Vstring_strcasecmp(tok, "ion") == 0) {
02993             Vnm_print(2, "parseGEOFLOW: WARNING! ion not implemented for geometric flow!\n");
02994         }
02995
02996         /* Pass the token through a series of parsers */
02997         rc = PBEparm_parseToken(pbeparm, tok, sock);
02998         if (rc == -1) {
02999             Vnm_print(0, "Nosh_parseGEOFLOW: parsePBE error!\n");
03000             break;
03001         } else if (rc == 0) {
03002             /* Pass the token to the generic GEOFLOW parser */
03003             rc = APOLparm_parseToken(apolparm, tok, sock);
03004             if (rc == -1) {
03005                 Vnm_print(0, "Nosh_parseAPOL: parseAPOL error!\n");
03006                 break;
03007             } else if (rc == 0) {
03008                 rc = GEOFLOWparm_parseToken(parm, tok, sock);
03009                 if (rc == -1) {
03010                     Vnm_print(0, "Nosh_parseGEOFLOW: parseGEOFLOW error!\n");
03011                     break;
03012                 } else if (rc == 0) {
03013                     /* We ran out of parsers! */
03014                     Vnm_print(2, "Nosh: Unrecognized keyword: %s\n", tok);
03015                     break;
03016                 }
03017             }
03018         }
03019     }
03020 }
03021
03022 pbeparm->setsrfm=1;
03023 pbeparm->srad=0.0;
03024 pbeparm->setsrad=1;
03025 pbeparm->settemp=1;
03026
03027 /* Handle various errors arising in the token-snarfing loop -- these all
03028    just result in simple returns right now */
03029 if (rc == -1) return 0;
03030 if (rc == 0) return 0;
03031
03032 /* Check the status of the parameter objects */
03033 if ((GEOFLOWparm_check(parm) == VRC_FAILURE) || (!PBEparm_check(pbeparm))) {
03034     Vnm_print(2, "Nosh: GEOFLOW parameters not set correctly!\n");
03035     return 0;

```

```

03036     }
03037     /*currently the only bc handle by geoflow is mdh so we check here if mdh was read*/
03038     if(pbeparm->bcfl != BCFL_MDH){
03039         Vnm_print(2, "Nosh_parseGEOFLOW: Geoflow currently only supports mdh boundary conditions!\n");
03040         Vnm_print(2, "Nosh_parseGEOFLOW: please change bcfl keyword.\n");
03041         return 0;
03042     }
03043
03044     return 1;
03045 }
03046
03047
03048 VPUBLIC int Nosh_parsePBAM(
03049     NOsh *thee,
03050     Vio *sock,
03051     NOsh_calc *elec
03052 ) {
03053
03054     char tok[VMAX_BUFSIZE];
03055     PBAMparm *parm = VNULL;
03056     PBEParm *pbeparm = VNULL;
03057     int rc;
03058
03059     /* Check the arguments */
03060     if (thee == VNULL) {
03061         Vnm_print(2, "Nosh: Got NULL thee!\n");
03062         return 0;
03063     }
03064     if (sock == VNULL) {
03065         Vnm_print(2, "Nosh: Got pointer to NULL socket!\n");
03066         return 0;
03067     }
03068     if (elec == VNULL) {
03069         Vnm_print(2, "Nosh: Got pointer to NULL elec object!\n");
03070         return 0;
03071     }
03072     parm = elec->pbamparm;
03073     if (parm == VNULL) {
03074         Vnm_print(2, "Nosh: Got pointer to NULL pbam object!\n");
03075         return 0;
03076     }
03077     pbeparm = elec->pbeparm;
03078     if (pbeparm == VNULL) {
03079         Vnm_print(2, "Nosh: Got pointer to NULL pbeparm object!\n");
03080         return 0;
03081     }
03082     Vnm_print(0, "Nosh_parsePBAM: Parsing parameters for PBAM calculation\n");
03083
03084     /* Start snarfing tokens from the input stream */
03085     rc = 1;
03086     while (Vio_scanf(sock, "%s", tok) == 1) {
03087
03088         Vnm_print(0, "Nosh_parsePBAM: Parsing %s...\n", tok);
03089
03090         /* See if it's an END token */
03091         if (Vstring_strcasecmp(tok, "end") == 0) {
03092             parm->parsed = 1;
03093             pbeparm->parsed = 1;
03094             rc = 1;
03095             break;
03096         }
03097
03098         if (Vstring_strcasecmp(tok, "ion") == 0) {
03099             Vnm_print(2, "parsePBAM: WARNING! PBAM only uses the conc parameter of ion!\n");
03100         }
03101
03102         /* Pass the token through a series of parsers */
03103         rc = PBEParm_parseToken(pbeparm, tok, sock);
03104         if (rc == -1) {
03105             Vnm_print(0, "Nosh_parsePBAM: parsePBE error!\n");
03106             break;
03107         } else if (rc == 0) {
03108             rc = PBAMparm_parseToken(parm, tok, sock);
03109             if (rc == -1) {
03110                 Vnm_print(0, "Nosh_parsePBAM: parsePBAM error!\n");
03111                 break;
03112             } else if (rc == 0) {
03113                 /* We ran out of parsers! */
03114                 Vnm_print(2, "Nosh: Unrecognized keyword: %s\n", tok);
03115                 break;
03116             }
03117         }
03118     }

```

```

03117     }
03118 }
03119
03120
03121
03122     pbeparm->setsrfm=1;
03123     pbeparm->setsrad=1;
03124     pbeparm->settemp=1; // do need temp, but have default, incase
03125     pbeparm->setmolid=1; // for unneeded mol flag
03126     pbeparm->setpbetype=1; // unneeded pbe type
03127     pbeparm->setbcfl=1; // unneeded bcfl
03128     pbeparm->setsdens=1;
03129
03130     //This is a hacky fix at best for issue 501. This is so we don't need to change PBAM's
03131     //external code.
03132     if(pbeparm->setnion){
03133         parm->salt = pbeparm->ionc[pbeparm->nion-1];
03134         parm->setsalt = 1;
03135     }
03136
03137     //This is also a hacky fix for issue 488
03138     if (pbeparm->writefmt[pbeparm->numwrite - 1] == VDF_DX) {
03139         strncpy(parm->dxname, pbeparm->writestem[pbeparm->numwrite - 1], CHR_MAXLEN);
03140         parm->setdxname = 1;
03141     }
03142     else {
03143         Vnm_print(2, "NOsh: PBAM only prints in dx format!\n");
03144         return 0;
03145     }
03146
03147     //Another hacky fix for issue 482
03148     if (pbeparm->pbam_3dmapflag == 1) {
03149         strcpy(parm->map3dname, pbeparm->pbam_3dmapstem);
03150         parm->set3dmap = 1;
03151     }
03152
03153     /* Handle various errors arising in the token-snarfing loop -- these all
03154        just result in simple returns right now */
03155     if (rc == -1) return 0;
03156     if (rc == 0) return 0;
03157
03158     /* Check the status of the parameter objects */
03159     if ((PBAMparm_check(parm) == VRC_FAILURE) || (!PBEparm_check(pbeparm))) {
03160         Vnm_print(2, "NOsh: PBAM parameters not set correctly!\n");
03161         return 0;
03162     }
03163     return 1;
03164 }
03165
03166 VPUBLIC int NOsh_parsePBSAM(
03167     NOsh *thee,
03168     Vio *sock,
03169     NOsh_calc *elec
03170 ) {
03171
03172     char tok[VMAX_BUFSIZE];
03173     PBAMparm *parm = VNULL;
03174     PBSAMparm *samparm = VNULL;
03175     PBEparm *pbeparm = VNULL;
03176     int rc;
03177
03178     /* Check the arguments */
03179     if (thee == VNULL) {
03180         Vnm_print(2, "NOsh: Got NULL thee!\n");
03181         return 0;
03182     }
03183     if (sock == VNULL) {
03184         Vnm_print(2, "NOsh: Got pointer to NULL socket!\n");
03185         return 0;
03186     }
03187     if (elec == VNULL) {
03188         Vnm_print(2, "NOsh: Got pointer to NULL elec object!\n");
03189         return 0;
03190     }
03191     parm = elec->pbamparm;
03192     if (parm == VNULL) {
03193         Vnm_print(2, "NOsh: Got pointer to NULL pbam object!\n");
03194         return 0;
03195     }
03196     samparm = elec->pbsamparm;
03197     if (samparm == VNULL) {

```

```

03198     Vnm_print(2, "Nosh: Got pointer to NULL pbsam object!\n");
03199     return 0;
03200 }
03201 pbeparm = elec->pbeparm;
03202 if (pbeparm == VNULL) {
03203     Vnm_print(2, "Nosh: Got pointer to NULL pbeparm object!\n");
03204     return 0;
03205 }
03206 Vnm_print(0, "Nosh_parsePBSAM: Parsing parameters for PBSAM calculation\n");
03207 /* Start snarfing tokens from the input stream */
03208 rc = 1;
03209 while (Vio_scanf(sock, "%s", tok) == 1) {
03210     Vnm_print(0, "Nosh_parsePBSAM: Parsing %s...\n", tok);
03211
03212     /* See if it's an END token */
03213     if (Vstring_strcasecmp(tok, "end") == 0) {
03214         parm->parsed = 1;
03215         samparm->parsed = 1;
03216         pbeparm->parsed = 1;
03217         rc = 1;
03218         break;
03219     }
03220
03221     if (Vstring_strcasecmp(tok, "ion") == 0) {
03222         Vnm_print(2, "parsePBSAM: WARNING! PBAM only uses the conc parameter of ion!\n");
03223     }
03224
03225     /* Pass the token through a series of parsers */
03226     rc = PBEParm_parseToken(pbeparm, tok, sock);
03227     if (rc == -1) {
03228         Vnm_print(0, "Nosh_parsePBSAM: parsePBE error!\n");
03229         break;
03230     } else if (rc == 0) {
03231         rc = PBAMparm_parseToken(parm, tok, sock);
03232         if (rc == -1) {
03233             Vnm_print(0, "Nosh_parsePBSAM: parsePBAM error!\n");
03234             break;
03235         } else if (rc == 0) {
03236             rc = PBSAMparm_parseToken(samparm, tok, sock);
03237             if (rc == -1) {
03238                 Vnm_print(0, "Nosh_parsePBSAM: parsePBSAM error!\n");
03239                 break;
03240             } else if (rc == 0) {
03241                 /* We ran out of parsers! */
03242                 Vnm_print(2, "Nosh: Unrecognized keyword: %s\n", tok);
03243                 break;
03244             }
03245         }
03246     }
03247 }
03248 }
03249 }
03250
03251 pbeparm->setsrfm=1;
03252 pbeparm->setsrad=1;
03253 pbeparm->settemp=1; // do need temp, but have default, incase
03254 pbeparm->setmolid=1; // for unneeded mol flag
03255 pbeparm->setpbetype=1; // unneeded pbe type
03256 pbeparm->setbcfl=1; // unneeded bcfl
03257 pbeparm->setsdens=1;
03258
03259 //This is a hacky fix at best for issue 501. This is so we don't need to change PBAM's
03260 //external code.
03261 if (pbeparm->setnion) {
03262     parm->salt = pbeparm->ionc[pbeparm->nion-1];
03263     parm->setsalt = 1;
03264 }
03265
03266 //This is also a hacky fix for issue 488
03267 if (pbeparm->writefmt[pbeparm->numwrite - 1] == VDF_DX) {
03268     strncpy(parm->dxname, pbeparm->writetestem[pbeparm->numwrite - 1], CHR_MAXLEN);
03269     parm->setdxname = 1;
03270 }
03271 else {
03272     Vnm_print(2, "Nosh: PBSAM only prints in dx format!\n");
03273     return 0;
03274 }
03275
03276 /* Handle various errors arising in the token-snarfing loop -- these all
03277 just result in simple returns right now */

```

```

03279     if (rc == -1) return 0;
03280     if (rc == 0) return 0;
03281
03282     /* Check the status of the parameter objects */
03283     if ((PBSAMparm_check(samparm) == VRC_FAILURE) ||
03284         (PBAMparm_check(parm) == VRC_FAILURE) ||
03285         (!PBEParm_check(pbeparm))) {
03286         Vnm_print(2, "Nosh: PBSAM parameters not set correctly!\n");
03287         return 0;
03288     }
03289     return 1;
03290 }

```

9.36 src/generic/nosh.h File Reference

Contains declarations for class NOsh.

```

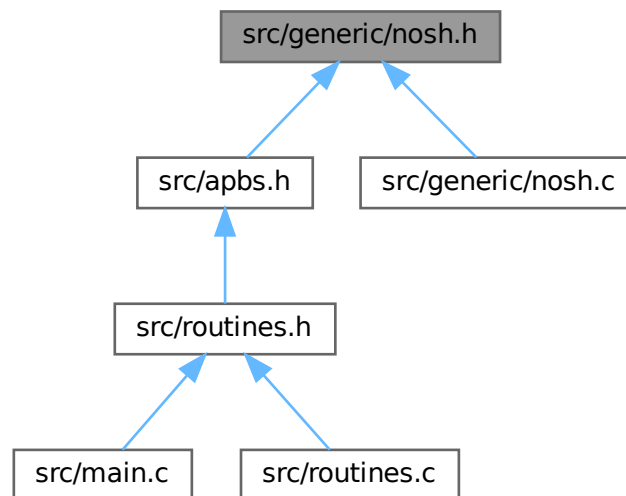
#include "apbscfg.h"
#include "maloc/maloc.h"
#include "generic/vhal.h"
#include "generic/vstring.h"
#include "generic/pbeparm.h"
#include "generic/mgparm.h"
#include "generic/apolparm.h"
#include "generic/femparm.h"
#include "generic/valist.h"
#include "generic/bemparm.h"
#include "generic/geoflowparm.h"
#include "generic/pbamparm.h"
#include "generic/pbsamparm.h"

```

Include dependency graph for nosh.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sNOsh_calc](#)
Calculation class for use when parsing fixed format input files.
- struct [sNOsh](#)
Class for parsing fixed format input files.

Macros

- #define [NOSH_MAXMOL](#) 20
Maximum number of molecules in a run.
- #define [NOSH_MAXCALC](#) 20
Maximum number of calculations in a run.
- #define [NOSH_MAXPRINT](#) 20
Maximum number of PRINT statements in a run.
- #define [NOSH_MAXPOP](#) 20
Maximum number of operations in a PRINT statement.

Typedefs

- typedef enum [eNOsh_MolFormat](#) [NOsh_MolFormat](#)
Declare NOsh_MolFormat type.
- typedef enum [eNOsh_CalcType](#) [NOsh_CalcType](#)
Declare NOsh_CalcType type.
- typedef enum [eNOsh_ParmFormat](#) [NOsh_ParmFormat](#)
Declare NOsh_ParmFormat type.

- typedef enum [eNosh_PrintType](#) [Nosh_PrintType](#)
Declare Nosh_PrintType type.
- typedef struct [sNosh_calc](#) [Nosh_calc](#)
Declaration of the Nosh_calc class as the Nosh_calc structure.
- typedef struct [sNosh](#) [Nosh](#)
Declaration of the Nosh class as the Nosh structure.

Enumerations

- enum [eNosh_MolFormat](#) { [NMF_PQR](#) =0 , [NMF_PDB](#) =1 , [NMF_XML](#) =2 }
Molecule file format types.
- enum [eNosh_CalcType](#) {
[NCT_MG](#) =0 , [NCT_FEM](#) =1 , [NCT_APOL](#) =2 , [NCT_BEM](#) =3 ,
[NCT_GEOFLOW](#) =4 , [NCT_PBAM](#) =5 , [NCT_PBSAM](#) =6 }
Nosh calculation types.
- enum [eNosh_ParmFormat](#) { [NPF_FLAT](#) =0 , [NPF_XML](#) =1 }
Parameter file format types.
- enum [eNosh_PrintType](#) {
[NPT_ENERGY](#) =0 , [NPT_FORCE](#) =1 , [NPT_ELECENERGY](#) , [NPT_ELECFORCE](#) ,
[NPT_APOLENERGY](#) , [NPT_APOLFORCE](#) }
Nosh print types.

Functions

- VEXTERNC char * [Nosh_getMolpath](#) ([Nosh](#) *thee, int imol)
Returns path to specified molecule.
- VEXTERNC char * [Nosh_getDielXpath](#) ([Nosh](#) *thee, int imap)
Returns path to specified x-shifted dielectric map.
- VEXTERNC char * [Nosh_getDielYpath](#) ([Nosh](#) *thee, int imap)
Returns path to specified y-shifted dielectric map.
- VEXTERNC char * [Nosh_getDielZpath](#) ([Nosh](#) *thee, int imap)
Returns path to specified z-shifted dielectric map.
- VEXTERNC char * [Nosh_getKappapath](#) ([Nosh](#) *thee, int imap)
Returns path to specified kappa map.
- VEXTERNC char * [Nosh_getPotpath](#) ([Nosh](#) *thee, int imap)
Returns path to specified potential map.
- VEXTERNC char * [Nosh_getChargepath](#) ([Nosh](#) *thee, int imap)
Returns path to specified charge distribution map.
- VEXTERNC [Nosh_calc](#) * [Nosh_getCalc](#) ([Nosh](#) *thee, int icalc)
Returns specified calculation object.
- VEXTERNC int [Nosh_getDielfmt](#) ([Nosh](#) *thee, int imap)
Returns format of specified dielectric map.
- VEXTERNC int [Nosh_getKappafmt](#) ([Nosh](#) *thee, int imap)
Returns format of specified kappa map.
- VEXTERNC int [Nosh_getPotfmt](#) ([Nosh](#) *thee, int imap)
Returns format of specified potential map.
- VEXTERNC int [Nosh_getChargefmt](#) ([Nosh](#) *thee, int imap)
Returns format of specified charge map.

- VEXTERNC [NOsh_PrintType](#) [NOsh_printWhat](#) ([NOsh](#) *thee, int iprint)
Return an integer ID of the observable to print (.
- VEXTERNC char * [NOsh_elecname](#) ([NOsh](#) *thee, int ielec)
Return an integer mapping of an ELEC statement to a calculation ID (.
- VEXTERNC int [NOsh_elec2calc](#) ([NOsh](#) *thee, int icalc)
Return the name of an elec statement.
- VEXTERNC int [NOsh_apol2calc](#) ([NOsh](#) *thee, int icalc)
Return the name of an apol statement.
- VEXTERNC int [NOsh_printNarg](#) ([NOsh](#) *thee, int iprint)
Return number of arguments to PRINT statement (.
- VEXTERNC int [NOsh_printOp](#) ([NOsh](#) *thee, int iprint, int iarg)
Return integer ID for specified operation (.
- VEXTERNC int [NOsh_printCalc](#) ([NOsh](#) *thee, int iprint, int iarg)
Return calculation ID for specified PRINT statement (.
- VEXTERNC [NOsh](#) * [NOsh_ctor](#) (int rank, int size)
Construct NOsh.
- VEXTERNC [NOsh_calc](#) * [NOsh_calc_ctor](#) ([NOsh_CalcType](#) calcType)
Construct NOsh_calc.
- VEXTERNC int [NOsh_calc_copy](#) ([NOsh_calc](#) *thee, [NOsh_calc](#) *source)
Copy NOsh_calc object into thee.
- VEXTERNC void [NOsh_calc_dtor](#) ([NOsh_calc](#) **thee)
Object destructor.
- VEXTERNC int [NOsh_ctor2](#) ([NOsh](#) *thee, int rank, int size)
FORTTRAN stub to construct NOsh.
- VEXTERNC void [NOsh_dtor](#) ([NOsh](#) **thee)
Object destructor.
- VEXTERNC void [NOsh_dtor2](#) ([NOsh](#) *thee)
FORTTRAN stub for object destructor.
- VEXTERNC int [NOsh_parseInput](#) ([NOsh](#) *thee, Vio *sock)
Parse an input file from a socket.
- VEXTERNC int [NOsh_parseInputFile](#) ([NOsh](#) *thee, char *filename)
Parse an input file only from a file.
- VEXTERNC int [NOsh_setupElecCalc](#) ([NOsh](#) *thee, [Valist](#) *alist[[NOSH_MAXMOL](#)])
Setup the series of electrostatics calculations.
- VEXTERNC int [NOsh_setupApolCalc](#) ([NOsh](#) *thee, [Valist](#) *alist[[NOSH_MAXMOL](#)])
Setup the series of non-polar calculations.

9.36.1 Detailed Description

Contains declarations for class NOsh.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```

*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
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* Pacific Northwest National Laboratory
*
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*
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* ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF
* THE POSSIBILITY OF SUCH DAMAGE.
*
*

```

Definition in file [nosh.h](#).

9.37 nosh.h

[Go to the documentation of this file.](#)

```

00001
00062 #ifndef _NOSH_H_
00063 #define _NOSH_H_
00064
00065 #include "apbscfg.h"
00066
00067 #include "maloc/maloc.h"
00068
00069 #include "generic/vhal.h"
00070 #include "generic/vstring.h"
00071 #include "generic/pbeparm.h"
00072 #include "generic/mgparm.h"
00073 #include "generic/apolparm.h"
00074 #include "generic/femparm.h"
00075 #include "generic/valist.h"

```

```
00076 #include "generic/bemparm.h"
00077 #include "generic/geoflowparm.h"
00078 #include "generic/pbamparm.h"
00079 #include "generic/pbsamparm.h" //path might change
00080
00083 #define NOSH_MAXMOL 20
00084
00087 #define NOSH_MAXCALC 20
00088
00091 #define NOSH_MAXPRINT 20
00092
00095 #define NOSH_MAXPOP 20
00096
00101 enum eNosh_MolFormat {
00102     NMF_PQR=0,
00103     NMF_PDB=1,
00104     NMF_XML=2
00105 };
00106
00111 typedef enum eNosh_MolFormat Nosh_MolFormat;
00112
00117 enum eNosh_CalcType {
00118     NCT_MG=0,
00119     NCT_FEM=1,
00120     NCT_APOL=2,
00121     NCT_BEM=3,
00122     NCT_GEOFLOW=4,
00123     NCT_PBAM=5,
00124     NCT_PBSAM=6
00125 };
00126
00131 typedef enum eNosh_CalcType Nosh_CalcType;
00132
00137 enum eNosh_ParmFormat {
00138     NPF_FLAT=0,
00139     NPF_XML=1
00140 };
00141
00146 typedef enum eNosh_ParmFormat Nosh_ParmFormat;
00147
00152 enum eNosh_PrintType {
00153     NPT_ENERGY=0,
00154     NPT_FORCE=1,
00155     NPT_ELECENERGY,
00156     NPT_ELECFORCE,
00157     NPT_APOLENERGY,
00158     NPT_APOLFORCE
00159 };
00160
00165 typedef enum eNosh_PrintType Nosh_PrintType;
00166
00172 struct sNosh_calc {
00173     MGparm *mgparm;
00174     FEMparm *femparm;
00175     BEMparm *bemparm;
00176     GEOFLOWparm *geoflowparm;
00177     PBAMparm *pbamparm;
00178     PBSAMparm *pbsamparm;
00179     PBEparm *pbeparm;
00180     APOLparm *apolparm;
00181     Nosh_CalcType calctype;
00182 };
00183
00188 typedef struct sNosh_calc Nosh_calc;
00189
00195 struct sNosh {
00196
00197     Nosh_calc *calc[NOSH_MAXCALC];
00200     int ncalc;
00202     Nosh_calc *elec[NOSH_MAXCALC];
00205     int nelec;
00208     Nosh_calc *apol[NOSH_MAXCALC];
00211     int napol;
00214     int ispara;
00215     int proc_rank;
00216     int proc_size;
00217     int bogus;
00221     int elec2calc[NOSH_MAXCALC];
00229     int apol2calc[NOSH_MAXCALC];
00231     int nmol;
00232     char molpath[NOSH_MAXMOL][VMAX_ARGLEN];
```

```

00233     Nosh_MolFormat molfmt[NOSH_MAXMOL];
00234     Valist *alist[NOSH_MAXMOL];
00235     int gotparm;
00236     char parmpath[VMAX_ARGLEN];
00237     Nosh_ParmFormat parmfmt;
00238     int ndiel;
00239     char dielXpath[NOSH_MAXMOL][VMAX_ARGLEN];
00240     char dielYpath[NOSH_MAXMOL][VMAX_ARGLEN];
00241     char dielZpath[NOSH_MAXMOL][VMAX_ARGLEN];
00242     Vdata_Format dielfmt[NOSH_MAXMOL];
00243     int nkappa;
00244     char kappapath[NOSH_MAXMOL][VMAX_ARGLEN];
00245     Vdata_Format kappafmt[NOSH_MAXMOL];
00246     int npot;
00247     char potpath[NOSH_MAXMOL][VMAX_ARGLEN];
00248     Vdata_Format potfmt[NOSH_MAXMOL];
00249     int ncharge;
00250     char chargepath[NOSH_MAXMOL][VMAX_ARGLEN];
00251     Vdata_Format chargefmt[NOSH_MAXMOL];
00252     int nmesh;
00253     char meshpath[NOSH_MAXMOL][VMAX_ARGLEN];
00254     Vdata_Format meshfmt[NOSH_MAXMOL];
00255     int nprint;
00256     Nosh_PrintType printwhat[NOSH_MAXPRINT];
00257     int printnarg[NOSH_MAXPRINT];
00258     int printcalc[NOSH_MAXPRINT][NOSH_MAXPOP];
00259     int printop[NOSH_MAXPRINT][NOSH_MAXPOP];
00260     int parsed;
00261     char elecname[NOSH_MAXCALC][VMAX_ARGLEN];
00262     char apolname[NOSH_MAXCALC][VMAX_ARGLEN];
00271 };
00272
00273 typedef struct sNosh Nosh;
00274
00275 /* ////////////////////////////////////////////////////
00276 // Class Nosh: Inlineable methods (mcsh.c)
00277 ////////////////////////////////////////////////////
00282 #if !defined(VINLINE_NOSH)
00283 VEXTERNC char* Nosh_getMolpath(Nosh *thee, int imol);
00284
00285 VEXTERNC char* Nosh_getDielXpath(Nosh *thee, int imap);
00286
00287 VEXTERNC char* Nosh_getDielYpath(Nosh *thee, int imap);
00288
00289 VEXTERNC char* Nosh_getDielZpath(Nosh *thee, int imap);
00290
00291 VEXTERNC char* Nosh_getKappapath(Nosh *thee, int imap);
00292
00293 VEXTERNC char* Nosh_getPotpath(Nosh *thee, int imap);
00294
00295 VEXTERNC char* Nosh_getChargepath(Nosh *thee, int imap);
00296
00297 VEXTERNC Nosh_calc* Nosh_getCalc(Nosh *thee, int icalc);
00298
00299 VEXTERNC int Nosh_getDielfmt(Nosh *thee, int imap);
00300
00301 VEXTERNC int Nosh_getKappafmt(Nosh *thee, int imap);
00302
00303 VEXTERNC int Nosh_getPotfmt(Nosh *thee, int imap);
00304
00305 VEXTERNC int Nosh_getChargefmt(Nosh *thee, int imap);
00306 #else
00307 #
00308 # define Nosh_getMolpath(thee, imol) ((thee)->molpath[(imol)])
00309 # define Nosh_getDielXpath(thee, imol) ((thee)->dielXpath[(imol)])
00310 # define Nosh_getDielYpath(thee, imol) ((thee)->dielYpath[(imol)])
00311 # define Nosh_getDielZpath(thee, imol) ((thee)->dielZpath[(imol)])
00312 # define Nosh_getKappapath(thee, imol) ((thee)->kappapath[(imol)])
00313 # define Nosh_getPotpath(thee, imol) ((thee)->potpath[(imol)])
00314 # define Nosh_getChargepath(thee, imol) ((thee)->chargepath[(imol)])
00315 # define Nosh_getCalc(thee, icalc) ((thee)->calc[(icalc)])
00316 # define Nosh_getDielfmt(thee, imap) ((thee)->dielfmt[(imap)])
00317 # define Nosh_getKappafmt(thee, imap) ((thee)->kappafmt[(imap)])
00318 # define Nosh_getPotfmt(thee, imap) ((thee)->potfmt[(imap)])
00319 # define Nosh_getChargefmt(thee, imap) ((thee)->chargefmt[(imap)])
00320 #endif
00321
00322 /* ////////////////////////////////////////////////////
00323 // Class Nosh: Non-inlineable methods (mcsh.c)
00324 ////////////////////////////////////////////////////

```

```

00412
00420 VEXTERNC NOsh_PrintType NOsh_printWhat(NOsh *thee, int iprint);
00421
00431 VEXTERNC char* NOsh_elecname(NOsh *thee, int ielec);
00432
00440 VEXTERNC int NOsh_elec2calc(NOsh *thee, int icalc);
00441
00449 VEXTERNC int NOsh_apol2calc(NOsh *thee, int icalc);
00450
00458 VEXTERNC int NOsh_printNarg(NOsh *thee, int iprint);
00459
00468 VEXTERNC int NOsh_printOp(NOsh *thee, int iprint, int iarg);
00469
00480 VEXTERNC int NOsh_printCalc(NOsh *thee, int iprint, int iarg);
00481
00491 VEXTERNC NOsh* NOsh_ctor(int rank, int size);
00492
00499 VEXTERNC NOsh_calc* NOsh_calc_ctor(
00500     NOsh_CalcType calcType
00501 );
00502
00509 VEXTERNC int NOsh_calc_copy(
00510     NOsh_calc *thee,
00511     NOsh_calc *source
00512 );
00513
00519 VEXTERNC void NOsh_calc_dtor(NOsh_calc **thee);
00520
00531 VEXTERNC int NOsh_ctor2(NOsh *thee, int rank, int size);
00532
00538 VEXTERNC void NOsh_dtor(NOsh **thee);
00539
00545 VEXTERNC void NOsh_dtor2(NOsh *thee);
00546
00555 VEXTERNC int NOsh_parseInput(NOsh *thee, Vio *sock);
00556
00566 VEXTERNC int NOsh_parseInputFile(NOsh *thee, char *filename);
00567
00577 VEXTERNC int NOsh_setupElecCalc(
00578     NOsh *thee, /**< NOsh object */
00579     Valist *alist[NOSH_MAXMOL]
00580 );
00581
00591 VEXTERNC int NOsh_setupApolCalc(
00592     NOsh *thee,
00593     Valist *alist[NOSH_MAXMOL]
00594 );
00595
00596 #endif
00597

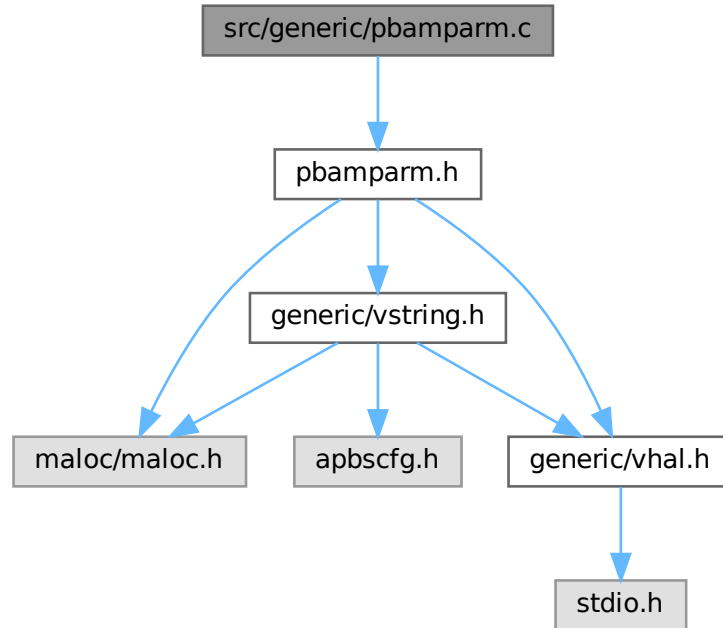
```

9.38 src/generic/pbamparm.c File Reference

Class PBAMparm methods.

```
#include "pbamparm.h"
```

Include dependency graph for pbamparm.c:



Functions

- VPUBLIC PBAMparm * PBAMparm_ctor (PBAMparm_CalcType type)
Construct PBAMparm object.
- VPUBLIC Vrc_Codes PBAMparm_ctor2 (PBAMparm *thee, PBAMparm_CalcType type)
FORTTRAN stub to construct PBAMparm object ????????!!!!!!
- VPUBLIC void PBAMparm_dtor (PBAMparm **thee)
Object destructor.
- VPUBLIC void PBAMparm_dtor2 (PBAMparm *thee)
FORTTRAN stub for object destructor ????????!!!!!!
- VPUBLIC Vrc_Codes PBAMparm_check (PBAMparm *thee)
Consistency check for parameter values stored in object.
- VPUBLIC void PBAMparm_copy (PBAMparm *thee, PBAMparm *parm)
copy PBAMparm object int thee.
- VPRIVATE Vrc_Codes PBAMparm_parseSalt (PBAMparm *thee, Vio *sock)
Find salt conc and save it as a structure variable.
- VPRIVATE Vrc_Codes PBAMparm_parseRunType (PBAMparm *thee, Vio *sock)
Find runType and save it as a structure variable.
- VPRIVATE Vrc_Codes PBAMparm_parseRunName (PBAMparm *thee, Vio *sock)
Find runName and save it as a structure variable.

- VPRIVATE Vrc_Codes [PBAMparm_parseRanorient](#) (PBAMparm *thee, Vio *sock)
Find ranomorientation flag and save it as a boolean.
- VPRIVATE Vrc_Codes [PBAMparm_parsePBCS](#) (PBAMparm *thee, Vio *sock)
Find PBC flag and save the type and the boxlength.
- VPRIVATE Vrc_Codes [PBAMparm_parseUnits](#) (PBAMparm *thee, Vio *sock)
Find units flag and save units.
- VPRIVATE Vrc_Codes [PBAMparm_parseGridPts](#) (PBAMparm *thee, Vio *sock)
Find Grid points and save them.
- VPRIVATE Vrc_Codes [PBAMparm_parse3Dmap](#) (PBAMparm *thee, Vio *sock)
Find 3D map filename and save it.
- VPRIVATE Vrc_Codes [PBAMparm_parseGrid2D](#) (PBAMparm *thee, Vio *sock)
Find 2D grid filename and save it.
- VPRIVATE Vrc_Codes [PBAMparm_parseDX](#) (PBAMparm *thee, Vio *sock)
Find DX filename and save it.
- VPRIVATE Vrc_Codes [PBAMparm_parseTermcombine](#) (PBAMparm *thee, Vio *sock)
Find Termination logic and save it.
- VPRIVATE Vrc_Codes [PBAMparm_parseNtraj](#) (PBAMparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [PBAMparm_parseDiff](#) (PBAMparm *thee, Vio *sock)
Find diffusion coeffs for each molecule and save them.
- VPRIVATE Vrc_Codes [PBAMparm_parseTerm](#) (PBAMparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [PBAMparm_parseXYZ](#) (PBAMparm *thee, Vio *sock)
Find xyz files for each molecule for each traj and save them.
- VPUBLIC Vrc_Codes [PBAMparm_parseToken](#) (PBAMparm *thee, char tok[VMAX_BUFSIZE], Vio *sock)
Parse an MG keyword from an input file.

9.38.1 Detailed Description

Class PBAMparm methods.

Author

Andrew Stevens

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
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* Pacific Northwest National Laboratory
*
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```

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*
*

```

Definition in file [pbamparm.c](#).

9.38.2 Function Documentation

9.38.2.1 PBAMparm_parseNtraj()

```

VPRIVATE Vrc_Codes PBAMparm_parseNtraj (
    PBAMparm * thee,
    Vio * sock )

```

Definition at line 458 of file [pbamparm.c](#).

9.38.2.2 PBAMparm_parseTerm()

```

VPRIVATE Vrc_Codes PBAMparm_parseTerm (
    PBAMparm * thee,
    Vio * sock )

```

Definition at line 549 of file [pbamparm.c](#).

9.39 pbamparm.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "pbamparm.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 #if !defined(VINLINE_MGPARM)
00062
00063 #endif /* if !defined(VINLINE_MGPARM) */

```

```

00064
00065
00066 VPUBLIC PBAMparm* PBAMparm_ctor(PBAMparm_CalcType type) {
00067
00068     /* Set up the structure */
00069     PBAMparm *thee = VNULL;
00070     thee = (PBAMparm*)Vmem_malloc(VNULL, 1, sizeof(PBAMparm));
00071     VASSERT( thee != VNULL);
00072     VASSERT( PBAMparm_ctor2(thee, type) == VRC_SUCCESS );
00073
00074     return thee;
00075 }
00076
00077 VPUBLIC Vrc_Codes PBAMparm_ctor2(PBAMparm *thee, PBAMparm_CalcType type) {
00078
00079     int i;
00080
00081     if (thee == VNULL) return VRC_FAILURE;
00082
00083     thee->parsed = 0;
00084     thee->type = type;
00085     thee->salt = 0;
00086
00087     thee->setsalt = 0;
00088     thee->setruntype = 0;
00089     thee->setrunname = 0;
00090     thee->setunits = 0;
00091
00092     thee->setrandorient = 0;
00093
00094     thee->setpbcs = 0;
00095     thee->pbcbboxlen = 1e15;
00096
00097     // Electrostatics
00098     thee->gridpt = 15;
00099     printf("Found a pts flag in ctor: %d\n", thee->gridpt);
00100     thee->setgridpt = 0;
00101     thee->set3dmap = 0;
00102     thee->setgrid2Dname = 0;
00103     thee->grid2Dct = 0;
00104     thee->setdxname = 0;
00105
00106     //Dynamics
00107     thee->ntraj = 1;
00108     thee->setntraj = 0;
00109
00110     thee->settermcombine = 0;
00111     thee->diffct = 0;
00112
00113     thee->termct = 0;
00114     thee->setterm = 0;
00115
00116     thee->setxyz = 0;
00117     for (i = 0; i<PBAMPARM_MAXMOL; i++) thee->xyzct[i] = 0;
00118
00119     return VRC_SUCCESS;
00120 }
00121
00122 VPUBLIC void PBAMparm_dtor(PBAMparm **thee) {
00123     if ((*thee) != VNULL) {
00124         PBAMparm_dtor2(*thee);
00125         Vmem_free(VNULL, 1, sizeof(PBAMparm), (void **)thee);
00126         (*thee) = VNULL;
00127     }
00128 }
00129
00130 VPUBLIC void PBAMparm_dtor2(PBAMparm *thee) { ; }
00131
00132 VPUBLIC Vrc_Codes PBAMparm_check(PBAMparm *thee) {
00133
00134     Vrc_Codes rc;
00135
00136     rc = VRC_SUCCESS;
00137
00138     Vnm_print(0, "PBAMparm_check:  checking PBAMparm object of type %d.\n",
00139             thee->type);
00140
00141     /* Check to see if we were even filled... */
00142     if (!thee->parsed) {
00143         Vnm_print(2, "PBAMparm_check:  not filled!\n");
00144         return VRC_FAILURE;

```

```

00145     }
00146
00147
00148     /* Check type settings */
00149     if (thee->type != PBAMCT_AUTO) {
00150         Vnm_print(2, "PBAMparm_check: type not set");
00151         rc = VRC_FAILURE;
00152     }
00153
00154     return rc;
00155 }
00156
00157 VPUBLIC void PBAMparm_copy(PBAMparm *thee, PBAMparm *parm) {
00158     int i, j, k;
00159     VASSERT(thee != VNULL);
00160     VASSERT(parm != VNULL);
00161
00162     thee->type = parm->type;
00163     thee->parsed = parm->parsed;
00164
00165     thee->salt = parm->salt;
00166     thee->setsalt = parm->setsalt;
00167     for (i=0; i<CHR_MAXLEN; i++) thee->runtype[i] = parm->runtype[i];
00168     thee->setruntype = parm->setruntype;
00169
00170     for (i=0; i<CHR_MAXLEN; i++) thee->runname[i] = parm->runname[i];
00171     thee->setrunname = parm->setrunname;
00172
00173     thee->setrandorient = parm->setrandorient;
00174
00175     thee->setpbcs = parm->setpbcs;
00176     thee->pbcbboxlen = parm->pbcbboxlen;
00177
00178     for (i=0; i<CHR_MAXLEN; i++) thee->units[i] = parm->units[i];
00179     thee->setunits = parm->setunits;
00180
00181     // Electrostatic parts
00182     thee->gridpt = parm->gridpt;
00183     thee->setgridpt = parm->setgridpt;
00184     for (i=0; i<CHR_MAXLEN; i++) thee->map3dname[i] = parm->map3dname[i];
00185     thee->set3dmap = parm->set3dmap;
00186
00187
00188     thee->grid2Dct = parm->grid2Dct;
00189     for (i=0; i<PBAMPARM_MAXWRITE; i++)
00190     {
00191         for (j=0; j<CHR_MAXLEN; j++)
00192         {
00193             thee->grid2Dname[i][j] = parm->grid2Dname[i][j];
00194             thee->grid2Dax[i][j] = parm->grid2Dax[i][j];
00195         }
00196         thee->grid2Dloc[i] = parm->grid2Dloc[i];
00197     }
00198
00199     for (i=0; i<CHR_MAXLEN; i++) thee->dxname[i] = parm->dxname[i];
00200     thee->setdxname = parm->setdxname;
00201
00202     // Dynamics parts
00203     thee->ntraj = parm->ntraj;
00204     thee->setntraj = parm->setntraj;
00205
00206     for (i=0; i<CHR_MAXLEN; i++) thee->termcombine[i] = parm->termcombine[i];
00207     thee->settermcombine = parm->settermcombine;
00208
00209     thee->diffct = parm->diffct;
00210
00211     for (i=0; i<PBAMPARM_MAXMOL; i++)
00212     {
00213         for (j=0; j<CHR_MAXLEN; j++)
00214         {
00215             thee->moveType[i][j] = parm->moveType[i][j];
00216         }
00217         thee->transDiff[i] = parm->transDiff[i];
00218         thee->rotDiff[i] = parm->rotDiff[i];
00219     }
00220
00221     thee->termct = parm->termct;
00222     thee->setterm = parm->setterm;
00223     thee->confilct = parm->confilct;
00224
00225     for (i=0; i<PBAMPARM_MAXWRITE; i++)

```

```

00226     {
00227         for (j=0; j<CHR_MAXLEN; j++)
00228         {
00229             thee->termnam[i][j] = parm->termnam[i][j];
00230             thee->confil[i][j] = parm->confil[i][j];
00231         }
00232         thee->termVal[i] = parm->termVal[i];
00233         thee->termnu[i][0] = parm->termnu[i][0];
00234     }
00235
00236     thee->setxyz = parm->setxyz;
00237     for (i = 0; i<PBAMPARM_MAXMOL; i++)
00238     {
00239         thee->xyzct[i] = parm->xyzct[i];
00240         for (j = 0; j<PBAMPARM_MAXWRITE; j++)
00241         {
00242             for (k = 0; k<CHR_MAXLEN; k++)
00243             {
00244                 thee->xyzfil[i][j][k] = parm->xyzfil[i][j][k];
00245             }
00246         }
00247     }
00248 }
00249 }
00250
00251
00252 VPRIVATE Vrc_Codes PBAMParm_parseSalt(PBAMParm *thee, Vio *sock){
00253     const char* name = "salt";
00254     char tok[VMAX_BUFSIZE];
00255     double tf;
00256     if(Vio_scanf(sock, "%s", tok) == 0) {
00257         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00258         return VRC_WARNING;
00259     }
00260
00261     if (sscanf(tok, "%lf", &tf) == 0){
00262         Vnm_print(2, "Nosh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00263         return VRC_WARNING;
00264     }else{
00265         thee->salt = tf;
00266     }
00267     thee->setsalt = 1;
00268     return VRC_SUCCESS;
00269 }
00270
00271 VPRIVATE Vrc_Codes PBAMParm_parseRunType(PBAMParm *thee, Vio *sock){
00272     const char* name = "runtype";
00273     char tok[VMAX_BUFSIZE];
00274
00275     if(Vio_scanf(sock, "%s", tok) == 0) {
00276         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00277         return VRC_WARNING;
00278     } else if(Vstring_strcasecmp(tok, "dynamics") == 0){
00279         Vnm_print(2, "parsePBAM: Dynamics has been moved out of the ELEC section!\n");
00280         return VRC_WARNING;
00281     } else {
00282         strncpy(thee->runtype, tok, CHR_MAXLEN);
00283         thee->setruntype=1;
00284     }
00285
00286     return VRC_SUCCESS;
00287 }
00288
00289 VPRIVATE Vrc_Codes PBAMParm_parseRunName(PBAMParm *thee, Vio *sock){
00290     const char* name = "runname";
00291     char tok[VMAX_BUFSIZE];
00292
00293     if(Vio_scanf(sock, "%s", tok) == 0) {
00294         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00295         return VRC_WARNING;
00296     } else {
00297         strncpy(thee->runname, tok, CHR_MAXLEN);
00298         thee->setrunname=1;
00299     }
00300
00301     return VRC_SUCCESS;
00302 }
00303
00304 VPRIVATE Vrc_Codes PBAMParm_parseRandonrient(PBAMParm *thee, Vio *sock){
00305     const char* name = "randonrient";
00306     thee->setrandonrient=1;

```

```

00307     return VRC_SUCCESS;
00308 }
00309
00310 VPRIVATE Vrc_Codes PBAMparm_parsePBCS(PBAMparm *thee, Vio *sock){
00311     const char* name = "pbc";
00312     char tok[VMAX_BUFSIZE];
00313     double tf;
00314     int td;
00315     if(Vio_scanf(sock, "%s", tok) == 0) {
00316         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00317         return VRC_WARNING;
00318     }
00319
00320     if (sscanf(tok, "%d", &td) == 0) {
00321         Vnm_print(2, "parsePBAM: Read non-int (%s) while parsing pbc keyword!\n", tok);
00322         return VRC_FAILURE;
00323     } else{
00324         thee->setpbc = td;
00325     }
00326
00327     if (sscanf(tok, "%lf", &tf) == 0){
00328         Vnm_print(2, "Nosh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00329         return VRC_WARNING;
00330     }else{
00331         thee->pbcboxlen = tf;
00332     }
00333     return VRC_SUCCESS;
00334 }
00335
00336 VPRIVATE Vrc_Codes PBAMparm_parseUnits(PBAMparm *thee, Vio *sock){
00337     const char* name = "units";
00338     char tok[VMAX_BUFSIZE];
00339
00340     if(Vio_scanf(sock, "%s", tok) == 0) {
00341         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00342         return VRC_WARNING;
00343     } else {
00344         strncpy(thee->units, tok, CHR_MAXLEN);
00345         thee->setunits=1;
00346     }
00347
00348     return VRC_SUCCESS;
00349 }
00350
00351 VPRIVATE Vrc_Codes PBAMparm_parseGridPts(PBAMparm *thee, Vio *sock){
00352     const char* name = "dime";
00353     char tok[VMAX_BUFSIZE];
00354     int td;
00355     if(Vio_scanf(sock, "%s", tok) == 0) {
00356         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00357         return VRC_WARNING;
00358     }
00359
00360     if (sscanf(tok, "%d", &td) == 0){
00361         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing %s keyword!\n", tok, name);
00362         return VRC_WARNING;
00363     }else{
00364         printf("Found a dime flag in parse: %d\n", td);
00365         thee->gridpt = td;
00366     }
00367     thee->setgridpt = 1;
00368     return VRC_SUCCESS;
00369 }
00370
00371 VPRIVATE Vrc_Codes PBAMparm_parse3Dmap(PBAMparm *thee, Vio *sock){
00372     const char* name = "3dmap";
00373     char tok[VMAX_BUFSIZE];
00374
00375     Vnm_print(2, "PBAM: 3dmap keyword has been deprecated! Please use in conjunction with the write
keyword.");
00376     return VRC_FAILURE;
00377
00378     /*
00379     if(Vio_scanf(sock, "%s", tok) == 0) {
00380         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00381         return VRC_WARNING;
00382     } else {
00383         strncpy(thee->map3dname, tok, CHR_MAXLEN);
00384         thee->set3dmap=1;
00385     }
00386

```

```

00387     return VRC_SUCCESS;
00388  */
00389  }
00390
00391  VPRIVATE Vrc_Codes PBAMparm_parseGrid2D(PBAMparm *thee, Vio *sock){
00392     const char* name = "grid2d";
00393     char tok[VMAX_BUFSIZE];
00394     double tf;
00395
00396     if(Vio_scanf(sock, "%s", tok) == 0) {
00397         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00398         return VRC_WARNING;
00399     } else {
00400         strncpy(thee->grid2Dname[thee->grid2Dct], tok, CHR_MAXLEN);
00401         thee->setgrid2Dname=1;
00402     }
00403
00404     if(Vio_scanf(sock, "%s", tok) == 0) {
00405         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00406         return VRC_WARNING;
00407     } else {
00408         strncpy(thee->grid2Dax[thee->grid2Dct], tok, CHR_MAXLEN);
00409     }
00410
00411     if(Vio_scanf(sock, "%s", tok) == 0) {
00412         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00413         return VRC_WARNING;
00414     }
00415
00416     if (sscanf(tok, "%lf", &tf) == 0){
00417         Vnm_print(2, "Nosh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00418         return VRC_WARNING;
00419     }else{
00420         thee->grid2Dloc[thee->grid2Dct] = tf;
00421         thee->grid2Dct = thee->grid2Dct+1;
00422     }
00423     return VRC_SUCCESS;
00424 }
00425
00426 VPRIVATE Vrc_Codes PBAMparm_parseDX(PBAMparm *thee, Vio *sock){
00427     Vnm_print(2, "PBAM's dx keyword is deprecated. Please use the write keyword!\n");
00428     return VRC_FAILURE;
00429  /*
00430     const char* name = "dx";
00431     char tok[VMAX_BUFSIZE];
00432
00433     if(Vio_scanf(sock, "%s", tok) == 0) {
00434         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00435         return VRC_WARNING;
00436     } else {
00437         strncpy(thee->dxname, tok, CHR_MAXLEN);
00438         thee->setdxname=1;
00439     }
00440     return VRC_SUCCESS;
00441  */
00442  }
00443
00444  VPRIVATE Vrc_Codes PBAMparm_parseTermcombine(PBAMparm *thee, Vio *sock){
00445     const char* name = "termcombine";
00446     char tok[VMAX_BUFSIZE];
00447
00448     if(Vio_scanf(sock, "%s", tok) == 0) {
00449         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00450         return VRC_WARNING;
00451     } else {
00452         strncpy(thee->termcombine, tok, CHR_MAXLEN);
00453         thee->settermcombine=1;
00454     }
00455     return VRC_SUCCESS;
00456  }
00457
00458  VPRIVATE Vrc_Codes PBAMparm_parseNtraj(PBAMparm *thee, Vio *sock){
00459     const char* name = "ntraj";
00460     char tok[VMAX_BUFSIZE];
00461     int td;
00462     if(Vio_scanf(sock, "%s", tok) == 0) {
00463         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00464         return VRC_WARNING;
00465     }
00466
00467     if (sscanf(tok, "%d", &td) == 0){

```

```
00468         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing %s keyword!\n", tok, name);
00469         return VRC_WARNING;
00470     }else{
00471         thee->ntraj = td;
00472     }
00473     thee->setntraj = 1;
00474     return VRC_SUCCESS;
00475 }
00476
00477 VPRIVATE Vrc_Codes PBAMparm_parseDiff(PBAMparm *thee, Vio *sock){
00478     const char* name = "diff";
00479     char tok[VMAX_BUFSIZE];
00480     int molind;
00481     double tf;
00482
00483     if(Vio_scanf(sock, "%s", tok) == 0) {
00484         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00485         return VRC_WARNING;
00486     }
00487
00488     // // looking for index
00489     if (sscanf(tok, "%d", &molind) == 0){
00490         Vnm_print(2, "Nosh: Read non-int (%s) while parsing %s keyword!\n", tok, name);
00491         return VRC_WARNING;
00492     }
00493
00494     molind -= 1;
00495     // looking for move type = move, stat, rot
00496     if(Vio_scanf(sock, "%s", tok) == 0) {
00497         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00498         return VRC_WARNING;
00499     } else {
00500         strncpy(thee->moveType[molind], tok, CHR_MAXLEN);
00501         thee->diffct += 1;
00502     }
00503
00504     if (strcmp(thee->moveType[molind], "move", 4) == 0)
00505     {
00506         if(Vio_scanf(sock, "%s", tok) == 0) {
00507             Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00508             return VRC_WARNING;
00509         }
00510         if (sscanf(tok, "%lf", &tf) == 0){
00511             Vnm_print(2, "Nosh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00512             return VRC_WARNING;
00513         }else{
00514             thee->transDiff[molind] = tf;
00515         }
00516
00517         // rot diffusion coeff
00518         if(Vio_scanf(sock, "%s", tok) == 0) {
00519             Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00520             return VRC_WARNING;
00521         }
00522         if (sscanf(tok, "%lf", &tf) == 0){
00523             Vnm_print(2, "Nosh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00524             return VRC_WARNING;
00525         }else{
00526             thee->rotDiff[molind] = tf;
00527         }
00528     } else if (strcmp(thee->moveType[molind], "rot", 3) == 0)
00529     {
00530         if(Vio_scanf(sock, "%s", tok) == 0) {
00531             Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00532             return VRC_WARNING;
00533         }
00534         if (sscanf(tok, "%lf", &tf) == 0){
00535             Vnm_print(2, "Nosh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00536             return VRC_WARNING;
00537         }else{
00538             thee->rotDiff[molind] = tf;
00539             thee->transDiff[molind] = 0.0;
00540         }
00541     } else{
00542         thee->transDiff[molind] = 0.0;
00543         thee->rotDiff[molind] = 0.0;
00544     }
00545
00546     return VRC_SUCCESS;
00547 }
00548
```

```

00549 VPRIVATE Vrc_Codes PBAMparm_parseTerm(PBAMparm *thee, Vio *sock){
00550     const char* name = "term";
00551     char tok[VMAX_BUFSIZE];
00552     double tf;
00553     int td;
00554
00555     // looking for term name
00556     if(Vio_scanf(sock, "%s", tok) == 0) {
00557         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00558         return VRC_WARNING;
00559     }else {
00560         if(strncmp(tok, "position", 8)==0){
00561             return PBAMparm_parseTerm(thee, sock);
00562         }else{
00563             strncpy(thee->termnam[thee->termct], tok, CHR_MAXLEN);
00564         }
00565     }
00566
00567     if (strncmp(thee->termnam[thee->termct], "contact", 7) == 0)
00568     {
00569         if(Vio_scanf(sock, "%s", tok) == 0) {
00570             Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00571             return VRC_WARNING;
00572         }else{
00573             strncpy(thee->confil[thee->confilct], tok, CHR_MAXLEN);
00574         }
00575
00576         if(Vio_scanf(sock, "%s", tok) == 0) {
00577             Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00578             return VRC_WARNING;
00579         }
00580         if (sscanf(tok, "%lf", &tf) == 0){
00581             Vnm_print(2, "NOsh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00582             return VRC_WARNING;
00583         }else
00584         {
00585             thee->termVal[thee->termct] = tf;
00586             thee->termnu[thee->termct][0] = 0;
00587             thee->confilct += 1;
00588         }
00589     } else if (strncmp(thee->termnam[thee->termct], "time", 4) == 0)
00590     {
00591         if(Vio_scanf(sock, "%s", tok) == 0) {
00592             Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00593             return VRC_WARNING;
00594         }
00595         if (sscanf(tok, "%lf", &tf) == 0){
00596             Vnm_print(2, "NOsh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00597             return VRC_WARNING;
00598         }else{
00599             thee->termVal[thee->termct] = tf;
00600             thee->termnu[thee->termct][0] = 0;
00601         }
00602     } else //if (strncmp(thee->termnam[thee->termct], "position", 8) == 0)
00603     {
00604         if(Vio_scanf(sock, "%s", tok) == 0) {
00605             Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00606             return VRC_WARNING;
00607         }
00608         if (sscanf(tok, "%lf", &tf) == 0){
00609             Vnm_print(2, "NOsh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00610             return VRC_WARNING;
00611         }else{
00612             thee->termVal[thee->termct] = tf;
00613         }
00614
00615         if(Vio_scanf(sock, "%s", tok) == 0) {
00616             Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00617             return VRC_WARNING;
00618         }
00619         if (sscanf(tok, "%d", &td) == 0){
00620             Vnm_print(2, "NOsh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00621             return VRC_WARNING;
00622         }else{
00623             thee->termnu[thee->termct][0] = td-1;
00624         }
00625     }
00626
00627     thee->setterm = 1;
00628     thee->termct += 1;
00629     return VRC_SUCCESS;

```



```

00630 }
00631
00632 VPRIVATE Vrc_Codes PBAMparm_parseXYZ(PBAMparm *thee, Vio *sock){
00633     const char* name = "xyz";
00634     char tok[VMAX_BUFSIZE];
00635     int td, mol;
00636
00637     if(Vio_scanf(sock, "%s", tok) == 0) {
00638         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00639         return VRC_WARNING;
00640     }
00641
00642     // // looking for index
00643     if (sscanf(tok, "%d", &td) == 0){
00644         Vnm_print(2, "Nosh: Read non-int (%s) while parsing %s keyword!\n", tok, name);
00645         return VRC_WARNING;
00646     } else{
00647         printf("This is my mol in parseXYZ: %d", td);
00648         mol = td-1;
00649     }
00650
00651     // looking for move type = move, stat, rot
00652     if(Vio_scanf(sock, "%s", tok) == 0) {
00653         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00654         return VRC_WARNING;
00655     } else {
00656         strncpy(thee->xyzfil[mol][thee->xyzct[mol]], tok, CHR_MAXLEN);
00657         thee->xyzct[mol] += 1;
00658     }
00659     return VRC_SUCCESS;
00660 }
00661
00662 VPUBLIC Vrc_Codes PBAMparm_parseToken(PBAMparm *thee, char tok[VMAX_BUFSIZE],
00663 Vio *sock) {
00664
00665     if (thee == VNULL) {
00666         Vnm_print(2, "parsePBAM: got NULL thee!\n");
00667         return VRC_WARNING;
00668     }
00669     if (sock == VNULL) {
00670         Vnm_print(2, "parsePBAM: got NULL socket!\n");
00671         return VRC_WARNING;
00672     }
00673
00674     Vnm_print(0, "PBAMparm_parseToken: trying %s...\n", tok);
00675
00676     // General terms to parse
00677     if (Vstring_strcasecmp(tok, "salt") == 0) {
00678         return PBAMparm_parseSalt(thee, sock);
00679     } else if (Vstring_strcasecmp(tok, "runtype") == 0) {
00680         return PBAMparm_parseRunType(thee, sock);
00681     } else if (Vstring_strcasecmp(tok, "runname") == 0) {
00682         return PBAMparm_parseRunName(thee, sock);
00683     } else if (Vstring_strcasecmp(tok, "randorient") == 0) {
00684         return PBAMparm_parseRandorient(thee, sock);
00685     } else if (Vstring_strcasecmp(tok, "pbc") == 0) {
00686         return PBAMparm_parsePBCS(thee, sock);
00687     } else if (Vstring_strcasecmp(tok, "units") == 0) {
00688         return PBAMparm_parseUnits(thee, sock);
00689     }
00690
00691     // Electrostatic parsing
00692     else if (Vstring_strcasecmp(tok, "dime") == 0) {
00693         return PBAMparm_parseGridPts(thee, sock);
00694     } else if (Vstring_strcasecmp(tok, "3dmap") == 0) {
00695         return PBAMparm_parse3Dmap(thee, sock);
00696     } else if (Vstring_strcasecmp(tok, "grid2d") == 0) {
00697         return PBAMparm_parseGrid2D(thee, sock);
00698     } else if (Vstring_strcasecmp(tok, "dx") == 0) {
00699         return PBAMparm_parseDX(thee, sock);
00700     }
00701
00702     // Dynamics parsing
00703     else if (Vstring_strcasecmp(tok, "ntraj") == 0) {
00704         return PBAMparm_parseNtraj(thee, sock);
00705     } else if (Vstring_strcasecmp(tok, "termcombine") == 0) {
00706         return PBAMparm_parseTermcombine(thee, sock);
00707     } else if (Vstring_strcasecmp(tok, "diff") == 0) {
00708         return PBAMparm_parseDiff(thee, sock);
00709     } else if (Vstring_strcasecmp(tok, "term") == 0) {
00710         return PBAMparm_parseTerm(thee, sock);

```

```

00711     }else if (Vstring_strcasecmp(tok, "xyz") == 0) {
00712         return PBAMparm_parseXYZ(thee, sock);
00713     }
00714
00715     else
00716         return 0;
00717
00718
00719     /*else {
00720         Vnm_print(2, "parsePBAM:  Unrecognized keyword (%s)!\n", tok);
00721         return VRC_WARNING;
00722     }
00723     return VRC_FAILURE;
00724 */
00725 }

```

9.40 src/generic/pbamparm.h File Reference

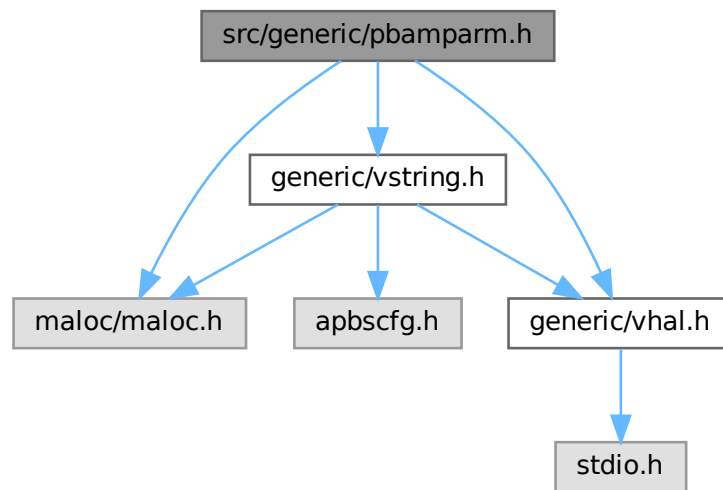
Contains declarations for class PBAMparm.

```
#include "maloc/maloc.h"
```

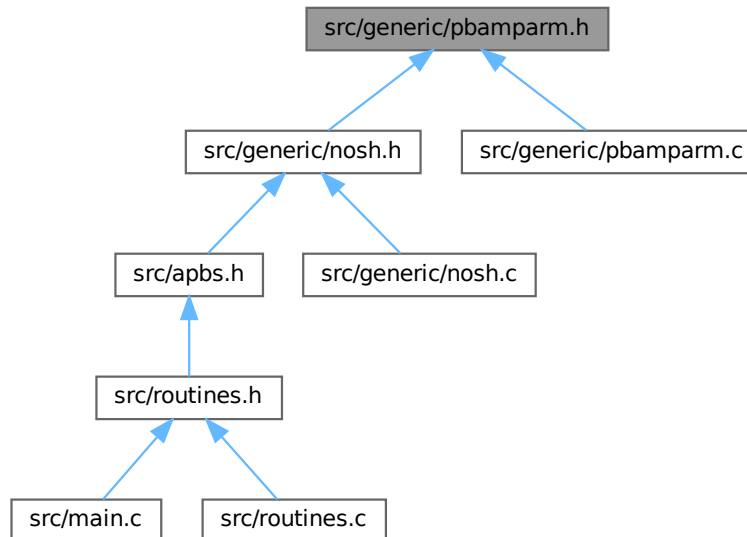
```
#include "generic/vhal.h"
```

```
#include "generic/vstring.h"
```

Include dependency graph for pbamparm.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sPBAMparm](#)
Parameter structure for PBAM-specific variables from input files.

Macros

- #define [CHR_MAXLEN](#) 1000
Number of things that can be written out in a single calculation.
- #define [PBAMPARM_MAXWRITE](#) 15
- #define [PBAMPARM_MAXMOL](#) 150

Typedefs

- typedef enum [ePBAMparm_CalcType](#) [PBAMparm_CalcType](#)
Declare PBAMparm_CalcType type.
- typedef struct [sPBAMparm](#) [PBAMparm](#)
Parameter structure for PBAM-specific variables from input files.

Enumerations

- enum [ePBAMparm_CalcType](#) { [PBAMCT_AUTO](#) =1 }
Calculation type.

Functions

- VEXTERNC PBAMparm * PBAMparm_ctor (PBAMparm_CalcType type)
Construct PBAMparm object.
- VEXTERNC Vrc_Codes PBAMparm_ctor2 (PBAMparm *thee, PBAMparm_CalcType type)
FORTTRAN stub to construct PBAMparm object ?????????!!!!!!!
- VEXTERNC void PBAMparm_dtor (PBAMparm **thee)
Object destructor.
- VEXTERNC void PBAMparm_dtor2 (PBAMparm *thee)
FORTTRAN stub for object destructor ?????????!!!!!!!
- VEXTERNC Vrc_Codes PBAMparm_check (PBAMparm *thee)
Consistency check for parameter values stored in object.
- VEXTERNC Vrc_Codes PBAMparm_parseToken (PBAMparm *thee, char tok[VMAX_BUFSIZE], Vio *sock)
Parse an MG keyword from an input file.
- VEXTERNC void PBAMparm_copy (PBAMparm *thee, PBAMparm *parm)
copy PBAMparm object into thee.
- VPRIVATE Vrc_Codes PBAMparm_parseSalt (PBAMparm *thee, Vio *sock)
Find salt conc and save it as a structure variable.
- VPRIVATE Vrc_Codes PBAMparm_parseRunType (PBAMparm *thee, Vio *sock)
Find runType and save it as a structure variable.
- VPRIVATE Vrc_Codes PBAMparm_parseRunName (PBAMparm *thee, Vio *sock)
Find runName and save it as a structure variable.
- VPRIVATE Vrc_Codes PBAMparm_parseRandorient (PBAMparm *thee, Vio *sock)
Find randomorientation flag and save it as a boolean.
- VPRIVATE Vrc_Codes PBAMparm_parsePBCS (PBAMparm *thee, Vio *sock)
Find PBC flag and save the type and the boxlength.
- VPRIVATE Vrc_Codes PBAMparm_parseUnits (PBAMparm *thee, Vio *sock)
Find units flag and save units.
- VPRIVATE Vrc_Codes PBAMparm_parse3Dmap (PBAMparm *thee, Vio *sock)
Find 3D map filename and save it.
- VPRIVATE Vrc_Codes PBAMparm_parseGrid2D (PBAMparm *thee, Vio *sock)
Find 2D grid filename and save it.
- VPRIVATE Vrc_Codes PBAMparm_parseDX (PBAMparm *thee, Vio *sock)
Find DX filename and save it.
- VPRIVATE Vrc_Codes PBAMparm_parseGridPts (PBAMparm *thee, Vio *sock)
Find Grid points and save them.
- VPRIVATE Vrc_Codes PBAMparm_parseTermcombine (PBAMparm *thee, Vio *sock)
Find Termination logic and save it.
- VPRIVATE Vrc_Codes PBAMparm_parseDiff (PBAMparm *thee, Vio *sock)
Find diffusion coeffs for each molecule and save them.
- VPRIVATE Vrc_Codes PBAMparm_parseXYZ (PBAMparm *thee, Vio *sock)
Find xyz files for each molecule for each traj and save them.

9.40.1 Detailed Description

Contains declarations for class PBAMparm.

Version

\$Id\$

Author

Lisa Felberg

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
*   Nathan A. Baker (nathan.baker@pnnl.gov)
*   Pacific Northwest National Laboratory
*
*   Additional contributing authors listed in the code documentation.
*
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*   THE POSSIBILITY OF SUCH DAMAGE.
*
*
```

Definition in file [pbamparm.h](#).

9.40.2 Macro Definition Documentation

9.40.2.1 PBAMPARM_MAXMOL

```
#define PBAMPARM_MAXMOL 150
```

Definition at line 78 of file [pbamparm.h](#).

9.40.2.2 PBAMPARM_MAXWRITE

```
#define PBAMPARM_MAXWRITE 15
```

Definition at line 77 of file [pbamparm.h](#).

9.41 pbamparm.h

[Go to the documentation of this file.](#)

```
00001
00064 #ifndef _PBAMPARM_H_
00065 #define _PBAMPARM_H_
00066
00067 /* Generic header files */
00068 #include "malloc/malloc.h"
00069
00070 #include "generic/vhal.h"
00071 #include "generic/vstring.h"
00072
00076 #define CHR_MAXLEN 1000
00077 #define PBAMPARM_MAXWRITE 15
00078 #define PBAMPARM_MAXMOL 150
00079
00084 enum ePBAMParm_CalcType {
00085     //other methods disabled for now only auto currently implemented.
00086     //PBAMCT_MANUAL=0,  /**< PBAM-manual */
00087     PBAMCT_AUTO=1,
00088     //PBAMCT_NONE=2 /**< not defined */
00089 };
00090
00095 typedef enum ePBAMParm_CalcType PBAMParm_CalcType;
00096
00105 typedef struct sPBAMParm {
00106
00107     PBAMParm_CalcType type;
00108     int parsed;
00110     /* *** GENERIC PARAMETERS *** */
00111     double salt;
00112     int setsalt;
00113
00114     // This is the type of run you want
00115     char runtype[CHR_MAXLEN];
00116     int setruntype;
00117
00118     // This is the name for output files
00119     char runname[CHR_MAXLEN];
00120     int setrunname;
00121
00122     // For setting random orientation of molecules
00123     int setrandorient;
00124
00125     // For periodic boundary conditions
00126     double pbcboxlen;
00127     int setpbcs;
00128
00129     // This is units of the calculation
00130     char units[CHR_MAXLEN];
00131     int setunits;
00132
00133     //
00134     // ELECTROSTATICS
00135     //
00136     // For the grid, store gridpt
00137     int gridpt;
00138     int setgridpt;
00139
00140     // For 3d map printing
00141     char map3dname[CHR_MAXLEN];
00142     int set3dmap;
```

```

00143
00144 // For 2D
00145 char grid2Dname[PBAMPARM_MAXWRITE][CHR_MAXLEN];
00146 char grid2Dax[PBAMPARM_MAXWRITE][CHR_MAXLEN];
00147 double grid2Dloc[PBAMPARM_MAXWRITE];
00148 int grid2Dct;
00149 int setgrid2Dname;
00150
00151 // For dx
00152 char dxname[CHR_MAXLEN];
00153 int setdxname;
00154
00155 //
00156 // DYNAMICS
00157 //
00158 int ntraj;
00159 int setntraj;
00160
00161 char termcombine[CHR_MAXLEN];
00162 int settermcombine;
00163
00164 int diffct;
00165 char moveType[PBAMPARM_MAXMOL][CHR_MAXLEN];
00166 double transDiff[PBAMPARM_MAXMOL];
00167 double rotDiff[PBAMPARM_MAXMOL];
00168
00169 int termct;
00170 int setterm;
00171
00172 char termnam[PBAMPARM_MAXWRITE][CHR_MAXLEN];
00173 int termnu[PBAMPARM_MAXWRITE][1];
00174 double termVal[PBAMPARM_MAXWRITE];
00175 char confil[PBAMPARM_MAXWRITE][CHR_MAXLEN];
00176 double conpad[PBAMPARM_MAXWRITE];
00177 int confilct;
00178
00179 int setxyz;
00180 int xyzct[PBAMPARM_MAXMOL];
00181 char xyzfil[PBAMPARM_MAXMOL][PBAMPARM_MAXWRITE][CHR_MAXLEN];
00182
00183 } PBAMParm;
00184
00191 VEXTERNC PBAMParm* PBAMParm_ctor(PBAMParm_CalcType type);
00192
00200 VEXTERNC Vrc_Codes PBAMParm_ctor2(PBAMParm *thee, PBAMParm_CalcType type);
00201
00207 VEXTERNC void PBAMParm_dtor(PBAMParm **thee);
00208
00214 VEXTERNC void PBAMParm_dtor2(PBAMParm *thee);
00215
00222 VEXTERNC Vrc_Codes PBAMParm_check(PBAMParm *thee);
00223
00233 VEXTERNC Vrc_Codes PBAMParm_parseToken(PBAMParm *thee, char tok[VMAX_BUFSIZE],
00234 Vio *sock);
00242 VEXTERNC void PBAMParm_copy(PBAMParm *thee, PBAMParm *parm);
00243
00251 VPRIVATE Vrc_Codes PBAMParm_parseSalt(PBAMParm *thee, Vio *sock);
00252
00260 VPRIVATE Vrc_Codes PBAMParm_parseRunType(PBAMParm *thee, Vio *sock);
00261
00269 VPRIVATE Vrc_Codes PBAMParm_parseRunName(PBAMParm *thee, Vio *sock);
00270
00278 VPRIVATE Vrc_Codes PBAMParm_parseRandorient(PBAMParm *thee, Vio *sock);
00279
00287 VPRIVATE Vrc_Codes PBAMParm_parsePBCS(PBAMParm *thee, Vio *sock);
00288
00296 VPRIVATE Vrc_Codes PBAMParm_parseUnits(PBAMParm *thee, Vio *sock);
00297
00305 VPRIVATE Vrc_Codes PBAMParm_parse3Dmap(PBAMParm *thee, Vio *sock);
00306
00314 VPRIVATE Vrc_Codes PBAMParm_parseGrid2D(PBAMParm *thee, Vio *sock);
00315
00323 VPRIVATE Vrc_Codes PBAMParm_parseDX(PBAMParm *thee, Vio *sock);
00324
00332 VPRIVATE Vrc_Codes PBAMParm_parseGridPts(PBAMParm *thee, Vio *sock);
00333
00341 VPRIVATE Vrc_Codes PBAMParm_parseTermcombine(PBAMParm *thee, Vio *sock);
00342
00350 VPRIVATE Vrc_Codes PBAMParm_parseDiff(PBAMParm *thee, Vio *sock);
00351
00359 VPRIVATE Vrc_Codes PBAMParm_parseXYZ(PBAMParm *thee, Vio *sock);

```

```

00360
00361
00362
00363
00364 #endif
00365

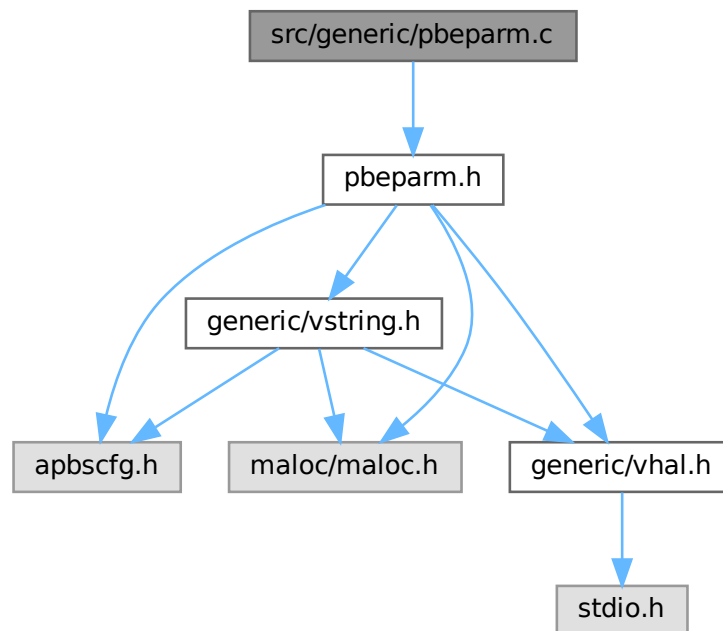
```

9.42 src/generic/pbeparm.c File Reference

Class PBEparm methods.

```
#include "pbeparm.h"
```

Include dependency graph for pbeparm.c:



Functions

- VPUBLIC double `PBEparm_getIonCharge` (`PBEparm *thee`, int `i`)
Get charge (e) of specified ion species.
- VPUBLIC double `PBEparm_getIonConc` (`PBEparm *thee`, int `i`)
Get concentration (M) of specified ion species.
- VPUBLIC double `PBEparm_getIonRadius` (`PBEparm *thee`, int `i`)
Get radius (A) of specified ion species.
- VPUBLIC double `PBEparm_getzmem` (`PBEparm *thee`)
- VPUBLIC double `PBEparm_getLmem` (`PBEparm *thee`)
- VPUBLIC double `PBEparm_getmembraneDiel` (`PBEparm *thee`)
- VPUBLIC double `PBEparm_getmemv` (`PBEparm *thee`)
- VPUBLIC `PBEparm *` `PBEparm_ctor` ()

Construct PBEparm object.

- VPUBLIC int [PBEparm_ctor2](#) ([PBEparm](#) *thee)

FORTTRAN stub to construct PBEparm object.

- VPUBLIC void [PBEparm_dtor](#) ([PBEparm](#) **thee)

Object destructor.

- VPUBLIC void [PBEparm_dtor2](#) ([PBEparm](#) *thee)

FORTTRAN stub for object destructor.

- VPUBLIC int [PBEparm_check](#) ([PBEparm](#) *thee)

Consistency check for parameter values stored in object.

- VPUBLIC void [PBEparm_copy](#) ([PBEparm](#) *thee, [PBEparm](#) *parm)

Copy PBEparm object into thee.

- VPRIVATE int [PBEparm_parseLPBE](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parseNPBE](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parseMOL](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parseLRPBE](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parseNRPBE](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parseSMPBE](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parseBCFL](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parseION](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parsePDIE](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parseSDENS](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parseSDIE](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parseSRFM](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parseSRAD](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parseSWIN](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parseTEMP](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parseUSEMAP](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parseCALCENERGY](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parseCALCFORCE](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parseZMEM](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parseLMEM](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parseMDIE](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parseMEMV](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parseWRITE](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPRIVATE int [PBEparm_parseWRITEMAT](#) ([PBEparm](#) *thee, [Vio](#) *sock)
- VPUBLIC int [PBEparm_parseToken](#) ([PBEparm](#) *thee, char tok[VMAX_BUFSIZE], [Vio](#) *sock)

Parse a keyword from an input file.

9.42.1 Detailed Description

Class PBEparm methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```

*
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*
*

```

Definition in file [pbeparm.c](#).

9.42.2 Function Documentation**9.42.2.1 PBEparm_getLmem()**

```

VPUBLIC double PBEparm_getLmem (
    PBEparm * thee )

```

Definition at line 91 of file [pbeparm.c](#).

9.42.2.2 PBEparm_getmembraneDiel()

```

VPUBLIC double PBEparm_getmembraneDiel (

```

```
PBEparm * thee )
```

Definition at line 95 of file [pbeparm.c](#).

9.42.2.3 PBEparm_getmemv()

```
VPUBLIC double PBEparm_getmemv (
```

```
PBEparm * thee )
```

Definition at line 99 of file [pbeparm.c](#).

9.42.2.4 PBEparm_getzmem()

```
VPUBLIC double PBEparm_getzmem (
```

```
PBEparm * thee )
```

Definition at line 87 of file [pbeparm.c](#).

9.42.2.5 PBEparm_parseBCFL()

```
VPRIVATE int PBEparm_parseBCFL (
```

```
PBEparm * thee,
```

```
Vio * sock )
```

Definition at line 474 of file [pbeparm.c](#).

9.42.2.6 PBEparm_parseCALCENERGY()

```
VPRIVATE int PBEparm_parseCALCENERGY (
```

```
PBEparm * thee,
```

```
Vio * sock )
```

Definition at line 895 of file [pbeparm.c](#).

9.42.2.7 PBEparm_parseCALCFORCE()

```
VPRIVATE int PBEparm_parseCALCFORCE (
```

```
PBEparm * thee,
```

```
Vio * sock )
```

Definition at line 948 of file [pbeparm.c](#).

9.42.2.8 PBEparm_parseION()

```
VPRIVATE int PBEparm_parseION (
```

```
PBEparm * thee,
```

```
Vio * sock )
```

Definition at line 555 of file [pbeparm.c](#).

9.42.2.9 PBEparm_parseLMEM()

```
VPRIVATE int PBEparm_parseLMEM (
```

```
PBEparm * thee,
```

```
Vio * sock )
```

Definition at line 1025 of file [pbeparm.c](#).

9.42.2.10 PBEparm_parseLPBE()

```
VPRIVATE int PBEparm_parseLPBE (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 368 of file [pbeparm.c](#).

9.42.2.11 PBEparm_parseLRPBE()

```
VPRIVATE int PBEparm_parseLRPBE (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 401 of file [pbeparm.c](#).

9.42.2.12 PBEparm_parseMDIE()

```
VPRIVATE int PBEparm_parseMDIE (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 1044 of file [pbeparm.c](#).

9.42.2.13 PBEparm_parseMEMV()

```
VPRIVATE int PBEparm_parseMEMV (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 1063 of file [pbeparm.c](#).

9.42.2.14 PBEparm_parseMOL()

```
VPRIVATE int PBEparm_parseMOL (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 382 of file [pbeparm.c](#).

9.42.2.15 PBEparm_parseNPBE()

```
VPRIVATE int PBEparm_parseNPBE (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 375 of file [pbeparm.c](#).

9.42.2.16 PBEparm_parseNRPBE()

```
VPRIVATE int PBEparm_parseNRPBE (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 408 of file [pbeparm.c](#).

9.42.2.17 PBEparm_parsePDIE()

```
VPRIVATE int PBEparm_parsePDIE (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 652 of file [pbeparm.c](#).

9.42.2.18 PBEparm_parseSDENS()

```
VPRIVATE int PBEparm_parseSDENS (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 671 of file [pbeparm.c](#).

9.42.2.19 PBEparm_parseSDIE()

```
VPRIVATE int PBEparm_parseSDIE (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 690 of file [pbeparm.c](#).

9.42.2.20 PBEparm_parseSMPBE()

```
VPRIVATE int PBEparm_parseSMPBE (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 415 of file [pbeparm.c](#).

9.42.2.21 PBEparm_parseSRAD()

```
VPRIVATE int PBEparm_parseSRAD (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 780 of file [pbeparm.c](#).

9.42.2.22 PBEparm_parseSRFM()

```
VPRIVATE int PBEparm_parseSRFM (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 709 of file [pbeparm.c](#).

9.42.2.23 PBEparm_parseSWIN()

```
VPRIVATE int PBEparm_parseSWIN (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 799 of file [pbeparm.c](#).

9.42.2.24 PBEparm_parseTEMP()

```
VPRIVATE int PBEparm_parseTEMP (
    PBEparm * thee,
    Vio * sock )
```

Definition at line 818 of file [pbeparm.c](#).

9.42.2.25 PBEparm_parseUSEMAP()

```
VPRIVATE int PBEparm_parseUSEMAP (
    PBEparm * thee,
    Vio * sock )
```

Definition at line 837 of file [pbeparm.c](#).

9.42.2.26 PBEparm_parseWRITE()

```
VPRIVATE int PBEparm_parseWRITE (
    PBEparm * thee,
    Vio * sock )
```

Definition at line 1084 of file [pbeparm.c](#).

9.42.2.27 PBEparm_parseWRITEMAT()

```
VPRIVATE int PBEparm_parseWRITEMAT (
    PBEparm * thee,
    Vio * sock )
```

Definition at line 1178 of file [pbeparm.c](#).

9.42.2.28 PBEparm_parseZMEM()

```
VPRIVATE int PBEparm_parseZMEM (
    PBEparm * thee,
    Vio * sock )
```

Definition at line 1005 of file [pbeparm.c](#).

9.43 pbeparm.c

[Go to the documentation of this file.](#)

```
00001
00057 #include "pbeparm.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 #if !defined(VINLINE_MGPARM)
00062
00063 #endif /* if !defined(VINLINE_MGPARM) */
00064
00065 VPUBLIC double PBEparm_getIonCharge(PBEparm *thee, int i) {
00066     VASSERT(thee != VNULL);
00067     VASSERT(i < thee->nion);
00068     return thee->ionq[i];
00069 }
```

```

00070
00071 VPUBLIC double PBEparm_getIonConc(PBEparm *thee, int i) {
00072     VASSERT(thee != VNULL);
00073     VASSERT(i < thee->nion);
00074     return thee->ionc[i];
00075 }
00076
00077 VPUBLIC double PBEparm_getIonRadius(PBEparm *thee, int i) {
00078     VASSERT(thee != VNULL);
00079     VASSERT(i < thee->nion);
00080     return thee->ionr[i];
00081 }
00082
00083 /*-----*/
00084 /* Added by Michael Grabe */
00085 /*-----*/
00086
00087 VPUBLIC double PBEparm_getzmem(PBEparm *thee) {
00088     VASSERT(thee != VNULL);
00089     return thee->zmem;
00090 }
00091 VPUBLIC double PBEparm_getLmem(PBEparm *thee) {
00092     VASSERT(thee != VNULL);
00093     return thee->Lmem;
00094 }
00095 VPUBLIC double PBEparm_getmembraneDiel(PBEparm *thee) {
00096     VASSERT(thee != VNULL);
00097     return thee->mdie;
00098 }
00099 VPUBLIC double PBEparm_getmemv(PBEparm *thee) {
00100     VASSERT(thee != VNULL);
00101     return thee->memv;
00102 }
00103
00104 VPUBLIC PBEparm* PBEparm_ctor() {
00105
00106     /* Set up the structure */
00107     PBEparm *thee = VNULL;
00108     thee = (PBEparm*)Vmem_malloc(VNULL, 1, sizeof(PBEparm));
00109     VASSERT( thee != VNULL);
00110     VASSERT( PBEparm_ctor2(thee) );
00111
00112     return thee;
00113 }
00114
00115 VPUBLIC int PBEparm_ctor2(PBEparm *thee) {
00116
00117     int i;
00118
00119     if (thee == VNULL) return 0;
00120
00121     thee->parsed = 0;
00122
00123     thee->setmolid = 0;
00124     thee->setpbetype = 0;
00125     thee->setbcfl = 0;
00126     thee->setnion = 0;
00127     for (i=0; i<MAXION; i++){
00128         thee->setion[i] = 0;
00129         thee->iong[i] = 0.0;
00130         thee->ionc[i] = 0.0;
00131         thee->ionr[i] = 0.0;
00132     }
00133     thee->setpdie = 0;
00134     thee->setsdie = 0;
00135     thee->setsrfm = 0;
00136     thee->setsrad = 0;
00137     thee->setswin = 0;
00138     thee->settemp = 0;
00139     thee->setcalcenergy = 0;
00140     thee->setcalcforce = 0;
00141     thee->setsdens = 0;
00142     thee->numwrite = 0;
00143     thee->setwritemat = 0;
00144     thee->nion = 0;
00145     thee->sdens = 0;
00146     thee->swin = 0;
00147     thee->srad = 1.4;
00148     thee->useDielMap = 0;
00149     thee->useKappaMap = 0;
00150     thee->usePotMap = 0;

```

```

00151     thee->useChargeMap = 0;
00152
00153     /*-----*/
00154     /* Added by Michael Grabe */
00155     /*-----*/
00156
00157     thee->setzmem = 0;
00158     thee->setLmem = 0;
00159     thee->setmdie = 0;
00160     thee->setmemv = 0;
00161
00162     /*-----*/
00163
00164     thee->smsize = 0.0;
00165     thee->smvolume = 0.0;
00166
00167     thee->setsmsize = 0;
00168     thee->setsmvolume = 0;
00169
00170     return 1;
00171 }
00172
00173 VPUBLIC void PBEparm_dtor(PBEparm **thee) {
00174     if ((*thee) != VNULL) {
00175         PBEparm_dtor2(*thee);
00176         Vmem_free(VNULL, 1, sizeof(PBEparm), (void **)thee);
00177         (*thee) = VNULL;
00178     }
00179 }
00180
00181 VPUBLIC void PBEparm_dtor2(PBEparm *thee) { ; }
00182
00183 VPUBLIC int PBEparm_check(PBEparm *thee) {
00184     int i;
00185
00186     /* Check to see if we were even filled... */
00187     if (!thee->parsed) {
00188         Vnm_print(2, "PBEparm_check: not filled!\n");
00189         return 0;
00190     }
00191
00192     if (!thee->setmolid) {
00193         Vnm_print(2, "PBEparm_check: MOL not set!\n");
00194         return 0;
00195     }
00196
00197     if (!thee->setpbetype) {
00198         Vnm_print(2, "PBEparm_check: LPBE/NPBE/LRPBE/NRPBE/SMPBE not set!\n");
00199         return 0;
00200     }
00201     if (!thee->setbcfl) {
00202         Vnm_print(2, "PBEparm_check: BCFL not set!\n");
00203         return 0;
00204     }
00205     if (!thee->setnion) {
00206         thee->setnion = 1;
00207         thee->nion = 0;
00208     }
00209     for (i=0; i<thee->nion; i++) {
00210         if (!thee->setion[i]) {
00211             Vnm_print(2, "PBEparm_check: ION #%d not set!\n",i);
00212             return 0;
00213         }
00214     }
00215     if (!thee->setpdie) {
00216         Vnm_print(2, "PBEparm_check: PDIE not set!\n");
00217         return 0;
00218     }
00219     if (((thee->srfm==VSM_MOL) || (thee->srfm==VSM_MOLSMOOTH)) \
00220         && (!thee->setsdens) && (thee->srad > VSMALL)) {
00221         Vnm_print(2, "PBEparm_check: SDENS not set!\n");
00222         return 0;
00223     }
00224     if (!thee->setsdie) {
00225         Vnm_print(2, "PBEparm_check: SDIE not set!\n");
00226         return 0;
00227     }
00228     if (!thee->setsrfm) {
00229         Vnm_print(2, "PBEparm_check: SRFM not set!\n");
00230         return 0;
00231     }

```



```

00232     if (((thee->srfm==VSM_MOL) || (thee->srfm==VSM_MOLSMOOTH)) \
00233         && (!thee->setsrad)) {
00234         Vnm_print(2, "PBeparm_check: SRAD not set!\n");
00235         return 0;
00236     }
00237     if ((thee->srfm==VSM_SPLINE) && (!thee->setswin)) {
00238         Vnm_print(2, "PBeparm_check: SWIN not set!\n");
00239         return 0;
00240     }
00241     if ((thee->srfm==VSM_SPLINE3) && (!thee->setswin)) {
00242         Vnm_print(2, "PBeparm_check: SWIN not set!\n");
00243         return 0;
00244     }
00245     if ((thee->srfm==VSM_SPLINE4) && (!thee->setswin)) {
00246         Vnm_print(2, "PBeparm_check: SWIN not set!\n");
00247         return 0;
00248     }
00249     if (!thee->settemp) {
00250         Vnm_print(2, "PBeparm_check: TEMP not set!\n");
00251         return 0;
00252     }
00253     if (!thee->setcalcenergy) thee->calcenergy = PCE_NO;
00254     if (!thee->setcalcforce) thee->calcforce = PCF_NO;
00255     if (!thee->setwritemat) thee->writemat = 0;
00256
00257     /*-----*/
00258     /* Added by Michael Grabe */
00259     /*-----*/
00260
00261     if (!thee->setzmem) && (thee->bcfl == 3){
00262         Vnm_print(2, "PBeparm_check: ZMEM not set!\n");
00263         return 0;
00264     }
00265     if (!thee->setlmem) && (thee->bcfl == 3){
00266         Vnm_print(2, "PBeparm_check: LMEM not set!\n");
00267         return 0;
00268     }
00269     if (!thee->setmdie) && (thee->bcfl == 3){
00270         Vnm_print(2, "PBeparm_check: MDIE not set!\n");
00271         return 0;
00272     }
00273     if (!thee->setmemv) && (thee->bcfl == 3){
00274         Vnm_print(2, "PBeparm_check: MEMV not set!\n");
00275         return 0;
00276     }
00277
00278     /*-----*/
00279
00280     return 1;
00281 }
00282
00283 VPUBLIC void PBeparm_copy(PBeparm *thee, PBeparm *parm) {
00284
00285     int i, j;
00286
00287     VASSERT(thee != VNULL);
00288     VASSERT(parm != VNULL);
00289
00290     thee->molid = parm->molid;
00291     thee->setmolid = parm->setmolid;
00292     thee->useDielMap = parm->useDielMap;
00293     thee->dielMapID = parm->dielMapID;
00294     thee->useKappaMap = parm->useKappaMap;
00295     thee->kappaMapID = parm->kappaMapID;
00296     thee->usePotMap = parm->usePotMap;
00297     thee->potMapID = parm->potMapID;
00298     thee->useChargeMap = parm->useChargeMap;
00299     thee->chargeMapID = parm->chargeMapID;
00300     thee->pbetype = parm->pbetype;
00301     thee->setpbetype = parm->setpbetype;
00302     thee->bcfl = parm->bcfl;
00303     thee->setbcfl = parm->setbcfl;
00304     thee->nion = parm->nion;
00305     thee->setnion = parm->setnion;
00306     for (i=0; i<MAXION; i++) {
00307         thee->ionq[i] = parm->ionq[i];
00308         thee->ionc[i] = parm->ionc[i];
00309         thee->ionr[i] = parm->ionr[i];
00310         thee->setion[i] = parm->setion[i];
00311     };
00312     thee->pdie = parm->pdie;

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```

00313     thee->setpdie = parm->setpdie;
00314     thee->sdens = parm->sdens;
00315     thee->setsdens = parm->setsdens;
00316     thee->sdie = parm->sdie;
00317     thee->setsdie = parm->setsdie;
00318     thee->srfr = parm->srfr;
00319     thee->setsrfr = parm->setsrfr;
00320     thee->srdr = parm->srdr;
00321     thee->setsrdr = parm->setsrdr;
00322     thee->swin = parm->swin;
00323     thee->setswin = parm->setswin;
00324     thee->temp = parm->temp;
00325     thee->settemp = parm->settemp;
00326     thee->calcenergy = parm->calcenergy;
00327     thee->setcalcenergy = parm->setcalcenergy;
00328     thee->calcforce = parm->calcforce;
00329     thee->setcalcforce = parm->setcalcforce;
00330
00331     /*-----*/
00332     /* Added by Michael Grabe */
00333     /*-----*/
00334
00335     thee->zmem = parm->zmem;
00336     thee->setzmem = parm->setzmem;
00337     thee->Lmem = parm->Lmem;
00338     thee->setLmem = parm->setLmem;
00339     thee->mdie = parm->mdie;
00340     thee->setmdie = parm->setmdie;
00341     thee->memv = parm->memv;
00342     thee->setmemv = parm->setmemv;
00343
00344     /*-----*/
00345
00346     thee->numwrite = parm->numwrite;
00347     for (i=0; i<PBEPARM_MAXWRITE; i++) {
00348         thee->writetype[i] = parm->writetype[i];
00349         thee->writefmt[i] = parm->writefmt[i];
00350         for (j=0; j<VMAX_ARGLEN; j++)
00351             thee->writestem[i][j] = parm->writestem[i][j];
00352     }
00353     thee->writemat = parm->writemat;
00354     thee->setwritemat = parm->setwritemat;
00355     for (i=0; i<VMAX_ARGLEN; i++) thee->writematstem[i] = parm->writematstem[i];
00356     thee->writematflag = parm->writematflag;
00357
00358     thee->smsize = parm->smsize;
00359     thee->smvolume = parm->smvolume;
00360
00361     thee->setsmsize = parm->setsmsize;
00362     thee->setsmvolume = parm->setsmvolume;
00363
00364     thee->parsed = parm->parsed;
00365 }
00366
00367 VPRIVATE int PBEParm_parseLPBE(PBEParm *thee, Vio *sock) {
00368     Vnm_print(0, "Nosh: parsed lpbe\n");
00369     thee->pbetype = PBE_LPBE;
00370     thee->setpbetype = 1;
00371     return 1;
00372 }
00373
00374 VPRIVATE int PBEParm_parseNPBE(PBEParm *thee, Vio *sock) {
00375     Vnm_print(0, "Nosh: parsed npbe\n");
00376     thee->pbetype = PBE_NPBE;
00377     thee->setpbetype = 1;
00378     return 1;
00379 }
00380
00381 VPRIVATE int PBEParm_parseMOL(PBEParm *thee, Vio *sock) {
00382     int ti;
00383     char tok[VMAX_BUFSIZE];
00384
00385     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00386     if (sscanf(tok, "%d", &ti) == 0) {
00387         Vnm_print(2, "Nosh: Read non-int (%s) while parsing MOL \
00388 keyword!\n", tok);
00389         return -1;
00390     }
00391     thee->molid = ti;
00392     thee->setmolid = 1;

```

```

00394     return 1;
00395
00396     ERROR1:
00397         Vnm_print(2, "parsePBE: ran out of tokens!\n");
00398         return -1;
00399 }
00400
00401 VPRIVATE int PBEparm_parseLRPBE(PBEparm *thee, Vio *sock) {
00402     Vnm_print(0, "Nosh: parsed lrpbe\n");
00403     thee->pbetype = PBE_LRPBE;
00404     thee->setpbetype = 1;
00405     return 1;
00406 }
00407
00408 VPRIVATE int PBEparm_parseNRPBE(PBEparm *thee, Vio *sock) {
00409     Vnm_print(0, "Nosh: parsed nrpbe\n");
00410     thee->pbetype = PBE_NRPBE;
00411     thee->setpbetype = 1;
00412     return 1;
00413 }
00414
00415 VPRIVATE int PBEparm_parseSMPBE(PBEparm *thee, Vio *sock) {
00416     int i;
00417
00418     char type[VMAX_BUFSIZE]; /* vol or size (keywords) */
00419     char value[VMAX_BUFSIZE]; /* floating point value */
00420
00421     char setVol = 1;
00422     char setSize = 1;
00423     char keyValuePairs = 2;
00424
00425     double size, volume;
00426
00427     for(i=0; i<keyValuePairs; i++){
00428
00429         /* The line two tokens at a time */
00430         VJMPERR1(Vio_scanf(sock, "%s", type) == 1);
00431         VJMPERR1(Vio_scanf(sock, "%s", value) == 1);
00432
00433         if(!strcmp(type, "vol")){
00434             if ((setVol = sscanf(value, "%lf", &volume)) == 0){
00435                 Vnm_print(2, "Nosh: Read non-float (%s) while parsing smpbe keyword!\n", value);
00436                 return VRC_FAILURE;
00437             }
00438         }else if(!strcmp(type, "size")){
00439             if ((setSize = sscanf(value, "%lf", &size)) == 0){
00440                 Vnm_print(2, "Nosh: Read non-float (%s) while parsing smpbe keyword!\n", value);
00441                 return VRC_FAILURE;
00442             }
00443         }else{
00444             Vnm_print(2, "Nosh: Read non-float (%s) while parsing smpbe keyword!\n", value);
00445             return VRC_FAILURE;
00446         }
00447     }
00448
00449     /* If either the volume or size isn't set, throw an error */
00450     if((setVol == 0) || (setSize == 0)){
00451         Vnm_print(2, "Nosh: Error while parsing smpbe keywords! Only size or vol was specified.\n");
00452         return VRC_FAILURE;
00453     }
00454
00455     Vnm_print(0, "Nosh: parsed smpbe\n");
00456     thee->pbetype = PBE_SMPBE;
00457     thee->setpbetype = 1;
00458
00459     thee->smsize = size;
00460     thee->setsmsize = 1;
00461
00462     thee->smvolume = volume;
00463     thee->setsmvolume = 1;
00464
00465     return VRC_SUCCESS;
00466
00467     ERROR1:
00468     Vnm_print(2, "parsePBE: ran out of tokens!\n");
00469     return VRC_FAILURE;
00470 }
00471
00472 }
00473
00474 VPRIVATE int PBEparm_parseBCFL(PBEparm *thee, Vio *sock) {

```

```

00475     char tok[VMAX_BUFSIZE];
00476     int ti;
00477
00478     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00479
00480     /* We can either parse int flag... */
00481     if (sscanf(tok, "%d", &ti) == 1) {
00482
00483         thee->bcfl = (Vbcfl)ti;
00484         thee->setbcfl = 1;
00485         /* Warn that this usage is deprecated */
00486         Vnm_print(2, "parsePBE: Warning -- parsed deprecated \"bcfl %d\" \"
00487 statement\\n\", ti);
00488         Vnm_print(2, "parsePBE: Please use \"bcfl \");
00489         switch (thee->bcfl) {
00490             case BCFL_ZERO:
00491                 Vnm_print(2, "zero");
00492                 break;
00493             case BCFL_SDH:
00494                 Vnm_print(2, "sdh");
00495                 break;
00496             case BCFL_MDH:
00497                 Vnm_print(2, "mdh");
00498                 break;
00499             case BCFL_FOCUS:
00500                 Vnm_print(2, "focus");
00501                 break;
00502             case BCFL_MEM:
00503                 Vnm_print(2, "mem");
00504                 break;
00505             case BCFL_MAP:
00506                 Vnm_print(2, "map");
00507                 break;
00508             default:
00509                 Vnm_print(2, "UNKNOWN");
00510                 break;
00511         }
00512         Vnm_print(2, "\" instead.\\n");
00513         return 1;
00514
00515     /* ...or the word */
00516     } else {
00517
00518         if (Vstring_strcasecmp(tok, "zero") == 0) {
00519             thee->bcfl = BCFL_ZERO;
00520             thee->setbcfl = 1;
00521             return 1;
00522         } else if (Vstring_strcasecmp(tok, "sdh") == 0) {
00523             thee->bcfl = BCFL_SDH;
00524             thee->setbcfl = 1;
00525             return 1;
00526         } else if (Vstring_strcasecmp(tok, "mdh") == 0) {
00527             thee->bcfl = BCFL_MDH;
00528             thee->setbcfl = 1;
00529             return 1;
00530         } else if (Vstring_strcasecmp(tok, "focus") == 0) {
00531             thee->bcfl = BCFL_FOCUS;
00532             thee->setbcfl = 1;
00533             return 1;
00534         } else if (Vstring_strcasecmp(tok, "mem") == 0) {
00535             thee->bcfl = BCFL_MEM;
00536             thee->setbcfl = 1;
00537             return 1;
00538         } else if (Vstring_strcasecmp(tok, "map") == 0) {
00539             thee->bcfl = BCFL_MAP;
00540             thee->setbcfl = 1;
00541             return 1;
00542         } else {
00543             Vnm_print(2, "NOsh: parsed unknown BCFL parameter (%s)!\\n",
00544                 tok);
00545             return -1;
00546         }
00547     }
00548     return 0;
00549
00550     ERROR1:
00551     Vnm_print(2, "parsePBE: ran out of tokens!\\n");
00552     return -1;
00553 }
00554
00555 VPRIVATE int PBEparm_parseION(PBEparm *thee, Vio *sock) {

```

```

00556
00557     int i;
00558     int meth = 0;
00559
00560     char tok[VMAX_BUFSIZE];
00561     char value[VMAX_BUFSIZE];
00562
00563     double tf;
00564     double charge, conc, radius;
00565
00566     int setCharge = 0;
00567     int setConc = 0;
00568     int setRadius = 0;
00569     int keyValuePairs = 3;
00570
00571     /* Get the initial token for the ION statement */
00572     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00573
00574     /* Scan the token once to determine the type (old style or new keyValue pair) */
00575     meth = sscanf(tok, "%lf", &tf);
00576     /* If tok is a non-zero float value, we are using the old method */
00577     if(meth != 0){
00578
00579         Vnm_print(2, "Nosh: Deprecated use of ION keyword! Use key-value pairs\n", tok);
00580
00581         if (sscanf(tok, "%lf", &tf) == 0) {
00582             Vnm_print(2, "Nosh: Read non-float (%s) while parsing ION keyword!\n", tok);
00583             return VRC_FAILURE;
00584         }
00585         thee->ionq[thee->nion] = tf;
00586         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00587         if (sscanf(tok, "%lf", &tf) == 0) {
00588             Vnm_print(2, "Nosh: Read non-float (%s) while parsing ION keyword!\n", tok);
00589             return VRC_FAILURE;
00590         }
00591         thee->ionc[thee->nion] = tf;
00592         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00593         if (sscanf(tok, "%lf", &tf) == 0) {
00594             Vnm_print(2, "Nosh: Read non-float (%s) while parsing ION keyword!\n", tok);
00595             return VRC_FAILURE;
00596         }
00597         thee->ionr[thee->nion] = tf;
00598     }else{
00599
00600         /* Three key-value pairs (charge, radius and conc) */
00601         for(i=0;i<keyValuePairs;i++){
00602
00603             /* Now scan for the value (float) to be used with the key token parsed
00604              * above the if-else statement */
00605             VJMPERR1(Vio_scanf(sock, "%s", value) == 1);
00606             if(!strcmp(tok,"charge")){
00607                 setCharge = sscanf(value, "%lf", &charge);
00608                 if (setCharge == 0){
00609                     Vnm_print(2,"Nosh: Read non-float (%s) while parsing ION %s keyword!\n", value, tok);
00610                     return VRC_FAILURE;
00611                 }
00612                 thee->ionq[thee->nion] = charge;
00613             }else if(!strcmp(tok,"radius")){
00614                 setRadius = sscanf(value, "%lf", &radius);
00615                 if (setRadius == 0){
00616                     Vnm_print(2,"Nosh: Read non-float (%s) while parsing ION %s keyword!\n", value, tok);
00617                     return VRC_FAILURE;
00618                 }
00619                 thee->ionr[thee->nion] = radius;
00620             }else if(!strcmp(tok,"conc")){
00621                 setConc = sscanf(value, "%lf", &conc);
00622                 if (setConc == 0){
00623                     Vnm_print(2,"Nosh: Read non-float (%s) while parsing ION %s keyword!\n", value, tok);
00624                     return VRC_FAILURE;
00625                 }
00626                 thee->ionc[thee->nion] = conc;
00627             }else{
00628                 Vnm_print(2,"Nosh: Illegal or missing key-value pair for ION keyword!\n");
00629                 return VRC_FAILURE;
00630             }
00631         }
00632
00633         /* If all three values haven't be set (setValue = 0) then read the next token */
00634         if((setCharge != 1) || (setConc != 1) || (setRadius != 1)){
00635             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00636         }

```

```

00637         } /* end for */
00638     } /* end if */
00639 } /* end if */
00640
00641 /* Finally set the setion, nion and setnion flags and return success */
00642 thee->setion[thee->nion] = 1;
00643 (thee->nion)++;
00644 thee->setnion = 1;
00645 return VRC_SUCCESS;
00646
00647 ERROR1:
00648     Vnm_print(2, "parsePBE: ran out of tokens!\n");
00649     return VRC_FAILURE;
00650 }
00651
00652 VPRIVATE int PBEparm_parsePDIE(PBEparm *thee, Vio *sock) {
00653     char tok[VMAX_BUFSIZE];
00654     double tf;
00655
00656     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00657     if (sscanf(tok, "%lf", &tf) == 0) {
00658         Vnm_print(2, "Nosh: Read non-float (%s) while parsing PDIE \
00659 keyword!\n", tok);
00660         return -1;
00661     }
00662     thee->pdie = tf;
00663     thee->setpdie = 1;
00664     return 1;
00665
00666     ERROR1:
00667         Vnm_print(2, "parsePBE: ran out of tokens!\n");
00668         return -1;
00669 }
00670
00671 VPRIVATE int PBEparm_parseSDENS(PBEparm *thee, Vio *sock) {
00672     char tok[VMAX_BUFSIZE];
00673     double tf;
00674
00675     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00676     if (sscanf(tok, "%lf", &tf) == 0) {
00677         Vnm_print(2, "Nosh: Read non-float (%s) while parsing SDENS \
00678 keyword!\n", tok);
00679         return -1;
00680     }
00681     thee->sdens = tf;
00682     thee->setsdens = 1;
00683     return 1;
00684
00685     ERROR1:
00686         Vnm_print(2, "parsePBE: ran out of tokens!\n");
00687         return -1;
00688 }
00689
00690 VPRIVATE int PBEparm_parseSDIE(PBEparm *thee, Vio *sock) {
00691     char tok[VMAX_BUFSIZE];
00692     double tf;
00693
00694     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00695     if (sscanf(tok, "%lf", &tf) == 0) {
00696         Vnm_print(2, "Nosh: Read non-float (%s) while parsing SDIE \
00697 keyword!\n", tok);
00698         return -1;
00699     }
00700     thee->sdie = tf;
00701     thee->setsdie = 1;
00702     return 1;
00703
00704     ERROR1:
00705         Vnm_print(2, "parsePBE: ran out of tokens!\n");
00706         return -1;
00707 }
00708
00709 VPRIVATE int PBEparm_parseSRFM(PBEparm *thee, Vio *sock) {
00710     char tok[VMAX_BUFSIZE];
00711     int ti;
00712
00713     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00714
00715     /* Parse old-style int arg */
00716     if (sscanf(tok, "%d", &ti) == 1) {
00717         thee->srfm = (Vsurf_Meth)ti;

```

```

00718     thee->setsrfm = 1;
00719
00720     Vnm_print(2, "parsePBE: Warning -- parsed deprecated \"srfm %d\" \
00721 statement.\n", ti);
00722     Vnm_print(2, "parsePBE: Please use \"srfm \");
00723     switch (thee->srfm) {
00724     case VSM_MOL:
00725         Vnm_print(2, "mol");
00726         break;
00727     case VSM_MOLSMOOTH:
00728         Vnm_print(2, "smol");
00729         break;
00730     case VSM_SPLINE:
00731         Vnm_print(2, "spl2");
00732         break;
00733     case VSM_SPLINE3:
00734         Vnm_print(2, "spl3");
00735         break;
00736     case VSM_SPLINE4:
00737         Vnm_print(2, "spl4");
00738         break;
00739     default:
00740         Vnm_print(2, "UNKNOWN");
00741         break;
00742     }
00743     Vnm_print(2, "\" instead.\n");
00744     return 1;
00745
00746     /* Parse newer text-based args */
00747     } else if (Vstring_strcasecmp(tok, "mol") == 0) {
00748         thee->srfm = VSM_MOL;
00749         thee->setsrfm = 1;
00750         return 1;
00751     } else if (Vstring_strcasecmp(tok, "smol") == 0) {
00752         thee->srfm = VSM_MOLSMOOTH;
00753         thee->setsrfm = 1;
00754         return 1;
00755     } else if (Vstring_strcasecmp(tok, "spl2") == 0) {
00756         thee->srfm = VSM_SPLINE;
00757         thee->setsrfm = 1;
00758         return 1;
00759     } else if (Vstring_strcasecmp(tok, "spl3") == 0) {
00760         thee->srfm = VSM_SPLINE3;
00761         thee->setsrfm = 1;
00762         return 1;
00763     } else if (Vstring_strcasecmp(tok, "spl4") == 0) {
00764         thee->srfm = VSM_SPLINE4;
00765         thee->setsrfm = 1;
00766         return 1;
00767     } else {
00768         Vnm_print(2, "Nosh: Unrecongized keyword (%s) when parsing \
00769 srfm!\n", tok);
00770         return -1;
00771     }
00772
00773     return 0;
00774
00775     ERROR1:
00776     Vnm_print(2, "parsePBE: ran out of tokens!\n");
00777     return -1;
00778 }
00779
00780 VPRIVATE int PBEparm_parseSRAD(PBEparm *thee, Vio *sock) {
00781     char tok[VMAX_BUFSIZE];
00782     double tf;
00783
00784     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00785     if (sscanf(tok, "%lf", &tf) == 0) {
00786         Vnm_print(2, "Nosh: Read non-float (%s) while parsing SRAD \
00787 keyword!\n", tok);
00788         return -1;
00789     }
00790     thee->srad = tf;
00791     thee->setsrad = 1;
00792     return 1;
00793
00794     ERROR1:
00795     Vnm_print(2, "parsePBE: ran out of tokens!\n");
00796     return -1;
00797 }
00798

```

```

00799 VPRIVATE int PBEparm_parseSWIN(PBEparm *thee, Vio *sock) {
00800     char tok[VMAX_BUFSIZE];
00801     double tf;
00802
00803     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00804     if (sscanf(tok, "%lf", &tf) == 0) {
00805         Vnm_print(2, "Nosh: Read non-float (%s) while parsing SWIN \
00806 keyword!\n", tok);
00807         return -1;
00808     }
00809     thee->swin = tf;
00810     thee->setswin = 1;
00811     return 1;
00812
00813     ERROR1:
00814     Vnm_print(2, "parsePBE: ran out of tokens!\n");
00815     return -1;
00816 }
00817
00818 VPRIVATE int PBEparm_parseTEMP(PBEparm *thee, Vio *sock) {
00819     char tok[VMAX_BUFSIZE];
00820     double tf;
00821
00822     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00823     if (sscanf(tok, "%lf", &tf) == 0) {
00824         Vnm_print(2, "Nosh: Read non-float (%s) while parsing TEMP \
00825 keyword!\n", tok);
00826         return -1;
00827     }
00828     thee->temp = tf;
00829     thee->settemp = 1;
00830     return 1;
00831
00832     ERROR1:
00833     Vnm_print(2, "parsePBE: ran out of tokens!\n");
00834     return -1;
00835 }
00836
00837 VPRIVATE int PBEparm_parseUSEMAP(PBEparm *thee, Vio *sock) {
00838     char tok[VMAX_BUFSIZE];
00839     int ti;
00840
00841     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00842     Vnm_print(0, "PBEparm_parseToken: Read %s...\n", tok);
00843     if (Vstring_strcasecmp(tok, "diel") == 0) {
00844         thee->useDielMap = 1;
00845         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00846         if (sscanf(tok, "%d", &ti) == 0) {
00847             Vnm_print(2, "Nosh: Read non-int (%s) while parsing \
00848 USEMAP DIEL keyword!\n", tok);
00849             return -1;
00850         }
00851         thee->dielMapID = ti;
00852         return 1;
00853     } else if (Vstring_strcasecmp(tok, "kappa") == 0) {
00854         thee->useKappaMap = 1;
00855         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00856         if (sscanf(tok, "%d", &ti) == 0) {
00857             Vnm_print(2, "Nosh: Read non-int (%s) while parsing \
00858 USEMAP KAPPA keyword!\n", tok);
00859             return -1;
00860         }
00861         thee->kappaMapID = ti;
00862         return 1;
00863     } else if (Vstring_strcasecmp(tok, "pot") == 0) {
00864         thee->usePotMap = 1;
00865         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00866         if (sscanf(tok, "%d", &ti) == 0) {
00867             Vnm_print(2, "Nosh: Read non-int (%s) while parsing \
00868 USEMAP POT keyword!\n", tok);
00869             return -1;
00870         }
00871         thee->potMapID = ti;
00872         return 1;
00873     } else if (Vstring_strcasecmp(tok, "charge") == 0) {
00874         thee->useChargeMap = 1;
00875         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00876         if (sscanf(tok, "%d", &ti) == 0) {
00877             Vnm_print(2, "Nosh: Read non-int (%s) while parsing \
00878 USEMAP CHARGE keyword!\n", tok);
00879             return -1;

```



```

00880     }
00881     thee->chargeMapID = ti;
00882     return 1;
00883 } else {
00884     Vnm_print(2, "Nosh: Read undefined keyword (%s) while parsing \
00885 USEMAP statement!\n", tok);
00886     return -1;
00887 }
00888 return 0;
00889
00890 ERROR1:
00891     Vnm_print(2, "parsePBE: ran out of tokens!\n");
00892     return -1;
00893 }
00894
00895 VPRIVATE int PBEparm_parseCALCENERGY(PBEparm *thee, Vio *sock) {
00896     char tok[VMAX_BUFSIZE];
00897     int ti;
00898
00899     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00900     /* Parse number */
00901     if (sscanf(tok, "%d", &ti) == 1) {
00902         thee->calcenergy = (PBEparm_calcEnergy)ti;
00903         thee->setcalcenergy = 1;
00904
00905         Vnm_print(2, "parsePBE: Warning -- parsed deprecated \"calcenergy \
00906 %d\" statement.\n", ti);
00907         Vnm_print(2, "parsePBE: Please use \"calcenergy ");
00908         switch (thee->calcenergy) {
00909             case PCE_NO:
00910                 Vnm_print(2, "no");
00911                 break;
00912             case PCE_TOTAL:
00913                 Vnm_print(2, "total");
00914                 break;
00915             case PCE_COMPS:
00916                 Vnm_print(2, "comps");
00917                 break;
00918             default:
00919                 Vnm_print(2, "UNKNOWN");
00920                 break;
00921         }
00922         Vnm_print(2, "\" instead.\n");
00923         return 1;
00924     } else if (Vstring_strcasecmp(tok, "no") == 0) {
00925         thee->calcenergy = PCE_NO;
00926         thee->setcalcenergy = 1;
00927         return 1;
00928     } else if (Vstring_strcasecmp(tok, "total") == 0) {
00929         thee->calcenergy = PCE_TOTAL;
00930         thee->setcalcenergy = 1;
00931         return 1;
00932     } else if (Vstring_strcasecmp(tok, "comps") == 0) {
00933         thee->calcenergy = PCE_COMPS;
00934         thee->setcalcenergy = 1;
00935         return 1;
00936     } else {
00937         Vnm_print(2, "Nosh: Unrecognized parameter (%s) while parsing \
00938 calcenergy!\n", tok);
00939         return -1;
00940     }
00941     return 0;
00942
00943 ERROR1:
00944     Vnm_print(2, "parsePBE: ran out of tokens!\n");
00945     return -1;
00946 }
00947
00948 VPRIVATE int PBEparm_parseCALCFORCE(PBEparm *thee, Vio *sock) {
00949     char tok[VMAX_BUFSIZE];
00950     int ti;
00951
00952     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00953     /* Parse number */
00954     if (sscanf(tok, "%d", &ti) == 1) {
00955         thee->calcforce = (PBEparm_calcForce)ti;
00956         thee->setcalcforce = 1;
00957
00958         Vnm_print(2, "parsePBE: Warning -- parsed deprecated \"calcforce \
00959 %d\" statement.\n", ti);
00960         Vnm_print(2, "parsePBE: Please use \"calcforce ");

```

```

00961         switch (thee->calcenergy) {
00962             case PCF_NO:
00963                 Vnm_print(2, "no");
00964                 break;
00965             case PCF_TOTAL:
00966                 Vnm_print(2, "total");
00967                 break;
00968             case PCF_COMPS:
00969                 Vnm_print(2, "comps");
00970                 break;
00971             default:
00972                 Vnm_print(2, "UNKNOWN");
00973                 break;
00974         }
00975         Vnm_print(2, "\" instead.\n");
00976         return 1;
00977     } else if (Vstring_strcasecmp(tok, "no") == 0) {
00978         thee->calcforce = PCF_NO;
00979         thee->setcalcforce = 1;
00980         return 1;
00981     } else if (Vstring_strcasecmp(tok, "total") == 0) {
00982         thee->calcforce = PCF_TOTAL;
00983         thee->setcalcforce = 1;
00984         return 1;
00985     } else if (Vstring_strcasecmp(tok, "comps") == 0) {
00986         thee->calcforce = PCF_COMPS;
00987         thee->setcalcforce = 1;
00988         return 1;
00989     } else {
00990         Vnm_print(2, "Nosh: Unrecognized parameter (%s) while parsing \
00991 calcforce!\n", tok);
00992         return -1;
00993     }
00994     return 0;
00995
00996     ERROR1:
00997         Vnm_print(2, "parsePBE: ran out of tokens!\n");
00998         return -1;
00999 }
01000
01001 /*-----*/
01002 /* Added by Michael Grabe */
01003 /*-----*/
01004
01005 VPRIVATE int PBEparm_parseZMEM(PBEparm *thee, Vio *sock) {
01006     char tok[VMAX_BUFSIZE];
01007     double tf;
01008
01009     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01010     if (sscanf(tok, "%lf", &tf) == 0) {
01011         Vnm_print(2, "Nosh: Read non-float (%s) while parsing ZMEM \
01012 keyword!\n", tok);
01013         return -1;
01014     }
01015     thee->zmem = tf;
01016     thee->setzmem = 1;
01017     return 1;
01018
01019     ERROR1:
01020         Vnm_print(2, "parsePBE: ran out of tokens!\n");
01021         return -1;
01022 }
01023
01024
01025 VPRIVATE int PBEparm_parseLMEM(PBEparm *thee, Vio *sock) {
01026     char tok[VMAX_BUFSIZE];
01027     double tf;
01028
01029     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01030     if (sscanf(tok, "%lf", &tf) == 0) {
01031         Vnm_print(2, "Nosh: Read non-float (%s) while parsing LMEM \
01032 keyword!\n", tok);
01033         return -1;
01034     }
01035     thee->Lmem = tf;
01036     thee->setLmem = 1;
01037     return 1;
01038
01039     ERROR1:
01040         Vnm_print(2, "parsePBE: ran out of tokens!\n");
01041         return -1;

```

```

01042 }
01043
01044 VPRIVATE int PBeparm_parseMDIE(PBeparm *thee, Vio *sock) {
01045     char tok[VMAX_BUFSIZE];
01046     double tf;
01047
01048     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01049     if (sscanf(tok, "%lf", &tf) == 0) {
01050         Vnm_print(2, "NOSH: Read non-float (%s) while parsing MDIE \
01051             keyword!\n", tok);
01052         return -1;
01053     }
01054     thee->mdie = tf;
01055     thee->setmdie = 1;
01056     return 1;
01057
01058 ERROR1:
01059     Vnm_print(2, "parsePBE: ran out of tokens!\n");
01060     return -1;
01061 }
01062
01063 VPRIVATE int PBeparm_parseMEMV(PBeparm *thee, Vio *sock) {
01064     char tok[VMAX_BUFSIZE];
01065     double tf;
01066
01067     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01068     if (sscanf(tok, "%lf", &tf) == 0) {
01069         Vnm_print(2, "NOSH: Read non-float (%s) while parsing MEMV \
01070             keyword!\n", tok);
01071         return -1;
01072     }
01073     thee->memv = tf;
01074     thee->setmemv = 1;
01075     return 1;
01076
01077 ERROR1:
01078     Vnm_print(2, "parsePBE: ran out of tokens!\n");
01079     return -1;
01080 }
01081
01082 /*-----*/
01083
01084 VPRIVATE int PBeparm_parseWRITE(PBeparm *thee, Vio *sock) {
01085     char tok[VMAX_BUFSIZE], str[VMAX_BUFSIZE]="", strnew[VMAX_BUFSIZE]="";
01086     Vdata_Type writetype;
01087     Vdata_Format writefmt;
01088
01089     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01090     if (Vstring_strcasecmp(tok, "pot") == 0) {
01091         writetype = VDT_POT;
01092     } else if (Vstring_strcasecmp(tok, "atompot") == 0) {
01093         writetype = VDT_ATOMPOT;
01094     } else if (Vstring_strcasecmp(tok, "charge") == 0) {
01095         writetype = VDT_CHARGE;
01096     } else if (Vstring_strcasecmp(tok, "smol") == 0) {
01097         writetype = VDT_SMOL;
01098     } else if (Vstring_strcasecmp(tok, "dielx") == 0) {
01099         writetype = VDT_DIELX;
01100     } else if (Vstring_strcasecmp(tok, "diely") == 0) {
01101         writetype = VDT_DIELY;
01102     } else if (Vstring_strcasecmp(tok, "dielz") == 0) {
01103         writetype = VDT_DIELZ;
01104     } else if (Vstring_strcasecmp(tok, "kappa") == 0) {
01105         writetype = VDT_KAPPA;
01106     } else if (Vstring_strcasecmp(tok, "sspl") == 0) {
01107         writetype = VDT_SSPL;
01108     } else if (Vstring_strcasecmp(tok, "vdw") == 0) {
01109         writetype = VDT_VDW;
01110     } else if (Vstring_strcasecmp(tok, "ivdw") == 0) {
01111         writetype = VDT_IVDW;
01112     } else if (Vstring_strcasecmp(tok, "lap") == 0) {
01113         writetype = VDT_LAP;
01114     } else if (Vstring_strcasecmp(tok, "edens") == 0) {
01115         writetype = VDT_EDENS;
01116     } else if (Vstring_strcasecmp(tok, "ndens") == 0) {
01117         writetype = VDT_NDENS;
01118     } else if (Vstring_strcasecmp(tok, "qdens") == 0) {
01119         writetype = VDT_QDENS;
01120     } else if (Vstring_strcasecmp(tok, "3dmap") == 0) {
01121         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01122         strcpy(thee->pbam_3dmapstem, tok);

```

```

01123     thee->pbam_3dmapflag = 1;
01124     return 1;
01125     } else {
01126         Vnm_print(2, "PBEparam_parse: Invalid data type (%s) to write!\n",
01127             tok);
01128         return -1;
01129     }
01130
01131     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01132     if (Vstring_strcasecmp(tok, "dx") == 0) {
01133         writefmt = VDF_DX;
01134     }
01135     else if (Vstring_strcasecmp(tok, "dxbin") == 0) {
01136         writefmt = VDF_DXBIN;
01137     } else if (Vstring_strcasecmp(tok, "uhbd") == 0) {
01138         writefmt = VDF_UHBD;
01139     } else if (Vstring_strcasecmp(tok, "avs") == 0) {
01140         writefmt = VDF_AVIS;
01141     } else if (Vstring_strcasecmp(tok, "gz") == 0) {
01142         writefmt = VDF_GZ;
01143     } else if (Vstring_strcasecmp(tok, "flat") == 0) {
01144         writefmt = VDF_FLAT;
01145     } else {
01146         Vnm_print(2, "PBEparam_parse: Invalid data format (%s) to write!\n",
01147             tok);
01148         return -1;
01149     }
01150     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01151     if (tok[0]!='\n') {
01152         strcpy(strnew, "");
01153         while (tok[strlen(tok)-1] != '\n') {
01154             strcat(str, tok);
01155             strcat(str, " ");
01156             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01157         }
01158         strcat(str, tok);
01159         strncpy(strnew, str+1, strlen(str)-2);
01160         strcpy(tok, strnew);
01161     }
01162     if (thee->numwrite < (PBEPARAM_MAXWRITE-1)) {
01163         strcpy(thee->writestem[thee->numwrite], tok, VMAX_ARGLEN);
01164         thee->writetype[thee->numwrite] = writetype;
01165         thee->writefmt[thee->numwrite] = writefmt;
01166         (thee->numwrite)++;
01167     } else {
01168         Vnm_print(2, "PBEparam_parse: You have exceeded the maximum number of write statements!\n");
01169         Vnm_print(2, "PBEparam_parse: Ignoring additional write statements!\n");
01170     }
01171     return 1;
01172
01173     VERR01:
01174     Vnm_print(2, "parsePBE: ran out of tokens!\n");
01175     return -1;
01176 }
01177
01178 VPRIVATE int PBEparam_parseWRITEMAT(PBEparam *thee, Vio *sock) {
01179     char tok[VMAX_BUFSIZE], str[VMAX_BUFSIZE]="", strnew[VMAX_BUFSIZE]="";
01180
01181     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01182     if (Vstring_strcasecmp(tok, "poisson") == 0) {
01183         thee->writematflag = 0;
01184     } else if (Vstring_strcasecmp(tok, "full") == 0) {
01185         thee->writematflag = 1;
01186     } else {
01187         Vnm_print(2, "NOSH: Invalid format (%s) while parsing \
01188 WRITEMAT keyword!\n", tok);
01189         return -1;
01190     }
01191
01192     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01193     if (tok[0]!='\n') {
01194         strcpy(strnew, "");
01195         while (tok[strlen(tok)-1] != '\n') {
01196             strcat(str, tok);
01197             strcat(str, " ");
01198             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01199         }
01200         strcat(str, tok);
01201         strncpy(strnew, str+1, strlen(str)-2);
01202         strcpy(tok, strnew);
01203     }

```

```

01204     strncpy(thee->writematstem, tok, VMAX_ARGLEN);
01205     thee->setwritemat = 1;
01206     thee->writemat = 1;
01207     return 1;
01208
01209     VERROR1:
01210         Vnm_print(2, "parsePBE: ran out of tokens!\n");
01211         return -1;
01212
01213 }
01214
01215 VPUBLIC int PBEparm_parseToken(PBEparm *thee, char tok[VMAX_BUFSIZE],
01216     Vio *sock) {
01217
01218     if (thee == VNULL) {
01219         Vnm_print(2, "parsePBE: got NULL thee!\n");
01220         return -1;
01221     }
01222     if (sock == VNULL) {
01223         Vnm_print(2, "parsePBE: got NULL socket!\n");
01224         return -1;
01225     }
01226
01227     Vnm_print(0, "PBEparm_parseToken: trying %s...\n", tok);
01228
01229     if (Vstring_strcasecmp(tok, "mol") == 0) {
01230         return PBEparm_parseMOL(thee, sock);
01231     } else if (Vstring_strcasecmp(tok, "lpbe") == 0) {
01232         return PBEparm_parseLPBE(thee, sock);
01233     } else if (Vstring_strcasecmp(tok, "npbe") == 0) {
01234         return PBEparm_parseNPBE(thee, sock);
01235     } else if (Vstring_strcasecmp(tok, "lrpbe") == 0) {
01236         return PBEparm_parseLRPBE(thee, sock);
01237     } else if (Vstring_strcasecmp(tok, "nrpbe") == 0) {
01238         return PBEparm_parseNRPBE(thee, sock);
01239     } else if (Vstring_strcasecmp(tok, "smpbe") == 0) {
01240         return PBEparm_parseSMPBE(thee, sock);
01241     } else if (Vstring_strcasecmp(tok, "bcfl") == 0) {
01242         return PBEparm_parseBCFL(thee, sock);
01243     } else if (Vstring_strcasecmp(tok, "ion") == 0) {
01244         return PBEparm_parseION(thee, sock);
01245     } else if (Vstring_strcasecmp(tok, "pdie") == 0) {
01246         return PBEparm_parsePDIE(thee, sock);
01247     } else if (Vstring_strcasecmp(tok, "sdens") == 0) {
01248         return PBEparm_parseSDENS(thee, sock);
01249     } else if (Vstring_strcasecmp(tok, "sdie") == 0) {
01250         return PBEparm_parseSDIE(thee, sock);
01251     } else if (Vstring_strcasecmp(tok, "srfm") == 0) {
01252         return PBEparm_parseSRFM(thee, sock);
01253     } else if (Vstring_strcasecmp(tok, "srad") == 0) {
01254         return PBEparm_parseSRAD(thee, sock);
01255     } else if (Vstring_strcasecmp(tok, "swin") == 0) {
01256         return PBEparm_parseSWIN(thee, sock);
01257     } else if (Vstring_strcasecmp(tok, "temp") == 0) {
01258         return PBEparm_parseTEMP(thee, sock);
01259     } else if (Vstring_strcasecmp(tok, "usemap") == 0) {
01260         return PBEparm_parseUSEMAP(thee, sock);
01261     } else if (Vstring_strcasecmp(tok, "calcenergy") == 0) {
01262         return PBEparm_parseCALCENERGY(thee, sock);
01263     } else if (Vstring_strcasecmp(tok, "calcforce") == 0) {
01264         return PBEparm_parseCALCFORCE(thee, sock);
01265     } else if (Vstring_strcasecmp(tok, "write") == 0) {
01266         return PBEparm_parseWRITE(thee, sock);
01267     } else if (Vstring_strcasecmp(tok, "writemat") == 0) {
01268         return PBEparm_parseWRITEMAT(thee, sock);
01269
01270     /*-----*/
01271     /* Added by Michael Grabe */
01272     /*-----*/
01273
01274     } else if (Vstring_strcasecmp(tok, "zmem") == 0) {
01275         return PBEparm_parseZMEM(thee, sock);
01276     } else if (Vstring_strcasecmp(tok, "lmem") == 0) {
01277         return PBEparm_parseLMEM(thee, sock);
01278     } else if (Vstring_strcasecmp(tok, "mdie") == 0) {
01279         return PBEparm_parseMDIE(thee, sock);
01280     } else if (Vstring_strcasecmp(tok, "memv") == 0) {
01281         return PBEparm_parseMEMV(thee, sock);
01282     }
01283
01284     /*-----*/

```

```

01285
01286     return 0;
01287
01288 }

```

9.44 src/generic/pbeparm.h File Reference

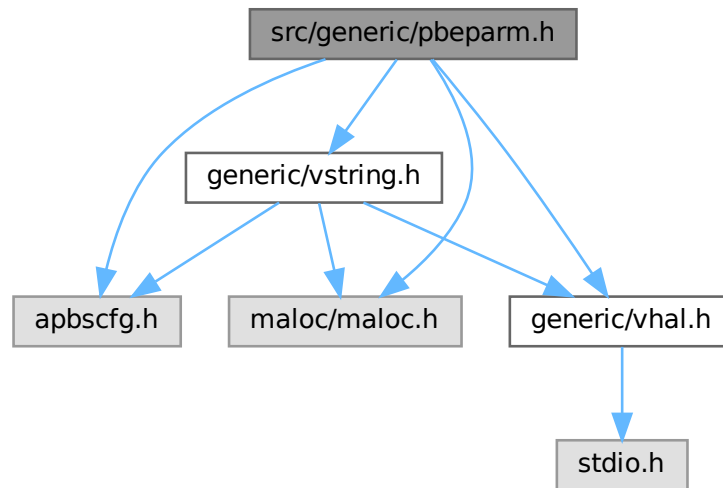
Contains declarations for class PBEparm.

```

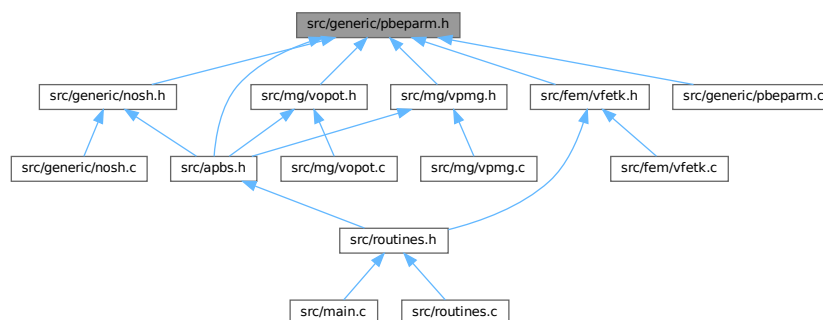
#include "apbscfg.h"
#include "malloc/malloc.h"
#include "generic/vhal.h"
#include "generic/vstring.h"

```

Include dependency graph for pbeparm.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sPBEparm](#)
Parameter structure for PBE variables from input files.

Macros

- #define [PBEARM_MAXWRITE](#) 20
Number of things that can be written out in a single calculation.

Typedefs

- typedef enum [ePBEparm_calcEnergy](#) [PBEparm_calcEnergy](#)
Define ePBEparm_calcEnergy enumeration as PBEparm_calcEnergy.
- typedef enum [ePBEparm_calcForce](#) [PBEparm_calcForce](#)
Define ePBEparm_calcForce enumeration as PBEparm_calcForce.
- typedef struct [sPBEparm](#) [PBEparm](#)
Declaration of the PBEparm class as the PBEparm structure.

Enumerations

- enum [ePBEparm_calcEnergy](#) { [PCE_NO](#) =0 , [PCE_TOTAL](#) =1 , [PCE_COMPS](#) =2 }
Define energy calculation enumeration.
- enum [ePBEparm_calcForce](#) { [PCF_NO](#) =0 , [PCF_TOTAL](#) =1 , [PCF_COMPS](#) =2 }
Define force calculation enumeration.

Functions

- VEXTERNC double [PBEparm_getIonCharge](#) ([PBEparm](#) *thee, int iion)
Get charge (e) of specified ion species.
- VEXTERNC double [PBEparm_getIonConc](#) ([PBEparm](#) *thee, int iion)
Get concentration (M) of specified ion species.
- VEXTERNC double [PBEparm_getIonRadius](#) ([PBEparm](#) *thee, int iion)
Get radius (A) of specified ion species.
- VEXTERNC [PBEparm](#) * [PBEparm_ctor](#) ()
Construct PBEparm object.
- VEXTERNC int [PBEparm_ctor2](#) ([PBEparm](#) *thee)
FORTTRAN stub to construct PBEparm object.
- VEXTERNC void [PBEparm_dtor](#) ([PBEparm](#) **thee)
Object destructor.
- VEXTERNC void [PBEparm_dtor2](#) ([PBEparm](#) *thee)
FORTTRAN stub for object destructor.
- VEXTERNC int [PBEparm_check](#) ([PBEparm](#) *thee)
Consistency check for parameter values stored in object.
- VEXTERNC void [PBEparm_copy](#) ([PBEparm](#) *thee, [PBEparm](#) *parm)
Copy PBEparm object into thee.
- VEXTERNC int [PBEparm_parseToken](#) ([PBEparm](#) *thee, char tok[VMAX_BUFSIZE], Vio *sock)
Parse a keyword from an input file.

9.44.1 Detailed Description

Contains declarations for class PBEparm.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```
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* Pacific Northwest National Laboratory
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*
*
```

Definition in file [pbeparm.h](#).

9.45 pbeparm.h

[Go to the documentation of this file.](#)


```

00001
00062 #ifndef _PBEPARM_H_
00063 #define _PBEPARM_H_
00064
00065 #include "apbscfg.h"
00066
00067 #include "malloc/malloc.h"
00068
00069 #include "generic/vhal.h"
00070 #include "generic/vstring.h"
00071
00075 #define PBEPARM_MAXWRITE 20
00076
00081 enum ePBEParm_calcEnergy {
00082     PCE_NO=0,
00083     PCE_TOTAL=1,
00084     PCE_COMPS=2
00085 };
00086
00091 typedef enum ePBEParm_calcEnergy PBEParm_calcEnergy;
00092
00097 enum ePBEParm_calcForce {
00098     PCF_NO=0,
00099     PCF_TOTAL=1,
00100     PCF_COMPS=2
00101 };
00102
00107 typedef enum ePBEParm_calcForce PBEParm_calcForce;
00108
00117 struct sPBEParm {
00118
00119     int molid;
00120     int setmolid;
00121     int useDielMap;
00123     int dielMapID;
00124     int useKappaMap;
00126     int kappaMapID;
00127     int usePotMap;
00129     int potMapID;
00131     int useChargeMap;
00133     int chargeMapID;
00134     Vhal_PBEType pbetype;
00135     int setpbetype;
00136     Vbcfl bcfl;
00137     int setbcfl;
00138     int nion;
00139     int setnion;
00140     double ionq[MAXION];
00141     double ionc[MAXION];
00142     double ionr[MAXION];
00143     int setion[MAXION];
00144     double pdie;
00145     int setpdie;
00146     double sdens;
00147     int setsdens;
00148     double sdie;
00149     int setsdie;
00150     Vsurf_Meth srfm;
00151     int setsrfm;
00152     double srad;
00153     int setsrad;
00154     double swin;
00155     int setswin;
00156     double temp;
00157     int settemp;
00159     double smsize;
00160     int setsmsize;
00162     double smvolume;
00163     int setsmvolume;
00165     PBEParm_calcEnergy calcenergy;
00166     int setcalcenergy;
00167     PBEParm_calcForce calcforce;
00168     int setcalcforce;
00170     /*-----*/
00171     /* Added by Michael Grabe */
00172     /*-----*/
00173
00174     double zmem;
00175     int setzmem;
00176     double Lmem;
00177     int setLmem;

```

```

00178     double mdie;
00179     int setmdie;
00180     double memv;
00181     int setmemv;
00183     /*-----*/
00184
00185     int numwrite;
00186     char writestem[PBE Parm_MAXWRITE][VMAX_ARGLEN];
00188     Vdata_Type writetype[PBE Parm_MAXWRITE];
00189     Vdata_Format writefmt[PBE Parm_MAXWRITE];
00191     int writemat;
00194     int setwritemat;
00195     char writematstem[VMAX_ARGLEN];
00196     int writematflag;
00201     /*Added for issue 482*/
00202     char pbam_3dmapstem[VMAX_ARGLEN];
00203     int pbam_3dmapflag;
00204
00205     int parsed;
00207 };
00208
00213 typedef struct sPBE Parm PBE Parm;
00214
00215 /* ////////////////////////////////////// */
00216 // Class NOsh: Non-inlineable methods (mcsh.c)
00218
00224 VEXTERNC double PBE Parm_getIonCharge(
00225     PBE Parm *thee, /**< PBE Parm object */
00226     int iion
00227 );
00228
00234 VEXTERNC double PBE Parm_getIonConc(
00235     PBE Parm *thee,
00236     int iion
00237 );
00238
00244 VEXTERNC double PBE Parm_getIonRadius(
00245     PBE Parm *thee,
00246     int iion
00247 );
00248
00249
00255 VEXTERNC PBE Parm* PBE Parm_ctor();
00256
00262 VEXTERNC int PBE Parm_ctor2(
00263     PBE Parm *thee
00264 );
00265
00270 VEXTERNC void PBE Parm_dtor(
00271     PBE Parm **thee
00272 );
00273
00278 VEXTERNC void PBE Parm_dtor2(
00279     PBE Parm *thee
00280 );
00281
00287 VEXTERNC int PBE Parm_check(
00288     PBE Parm *thee
00289 );
00290
00295 VEXTERNC void PBE Parm_copy(
00296     PBE Parm *thee,
00297     PBE Parm *parm
00298 );
00299
00306 VEXTERNC int PBE Parm_parseToken(
00307     PBE Parm *thee,
00308     char tok[VMAX_BUFSIZE],
00309     Vio *sock
00310 );
00311
00312
00313 #endif
00314

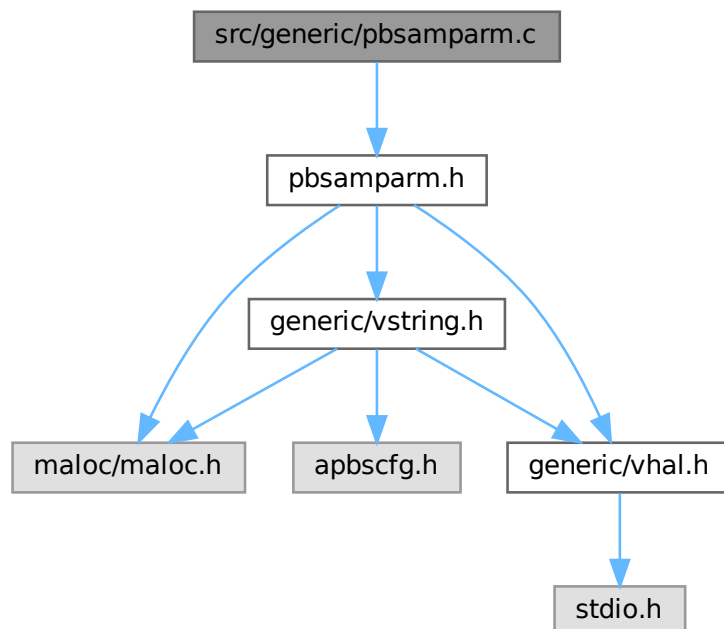
```

9.46 src/generic/pbsamparm.c File Reference

Class PBSAM Parm methods.

```
#include "pbsamparm.h"
```

Include dependency graph for pbsamparm.c:



Functions

- VPUBLIC PBSAMparm * PBSAMparm_ctor (PBSAMparm_CalcType type)
Construct PBSAMparm object.
- VPUBLIC Vrc_Codes PBSAMparm_ctor2 (PBSAMparm *thee, PBSAMparm_CalcType type)
FORTTRAN stub to construct PBSAMparm object ?????????!!!!!!!
- VPUBLIC void PBSAMparm_dtor (PBSAMparm **thee)
Object destructor.
- VPUBLIC void PBSAMparm_dtor2 (PBSAMparm *thee)
FORTTRAN stub for object destructor ?????????!!!!!!!
- VPUBLIC Vrc_Codes PBSAMparm_check (PBSAMparm *thee)
Consistency check for parameter values stored in object.
- VPUBLIC void PBSAMparm_copy (PBSAMparm *thee, PBSAMparm *parm)
copy PBSAMparm object into thee.
- VPRIVATE Vrc_Codes PBSAMparm_parseSurf (PBSAMparm *thee, Vio *sock)
Find vertex files for each molecule and save them.
- VPRIVATE Vrc_Codes PBSAMparm_parseMSMS (PBSAMparm *thee, Vio *sock)
Find msms flag for if MSMS is to be run.
- VPRIVATE Vrc_Codes PBSAMparm_parselmat (PBSAMparm *thee, Vio *sock)
Find IMAT files for each molecule and save them.

- VPRIVATE Vrc_Codes [PBSAMparm_parseExp](#) ([PBSAMparm](#) *thee, Vio *sock)
Find expansion files for each molecule and save them.
- VPRIVATE Vrc_Codes [PBSAMparm_parseTolsp](#) ([PBSAMparm](#) *thee, Vio *sock)
Find sphere tolerance for coarse-graining.
- VPUBLIC Vrc_Codes [PBSAMparm_parseToken](#) ([PBSAMparm](#) *thee, char tok[VMAX_BUFSIZE], Vio *sock)
Parse an MG keyword from an input file.

9.46.1 Detailed Description

Class PBSAMparm methods.

Author

Andrew Stevens

Version

\$Id\$

Attention

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*

```

Definition in file [pbsamparm.c](#).

9.47 pbsamparm.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "pbsamparm.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 #if !defined(VINLINE_MGPARM)
00062
00063 #endif /* if !defined(VINLINE_MGPARM) */
00064
00065
00066 VPUBLIC PBSamparm* PBSamparm_ctor(PBSamparm_CalcType type) {
00067
00068     /* Set up the structure */
00069     PBSamparm *thee = VNULL;
00070     thee = (PBSamparm*)Vmem_malloc(VNULL, 1, sizeof(PBSamparm));
00071     VASSERT( thee != VNULL);
00072     VASSERT( PBSamparm_ctor2(thee, type) == VRC_SUCCESS );
00073
00074     return thee;
00075 }
00076
00077 VPUBLIC Vrc_Codes PBSamparm_ctor2(PBSamparm *thee, PBSamparm_CalcType type) {
00078
00079     int i;
00080
00081     if (thee == VNULL) return VRC_FAILURE;
00082
00083     thee->tolsp = 2.5;
00084     thee->setmsms = 0;
00085     thee->probe_radius = 1.5;
00086     thee->density = 3.0;
00087
00088     thee->setsurf = 0;
00089     thee->surfct = 0;
00090
00091     thee->setimat = 0;
00092     thee->imatct = 0;
00093
00094     thee->setexp = 0;
00095     thee->expct = 0;
00096
00097     return VRC_SUCCESS;
00098 }
00099
00100 VPUBLIC void PBSamparm_dtor(PBSamparm **thee) {
00101     if ((*thee) != VNULL) {
00102         PBSamparm_dtor2(*thee);
00103         Vmem_free(VNULL, 1, sizeof(PBSamparm), (void **)thee);
00104         (*thee) = VNULL;
00105     }
00106 }
00107
00108 VPUBLIC void PBSamparm_dtor2(PBSamparm *thee) { ; }
00109
00110 VPUBLIC Vrc_Codes PBSamparm_check(PBSamparm *thee) {
00111
00112     Vrc_Codes rc;
00113
00114     rc = VRC_SUCCESS;
00115
00116     Vnm_print(0, "PBSamparm_check: checking PBSamparm object of type %d.\n",
00117               thee->type);
00118
00119     /* Check to see if we were even filled... */
00120     if (!thee->parsed) {
00121         Vnm_print(2, "PBSamparm_check: not filled!\n");
00122         return VRC_FAILURE;

```

```

00123     }
00124
00125
00126     /* Check type settings */
00127     if (thee->type != PBSAMCT_AUTO) {
00128         Vnm_print(2, "PBSAMparm_check: type not set");
00129         rc = VRC_FAILURE;
00130     }
00131
00132     return rc;
00133 }
00134
00135 VPUBLIC void PBSAMparm_copy(PBSAMparm *thee, PBSAMparm *parm) {
00136     int i, j;
00137     VASSERT(thee != VNULL);
00138     VASSERT(parm != VNULL);
00139
00140
00141     thee->settolsp = parm->settolsp;
00142     thee->tolsp = parm->tolsp;
00143
00144     thee->setmsms = parm->setmsms;
00145     thee->probe_radius = parm->probe_radius;
00146     thee->density = parm->density;
00147     thee->setsurf = parm->setsurf;
00148     thee->surfct = parm->surfct;
00149     thee->setimat = parm->setimat;
00150     thee->imatct = parm->imatct;
00151     thee->setexp = parm->setexp;
00152     thee->expct = parm->expct;
00153
00154     for (i=0; i<PBSAMPARM_MAXWRITE; i++)
00155     {
00156         for (j=0; j<CHR_MAXLEN; j++)
00157         {
00158             thee->surffil[i][j] = parm->surffil[i][j];
00159             thee->imatfil[i][j] = parm->imatfil[i][j];
00160             thee->expfil[i][j] = parm->expfil[i][j];
00161         }
00162     }
00163 }
00164
00165 //Parsing vertex file
00166 VPRIVATE Vrc_Codes PBSAMparm_parseSurf(PBSAMparm *thee, Vio *sock){
00167     const char* name = "usemesh";
00168     char tok[VMAX_BUFSIZE];
00169
00170     if (Vio_scanf(sock, "%s", tok) == 0) {
00171         Vnm_print(2, "parsePBSAM: ran out of tokens on %s!\n", name);
00172         return VRC_WARNING;
00173     } else {
00174         strncpy(thee->surffil[thee->surfct], tok, CHR_MAXLEN);
00175         thee->surfct += 1;
00176     }
00177     return VRC_SUCCESS;
00178 }
00179
00180
00181 //Parsing imat prefix file
00182 VPRIVATE Vrc_Codes PBSAMparm_parseMSMS(PBSAMparm *thee, Vio *sock){
00183     int td;
00184     char tok[VMAX_BUFSIZE];
00185     const char *name = "mesh";
00186
00187     if (Vio_scanf(sock, "%s", tok) == 0){
00188         Vnm_print(2, "parsePBSAM: ran out of tokens on %s!\n", name);
00189         return VRC_WARNING;
00190     }
00191
00192     if (strcmp(tok, "msms") == 0){
00193         thee->setmsms = 1;
00194     }
00195     else{
00196         Vnm_print(2, "parsePBSAM: %s is not currently supported in PBSAM! Change to msms\n", tok);
00197         return VRC_WARNING;
00198     }
00199
00200     return VRC_SUCCESS;
00201 }
00202 //Parsing imat prefix file
00203 VPRIVATE Vrc_Codes PBSAMparm_parseImat(PBSAMparm *thee, Vio *sock){

```

```

00204     const char* name = "imat";
00205     char tok[VMAX_BUFSIZE];
00206
00207     if (Vio_scanf(sock, "%s", tok) == 0) {
00208         Vnm_print(2, "parsePBSAM: ran out of tokens on %s!\n", name);
00209         return VRC_WARNING;
00210     } else {
00211         strncpy(thee->imatfil[thee->imatct], tok, CHR_MAXLEN);
00212         thee->imatct += 1;
00213     }
00214     return VRC_SUCCESS;
00215 }
00216
00217 //Parsing imat prefix file
00218 VPRIVATE Vrc_Codes PBSAMparm_parseExp(PBSAMparm *thee, Vio *sock){
00219     const char* name = "exp";
00220     char tok[VMAX_BUFSIZE];
00221
00222     if (Vio_scanf(sock, "%s", tok) == 0) {
00223         Vnm_print(2, "parsePBSAM: ran out of tokens on %s!\n", name);
00224         return VRC_WARNING;
00225     } else {
00226         strncpy(thee->expfil[thee->expct], tok, CHR_MAXLEN);
00227         thee->expct += 1;
00228     }
00229     return VRC_SUCCESS;
00230 }
00231
00232 VPRIVATE Vrc_Codes PBSAMparm_parseTolsp(PBSAMparm *thee, Vio *sock){
00233     const char* name = "tolsp";
00234     char tok[VMAX_BUFSIZE];
00235     double tf;
00236     if (Vio_scanf(sock, "%s", tok) == 0) {
00237         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00238         return VRC_WARNING;
00239     }
00240
00241     if (sscanf(tok, "%lf", &tf) == 0){
00242         Vnm_print(2, "Nosh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00243         return VRC_WARNING;
00244     }else{
00245         thee->tolsp = tf;
00246     }
00247     thee->settolsp = 1;
00248     return VRC_SUCCESS;
00249 }
00250
00251
00252 VPUBLIC Vrc_Codes PBSAMparm_parseToken(PBSAMparm *thee, char tok[VMAX_BUFSIZE],
00253     Vio *sock) {
00254
00255     if (thee == VNULL) {
00256         Vnm_print(2, "parsePBSAM: got NULL thee!\n");
00257         return VRC_WARNING;
00258     }
00259     if (sock == VNULL) {
00260         Vnm_print(2, "parsePBSAM: got NULL socket!\n");
00261         return VRC_WARNING;
00262     }
00263
00264     Vnm_print(0, "PBSAMparm_parseToken: trying %s...\n", tok);
00265
00266     // Molecule terms
00267     if (Vstring_strcasecmp(tok, "usemesh") == 0) {
00268         return PBSAMparm_parseSurf(thee, sock);
00269     }else if (Vstring_strcasecmp(tok, "mesh") == 0) {
00270         return PBSAMparm_parseMSMS(thee, sock);
00271     }else if (Vstring_strcasecmp(tok, "imat") == 0) {
00272         return PBSAMparm_parseImat(thee, sock);
00273     }else if (Vstring_strcasecmp(tok, "exp") == 0) {
00274         return PBSAMparm_parseExp(thee, sock);
00275     }else if (Vstring_strcasecmp(tok, "tolsp") == 0) {
00276         return PBSAMparm_parseTolsp(thee, sock);
00277     }
00278
00279     else {
00280         Vnm_print(2, "parsePBSAM: Unrecognized keyword (%s)!\n", tok);
00281         return VRC_WARNING;
00282     }
00283     return VRC_FAILURE;
00284 }

```

9.48 src/generic/pbsamparm.h File Reference

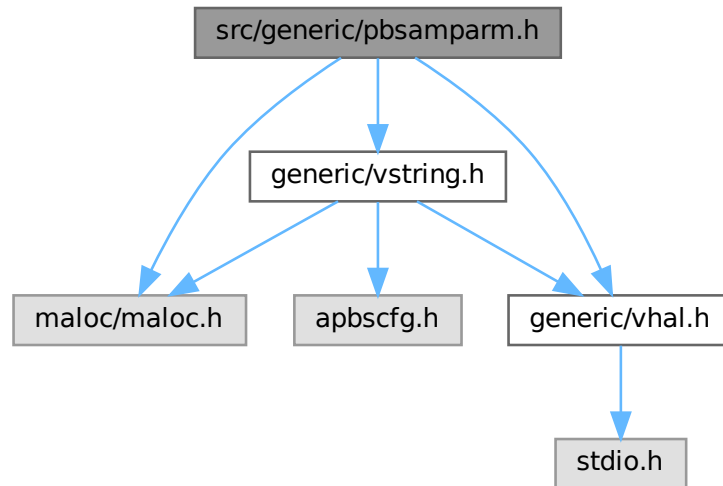
Contains declarations for class PBSAMparm.

```
#include "maloc/maloc.h"
```

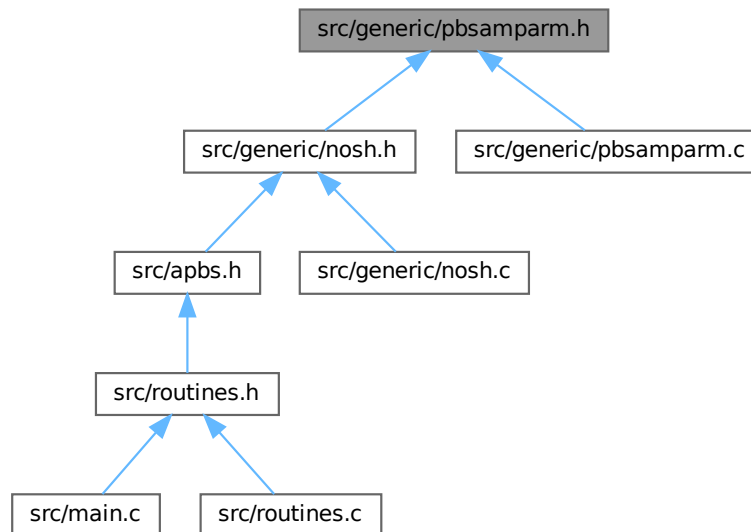
```
#include "generic/vhal.h"
```

```
#include "generic/vstring.h"
```

Include dependency graph for pbsamparm.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sPBSAMparm](#)
Parameter structure for PBSAM-specific variables from input files.

Macros

- #define [CHR_MAXLEN](#) 1000
Number of things that can be written out in a single calculation.
- #define [PBSAMPARM_MAXWRITE](#) 15
- #define [PBSAMPARM_MAXMOL](#) 150

Typedefs

- typedef enum [ePBSAMparm_CalcType](#) [PBSAMparm_CalcType](#)
Declare PBSAMparm_CalcType type.
- typedef struct [sPBSAMparm](#) [PBSAMparm](#)
Parameter structure for PBSAM-specific variables from input files.

Enumerations

- enum [ePBSAMparm_CalcType](#) { [PBSAMCT_AUTO](#) =1 }
- Calculation type.*

Functions

- VEXTERNC `PBSAMparm * PBSAMparm_ctor (PBSAMparm_CalcType type)`
Construct PBSAMparm object.
- VEXTERNC `Vrc_Codes PBSAMparm_ctor2 (PBSAMparm *thee, PBSAMparm_CalcType type)`
FORTTRAN stub to construct PBSAMparm object ?????????!!!!!!!
- VEXTERNC `void PBSAMparm_dtor (PBSAMparm **thee)`
Object destructor.
- VEXTERNC `void PBSAMparm_dtor2 (PBSAMparm *thee)`
FORTTRAN stub for object destructor ?????????!!!!!!!
- VEXTERNC `Vrc_Codes PBSAMparm_check (PBSAMparm *thee)`
Consistency check for parameter values stored in object.
- VEXTERNC `Vrc_Codes PBSAMparm_parseToken (PBSAMparm *thee, char tok[VMAX_BUFSIZE], Vio *sock)`
Parse an MG keyword from an input file.
- VEXTERNC `void PBSAMparm_copy (PBSAMparm *thee, PBSAMparm *parm)`
copy PBSAMparm object into thee.
- VPRIVATE `Vrc_Codes PBSAMparm_parseTolsp (PBSAMparm *thee, Vio *sock)`
Find sphere tolerance for coarse-graining.
- VPRIVATE `Vrc_Codes PBSAMparm_parseSurf (PBSAMparm *thee, Vio *sock)`
Find vertex files for each molecule and save them.
- VPRIVATE `Vrc_Codes PBSAMparm_parselmat (PBSAMparm *thee, Vio *sock)`
Find IMAT files for each molecule and save them.
- VPRIVATE `Vrc_Codes PBSAMparm_parseExp (PBSAMparm *thee, Vio *sock)`
Find expansion files for each molecule and save them.
- VPRIVATE `Vrc_Codes PBSAMparm_parseMSMS (PBSAMparm *thee, Vio *sock)`
Find msms flag for if MSMS is to be run.

9.48.1 Detailed Description

Contains declarations for class PBSAMparm.

Version

\$Id\$

Author

Lisa Felberg

Attention

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```

Definition in file [pbsamparm.h](#).

9.48.2 Macro Definition Documentation

9.48.2.1 PBSAMPARM_MAXMOL

```
#define PBSAMPARM_MAXMOL 150
```

Definition at line 78 of file [pbsamparm.h](#).

9.48.2.2 PBSAMPARM_MAXWRITE

```
#define PBSAMPARM_MAXWRITE 15
```

Definition at line 77 of file [pbsamparm.h](#).

9.49 pbsamparm.h

[Go to the documentation of this file.](#)

```

00001
00064 #ifndef _PBSAMPARM_H_
00065 #define _PBSAMPARM_H_
00066
00067 /* Generic header files */
00068 #include "malloc/malloc.h"
00069
00070 #include "generic/vhal.h"
00071 #include "generic/vstring.h"
00072
00076 #define CHR_MAXLEN 1000

```

```

00077 #define PBSAMPARM_MAXWRITE 15
00078 #define PBSAMPARM_MAXMOL 150
00079
00084 enum ePBSAMParm_CalcType {
00085     //other methods disabled for now only auto currently implemented.
00086     //PBSAMCT_MANUAL=0,  /**< PBSAM-manual */
00087     PBSAMCT_AUTO=1,
00088     //PBSAMCT_NONE=2 /**< not defined */
00089 };
00090
00095 typedef enum ePBSAMParm_CalcType PBSAMParm_CalcType;
00096
00105 typedef struct sPBSAMParm {
00106     PBSAMParm_CalcType type;
00107     int parsed;
00110     /* The only parms in addition to PBAM would be MSMS
00111        IMAT and Selfpol */
00112     int settolsp;
00113     double tolspl;
00114
00115     int setmsms;
00116     double probe_radius;
00117     double density;
00118
00119     int setsurf;
00120     int surfct;
00121     char surfhil[PBSAMPARM_MAXMOL][CHR_MAXLEN];
00122
00123     int setimat;
00124     int imatct;
00125     char imatfil[PBSAMPARM_MAXMOL][CHR_MAXLEN];
00126
00127     int setexp;
00128     int expct;
00129     char expfil[PBSAMPARM_MAXMOL][CHR_MAXLEN];
00130
00131 } PBSAMParm;
00132
00139 VEXTERNC PBSAMParm* PBSAMParm_ctor(PBSAMParm_CalcType type);
00140
00148 VEXTERNC Vrc_Codes PBSAMParm_ctor2(PBSAMParm *thee, PBSAMParm_CalcType type);
00149
00155 VEXTERNC void PBSAMParm_dtor(PBSAMParm **thee);
00156
00162 VEXTERNC void PBSAMParm_dtor2(PBSAMParm *thee);
00163
00170 VEXTERNC Vrc_Codes PBSAMParm_check(PBSAMParm *thee);
00171
00181 VEXTERNC Vrc_Codes PBSAMParm_parseToken(PBSAMParm *thee, char tok[VMAX_BUFSIZE],
00182     Vio *sock);
00190 VEXTERNC void PBSAMParm_copy(PBSAMParm *thee, PBSAMParm *parm);
00191
00199 VPRIVATE Vrc_Codes PBSAMParm_parseTolsp(PBSAMParm *thee, Vio *sock);
00200
00208 VPRIVATE Vrc_Codes PBSAMParm_parseSurf(PBSAMParm *thee, Vio *sock);
00209
00217 VPRIVATE Vrc_Codes PBSAMParm_parseImat(PBSAMParm *thee, Vio *sock);
00218
00226 VPRIVATE Vrc_Codes PBSAMParm_parseExp(PBSAMParm *thee, Vio *sock);
00227
00235 VPRIVATE Vrc_Codes PBSAMParm_parseMSMS(PBSAMParm *thee, Vio *sock);
00236
00237 #endif
00238

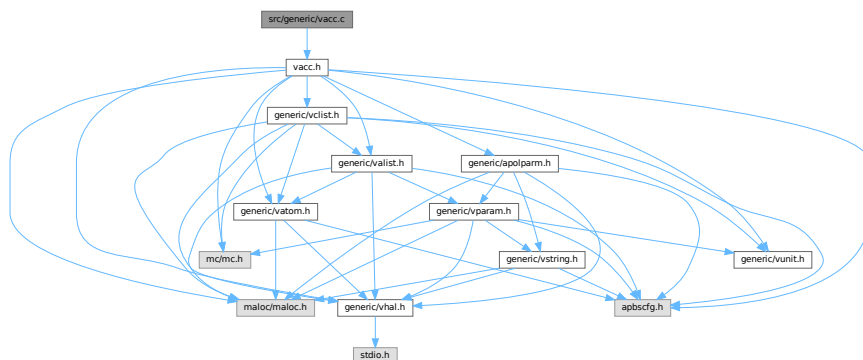
```

9.50 src/generic/vacc.c File Reference

Class Vacc methods.

```
#include "vacc.h"
```

Include dependency graph for vacc.c:



Functions

- VPUBLIC unsigned long int [Vacc_memChk](#) ([Vacc](#) *thee)
Get number of bytes in this object and its members.
- VPRIVATE int [ivdwAccExclus](#) ([Vacc](#) *thee, double center[3], double radius, int atomID)
Determines if a point is within the union of the spheres centered at the atomic centers with radii equal to the sum of their van der Waals radii and the probe radius. Does not include contributions from the specified atom.
- VPUBLIC [Vacc](#) * [Vacc_ctor](#) ([Valist](#) *alist, [Vclist](#) *clist, double surf_density)
Construct the accessibility object.
- VPRIVATE int [Vacc_storeParms](#) ([Vacc](#) *thee, [Valist](#) *alist, [Vclist](#) *clist, double surf_density)
- VPRIVATE int [Vacc_allocate](#) ([Vacc](#) *thee)
- VPUBLIC int [Vacc_ctor2](#) ([Vacc](#) *thee, [Valist](#) *alist, [Vclist](#) *clist, double surf_density)
FORTTRAN stub to construct the accessibility object.
- VPUBLIC void [Vacc_dtor](#) ([Vacc](#) **thee)
Destroy object.
- VPUBLIC void [Vacc_dtor2](#) ([Vacc](#) *thee)
FORTTRAN stub to destroy object.
- VPUBLIC double [Vacc_vdwAcc](#) ([Vacc](#) *thee, double center[3])
- VPUBLIC double [Vacc_ivdwAcc](#) ([Vacc](#) *thee, double center[3], double radius)
- VPUBLIC void [Vacc_splineAccGradAtomNorm](#) ([Vacc](#) *thee, double center[[VAPBS_DIM](#)], double win, double infrad, [Vatom](#) *atom, double *grad)
Report gradient of spline-based accessibility with respect to a particular atom normalized by the accessibility value due to that atom at that point (see [Vpmg_splineAccAtom](#))
- VPUBLIC void [Vacc_splineAccGradAtomUnnorm](#) ([Vacc](#) *thee, double center[[VAPBS_DIM](#)], double win, double infrad, [Vatom](#) *atom, double *grad)
Report gradient of spline-based accessibility with respect to a particular atom (see [Vpmg_splineAccAtom](#))
- VPUBLIC double [Vacc_splineAccAtom](#) ([Vacc](#) *thee, double center[[VAPBS_DIM](#)], double win, double infrad, [Vatom](#) *atom)
Report spline-based accessibility for a given atom.
- VPRIVATE double [splineAcc](#) ([Vacc](#) *thee, double center[[VAPBS_DIM](#)], double win, double infrad, [VclistCell](#) *cell)
Fast spline-based surface computation subroutine.
- VPUBLIC double [Vacc_splineAcc](#) ([Vacc](#) *thee, double center[[VAPBS_DIM](#)], double win, double infrad)

Report spline-based accessibility.

- VPUBLIC void `Vacc_splineAccGrad` (`Vacc` *thee, double center[`VAPBS_DIM`], double win, double infrad, double *grad)

Report gradient of spline-based accessibility.

- VPUBLIC double `Vacc_molAcc` (`Vacc` *thee, double center[`VAPBS_DIM`], double radius)

Report molecular accessibility.

- VPUBLIC double `Vacc_fastMolAcc` (`Vacc` *thee, double center[`VAPBS_DIM`], double radius)

Report molecular accessibility quickly.

- VPUBLIC void `Vacc_writeGMV` (`Vacc` *thee, double radius, int meth, Gem *gm, char *iodev, char *iofmt, char *iohost, char *iofile)
- VPUBLIC double `Vacc_SASA` (`Vacc` *thee, double radius)

Build the solvent accessible surface (SAS) and calculate the solvent accessible surface area.

- VPUBLIC double `Vacc_totalSASA` (`Vacc` *thee, double radius)

Return the total solvent accessible surface area (SASA)

- VPUBLIC double `Vacc_atomSASA` (`Vacc` *thee, double radius, `Vatom` *atom)

Return the atomic solvent accessible surface area (SASA)

- VPUBLIC `VaccSurf` * `VaccSurf_ctor` (`Vmem` *mem, double probe_radius, int nsphere)

Allocate and construct the surface object; do not assign surface points to positions.

- VPUBLIC int `VaccSurf_ctor2` (`VaccSurf` *thee, `Vmem` *mem, double probe_radius, int nsphere)

Construct the surface object using previously allocated memory; do not assign surface points to positions.

- VPUBLIC void `VaccSurf_dtor` (`VaccSurf` **thee)

Destroy the surface object and free its memory.

- VPUBLIC void `VaccSurf_dtor2` (`VaccSurf` *thee)

Destroy the surface object.

- VPUBLIC `VaccSurf` * `Vacc_atomSurf` (`Vacc` *thee, `Vatom` *atom, `VaccSurf` *ref, double prad)

Set up an array of points corresponding to the SAS due to a particular atom.

- VPUBLIC `VaccSurf` * `VaccSurf_refSphere` (`Vmem` *mem, int npts)

Set up an array of points for a reference sphere of unit radius.

- VPUBLIC `VaccSurf` * `Vacc_atomSASPoints` (`Vacc` *thee, double radius, `Vatom` *atom)

Get the set of points for this atom's solvent-accessible surface.

- VPUBLIC void `Vacc_splineAccGradAtomNorm4` (`Vacc` *thee, double center[`VAPBS_DIM`], double win, double infrad, `Vatom` *atom, double *grad)

Report gradient of spline-based accessibility with respect to a particular atom normalized by a 4th order accessibility value due to that atom at that point (see `Vpmsg_splineAccAtom`)

- VPUBLIC void `Vacc_splineAccGradAtomNorm3` (`Vacc` *thee, double center[`VAPBS_DIM`], double win, double infrad, `Vatom` *atom, double *grad)

Report gradient of spline-based accessibility with respect to a particular atom normalized by a 3rd order accessibility value due to that atom at that point (see `Vpmsg_splineAccAtom`)

- VPUBLIC void `Vacc_atomdSAV` (`Vacc` *thee, double srاد, `Vatom` *atom, double *dSA)

Get the derivatve of solvent accessible volume.

- VPRIVATE double `Vacc_SASAPos` (`Vacc` *thee, double radius)
- VPRIVATE double `Vacc_atomSASAPos` (`Vacc` *thee, double radius, `Vatom` *atom, int mode)
- VPUBLIC void `Vacc_atomdSASA` (`Vacc` *thee, double dpos, double srاد, `Vatom` *atom, double *dSA)

Get the derivatve of solvent accessible area.

- VPUBLIC void `Vacc_totalAtomdSASA` (`Vacc` *thee, double dpos, double srاد, `Vatom` *atom, double *dSA)

Testing purposes only.

- VPUBLIC void `Vacc_totalAtomdSAV` (`Vacc` *thee, double dpos, double srاد, `Vatom` *atom, double *dSA, `Vclist` *clist)

Total solvent accessible volume.

- VPUBLIC double [Vacc_totalSAV](#) ([Vacc](#) *thee, [Vclist](#) *clist, [APOLparm](#) *apolparm, double radius)

Return the total solvent accessible volume (SAV)

- int [Vacc_wcaEnergyAtom](#) ([Vacc](#) *thee, [APOLparm](#) *apolparm, [Valist](#) *alist, [Vclist](#) *clist, int iatom, double *value)

Calculate the WCA energy for an atom.

- VPUBLIC int [Vacc_wcaEnergy](#) ([Vacc](#) *acc, [APOLparm](#) *apolparm, [Valist](#) *alist, [Vclist](#) *clist)

Return the WCA integral energy.

- VPUBLIC int [Vacc_wcaForceAtom](#) ([Vacc](#) *thee, [APOLparm](#) *apolparm, [Vclist](#) *clist, [Vatom](#) *atom, double *force)

Return the WCA integral force.

9.50.1 Detailed Description

Class Vacc methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
*
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```

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*
*
```

Definition in file [vacc.c](#).

9.50.2 Function Documentation

9.50.2.1 ivdwAccExclus()

```

VPRIVATE int ivdwAccExclus (
    Vacc * thee,
    double center[3],
    double radius,
    int atomID )
```

Determines if a point is within the union of the spheres centered at the atomic centers with radii equal to the sum of their van der Waals radii and the probe radius. Does not include contributions from the specified atom.

Returns

1 if accessible (outside the inflated van der Waals radius), 0 otherwise

Author

Nathan Baker

Parameters

<i>center</i>	Accessibility object
<i>radius</i>	Position to test
<i>atomID</i>	Radius of probe ID of atom to ignore

Definition at line 80 of file [vacc.c](#).

9.50.2.2 splineAcc()

```

VPRIVATE double splineAcc (
    Vacc * thee,
    double center[VAPBS_DIM],
    double win,
    double infrad,
    VclistCell * cell )
```

Fast spline-based surface computation subroutine.

Returns

Spline value

Author

Todd Dolinsky and Nathan Baker

Parameters

<i>center</i>	Accessibility object
<i>win</i>	Point at which the acc is to be evaluated
<i>infrad</i>	Spline window
<i>cell</i>	Radius to inflate atomic radius Cell of atom objects

Definition at line 493 of file [vacc.c](#).

9.50.2.3 Vacc_allocate()

```
VPRIVATE int Vacc_allocate (  
    Vacc * thee )
```

Allocate (and clear) space for storage

Definition at line 193 of file [vacc.c](#).

9.50.2.4 Vacc_atomSASAPos()

```
VPRIVATE double Vacc_atomSASAPos (  
    Vacc * thee,  
    double radius,  
    Vatom * atom,  
    int mode )
```

Definition at line 1277 of file [vacc.c](#).

9.50.2.5 Vacc_ivdwAcc()

```
VPUBLIC double Vacc_ivdwAcc (  
    Vacc * thee,  
    double center[3],  
    double radius )
```

Definition at line 307 of file [vacc.c](#).

9.50.2.6 Vacc_SASAPos()

```
VPRIVATE double Vacc_SASAPos (  
    Vacc * thee,  
    double radius )
```

Definition at line 1252 of file [vacc.c](#).

9.50.2.7 Vacc_storeParms()

```
VPRIVATE int Vacc_storeParms (  
    Vacc * thee,  
    Valist * alist,
```

```

    Vclist * clist,
    double surf_density )

```

Check and store parameters passed to constructor

Definition at line 148 of file [vacc.c](#).

9.50.2.8 Vacc_vdwAcc()

```

VPUBLIC double Vacc_vdwAcc (
    Vacc * thee,
    double center[3] )

```

Definition at line 277 of file [vacc.c](#).

9.50.2.9 Vacc_writeGMV()

```

VPUBLIC void Vacc_writeGMV (
    Vacc * thee,
    double radius,
    int meth,
    Gem * gm,
    char * iodev,
    char * iofmt,
    char * iohost,
    char * iofile )

```

Definition at line 679 of file [vacc.c](#).

9.51 vacc.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "vacc.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 #if !defined(VINLINE_VACC)
00062
00063 VPUBLIC unsigned long int Vacc_memChk(Vacc *thee) {
00064     if (thee == VNULL)
00065         return 0;
00066     return Vmem_bytes(thee->mem);
00067 }
00068
00069 #endif /* if !defined(VINLINE_VACC) */
00070
00080 VPRIVATE int ivdwAccExclus(
00081     Vacc *thee,
00082     double center[3],
00083     double radius,
00084     int atomID
00085 ) {
00086
00087     int iatom;
00088     double dist2,
00089         *apos;
00090     Vatom *atom;
00091     VclistCell *cell;
00092
00093     VASSERT(thee != VNULL);
00094
00095     /* We can only test probes with radii less than the max specified */
00096     if (radius > Vclist_maxRadius(thee->clist)) {
00097         Vnm_print(2,
00098             "Vacc_ivdwAcc: got radius (%g) bigger than max radius (%g)\n",
00099             radius, Vclist_maxRadius(thee->clist));
00100         VASSERT(0);

```

```

00101     }
00102
00103     /* Get the relevant cell from the cell list */
00104     cell = Vclist_getCell(thee->clist, center);
00105
00106     /* If we have no cell, then no atoms are nearby and we're definitely
00107      * accessible */
00108     if (cell == VNULL) {
00109         return 1;
00110     }
00111
00112     /* Otherwise, check for overlap with the atoms in the cell */
00113     for (iatom=0; iatom<cell->natoms; iatom++) {
00114         atom = cell->atoms[iatom];
00115
00116         // We don't actually need to test this if the atom IDs do match; don't compute this if we're
00117         // comparing atom against itself.
00118         if (atom->id == atomID) continue;
00119
00120         apos = atom->position;
00121         dist2 = VSQR(center[0]-apos[0]) + VSQR(center[1]-apos[1])
00122             + VSQR(center[2]-apos[2]);
00123         if (dist2 < VSQR(atom->radius+radius)){
00124             return 0;
00125         }
00126     }
00127     /* If we're still here, then the point is accessible */
00128     return 1;
00129 }
00130
00131
00132 VPUBLIC Vacc* Vacc_ctor(Valist *alist,
00133                         Vclist *clist,
00134                         double surf_density /* Surface density */
00135 ) {
00136
00137     Vacc *thee = VNULL;
00138
00139     /* Set up the structure */
00140     thee = (Vacc*)Vmem_malloc(VNULL, 1, sizeof(Vacc) );
00141     VASSERT( thee != VNULL);
00142     VASSERT( Vacc_ctor2(thee, alist, clist, surf_density));
00143     return thee;
00144 }
00145
00146
00147 VPRIVATE int Vacc_storeParms(Vacc *thee,
00148                             Valist *alist,
00149                             Vclist *clist,
00150                             double surf_density /* Surface density */
00151 ) {
00152
00153     int nsphere,
00154         iatom;
00155     double maxrad = 0.0,
00156         maxarea,
00157         rad;
00158     Vatom *atom;
00159
00160     if (alist == VNULL) {
00161         Vnm_print(2, "Vacc_storeParms: Got NULL Valist!\n");
00162         return 0;
00163     } else thee->alist = alist;
00164     if (clist == VNULL) {
00165         Vnm_print(2, "Vacc_storeParms: Got NULL Vclist!\n");
00166         return 0;
00167     } else thee->clist = clist;
00168     thee->surf_density = surf_density;
00169
00170     /* Loop through the atoms to determine the maximum radius */
00171     maxrad = 0.0;
00172     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
00173         atom = Valist_getAtom(alist, iatom);
00174         rad = Vatom_getRadius(atom);
00175         if (rad > maxrad) maxrad = rad;
00176     }
00177     maxrad = maxrad + Vclist_maxRadius(thee->clist);
00178
00179     maxarea = 4.0*VPI*maxrad*maxrad;
00180     nsphere = (int)ceil(maxarea*surf_density);

```

```

00182
00183     Vnm_print(0, "Vacc_storeParms: Surf. density = %g\n", surf_density);
00184     Vnm_print(0, "Vacc_storeParms: Max area = %g\n", maxarea);
00185     thee->refSphere = VaccSurf_refSphere(thee->mem, nsphere);
00186     Vnm_print(0, "Vacc_storeParms: Using %d-point reference sphere\n",
00187             thee->refSphere->npts);
00188
00189     return 1;
00190 }
00191
00193 VPRIVATE int Vacc_allocate(Vacc *thee) {
00194     int i,
00195         natoms;
00196
00197     natoms = Valist_getNumberAtoms(thee->alist);
00198
00199     thee->atomFlags = (int*)Vmem_malloc(thee->mem, natoms, sizeof(int));
00200     if (thee->atomFlags == VNULL) {
00201         Vnm_print(2,
00202             "Vacc_allocate: Failed to allocate %d (int)s for atomFlags!\n",
00203             natoms);
00204         return 0;
00205     }
00206     for (i=0; i<natoms; i++) (thee->atomFlags)[i] = 0;
00207     return 1;
00208 }
00209
00210 }
00211
00212
00213 VPUBLIC int Vacc_ctor2(Vacc *thee,
00214                     Valist *alist,
00215                     Vclist *clist,
00216                     double surf_density
00217                     ) {
00218
00219     /* Check and store parameters */
00220     if (!Vacc_storeParms(thee, alist, clist, surf_density)) {
00221         Vnm_print(2, "Vacc_ctor2: parameter check failed!\n");
00222         return 0;
00223     }
00224
00225     /* Set up memory management object */
00226     thee->mem = Vmem_ctor("APBS::VACC");
00227     if (thee->mem == VNULL) {
00228         Vnm_print(2, "Vacc_ctor2: memory object setup failed!\n");
00229         return 0;
00230     }
00231
00232     /* Setup and check probe */
00233     thee->surf = VNULL;
00234
00235     /* Allocate space */
00236     if (!Vacc_allocate(thee)) {
00237         Vnm_print(2, "Vacc_ctor2: memory allocation failed!\n");
00238         return 0;
00239     }
00240
00241     return 1;
00242 }
00243
00244
00245 VPUBLIC void Vacc_dtor(Vacc **thee) {
00246     if ((*thee) != VNULL) {
00247         Vacc_dtor2(*thee);
00248         Vmem_free(VNULL, 1, sizeof(Vacc), (void **)thee);
00249         (*thee) = VNULL;
00250     }
00251 }
00252
00253 }
00254
00255 VPUBLIC void Vacc_dtor2(Vacc *thee) {
00256     int i,
00257         natoms;
00258
00259     natoms = Valist_getNumberAtoms(thee->alist);
00260     Vmem_free(thee->mem, natoms, sizeof(int), (void **)&(thee->atomFlags));
00261
00262     if (thee->refSphere != VNULL) {

```

```

00264     VaccSurf_dtor(&(thee->refSphere));
00265     thee->refSphere = VNULL;
00266 }
00267 if (thee->surf != VNULL) {
00268     for (i=0; i<natoms; i++) VaccSurf_dtor(&(thee->surf[i]));
00269     Vmem_free(thee->mem, natoms, sizeof(VaccSurf *),
00270             (void *)&(thee->surf));
00271     thee->surf = VNULL;
00272 }
00273
00274 Vmem_dtor(&(thee->mem));
00275 }
00276
00277 VPUBLIC double Vacc_vdwAcc(Vacc *thee,
00278     double center[3]
00279     ) {
00280
00281     VclistCell *cell;
00282     Vatom *atom;
00283     int iatom;
00284     double *apos,
00285            dist2;
00286
00287     /* Get the relevant cell from the cell list */
00288     cell = Vclist_getCell(thee->clist, center);
00289
00290     /* If we have no cell, then no atoms are nearby and we're definitely
00291      * accessible */
00292     if (cell == VNULL) return 1.0;
00293
00294     /* Otherwise, check for overlap with the atoms in the cell */
00295     for (iatom=0; iatom<cell->natoms; iatom++) {
00296         atom = cell->atoms[iatom];
00297         apos = Vatom_getPosition(atom);
00298         dist2 = VSQR(center[0]-apos[0]) + VSQR(center[1]-apos[1])
00299             + VSQR(center[2]-apos[2]);
00300         if (dist2 < VSQR(Vatom_getRadius(atom))) return 0.0;
00301     }
00302
00303     /* If we're still here, then the point is accessible */
00304     return 1.0;
00305 }
00306
00307 VPUBLIC double Vacc_ivdwAcc(Vacc *thee,
00308     double center[3],
00309     double radius
00310     ) {
00311
00312     return (double)ivdwAccExclus(thee, center, radius, -1);
00313 }
00314 }
00315
00316 VPUBLIC void Vacc_splineAccGradAtomNorm(Vacc *thee,
00317     double center[VAPBS_DIM],
00318     double win,
00319     double infrad,
00320     Vatom *atom,
00321     double *grad
00322     ) {
00323
00324     int i;
00325     double dist,
00326            *apos,
00327            arad,
00328            sm,
00329            sm2,
00330            w2i, /* inverse of win squared */
00331            w3i, /* inverse of win cubed */
00332            mygrad,
00333            mychi = 1.0; /* Char. func. value for given atom */
00334
00335     VASSERT(thee != NULL);
00336
00337     /* Inverse squared window parameter */
00338     w2i = 1.0/(win*win);
00339     w3i = 1.0/(win*win*win);
00340
00341     /* The grad is zero by default */
00342     for (i=0; i<VAPBS_DIM; i++) grad[i] = 0.0;
00343
00344     /* *** CALCULATE THE CHARACTERISTIC FUNCTION VALUE FOR THIS ATOM AND THE

```

```

00345     * *** MAGNITUDE OF THE FORCE *** */
00346     apos = Vatom_getPosition(atom);
00347     /* Zero-radius atoms don't contribute */
00348     if (Vatom_getRadius(atom) > 0.0) {
00349         arad = Vatom_getRadius(atom) + infrad;
00350         dist = VSQRT(VSQR(apos[0]-center[0]) + VSQR(apos[1]-center[1])
00351             + VSQR(apos[2]-center[2]));
00352         /* If we're inside an atom, the entire characteristic function
00353          * will be zero and the grad will be zero, so we can stop */
00354         if (dist < (arad - win)) return;
00355         /* Likewise, if we're outside the smoothing window, the characteristic
00356          * function is unity and the grad will be zero, so we can stop */
00357         else if (dist > (arad + win)) return;
00358         /* Account for floating point error at the border
00359          * NAB: COULDN'T THESE TESTS BE COMBINED AS BELOW
00360          * (Vacc_splineAccAtom)? */
00361         else if ((VABS(dist - (arad - win)) < VSMALL) ||
00362             (VABS(dist - (arad + win)) < VSMALL)) return;
00363         /* If we're inside the smoothing window */
00364         else {
00365             sm = dist - arad + win;
00366             sm2 = VSQR(sm);
00367             mychi = 0.75*sm2*w2i - 0.25*sm*sm2*w3i;
00368             mygrad = 1.5*sm*w2i - 0.75*sm2*w3i;
00369         }
00370         /* Now assemble the grad vector */
00371         VASSERT(mychi > 0.0);
00372         for (i=0; i<VAPBS_DIM; i++)
00373             grad[i] = -(mygrad/mychi)*((center[i] - apos[i])/dist);
00374     }
00375 }
00376
00377 VPUBLIC void Vacc_splineAccGradAtomUnnorm(Vacc *thee,
00378     double center[VAPBS_DIM],
00379     double win,
00380     double infrad,
00381     Vatom *atom,
00382     double *grad
00383 ) {
00384
00385     int i;
00386     double dist,
00387         *apos,
00388         arad,
00389         sm,
00390         sm2,
00391         w2i, /* Inverse of win squared */
00392         w3i, /* Inverse of win cubed */
00393         mygrad,
00394         mychi = 1.0; /* Char. func. value for given atom */
00395
00396     VASSERT(thee != NULL);
00397
00398     /* Inverse squared window parameter */
00399     w2i = 1.0/(win*win);
00400     w3i = 1.0/(win*win*win);
00401
00402     /* The grad is zero by default */
00403     for (i=0; i<VAPBS_DIM; i++) grad[i] = 0.0;
00404
00405     /* *** CALCULATE THE CHARACTERISTIC FUNCTION VALUE FOR THIS ATOM AND THE
00406      * *** MAGNITUDE OF THE FORCE *** */
00407     apos = Vatom_getPosition(atom);
00408     /* Zero-radius atoms don't contribute */
00409     if (Vatom_getRadius(atom) > 0.0) {
00410         arad = Vatom_getRadius(atom) + infrad;
00411         dist = VSQRT(VSQR(apos[0]-center[0]) + VSQR(apos[1]-center[1])
00412             + VSQR(apos[2]-center[2]));
00413         /* If we're inside an atom, the entire characteristic function
00414          * will be zero and the grad will be zero, so we can stop */
00415         if (dist < (arad - win)) return;
00416         /* Likewise, if we're outside the smoothing window, the characteristic
00417          * function is unity and the grad will be zero, so we can stop */
00418         else if (dist > (arad + win)) return;
00419         /* Account for floating point error at the border
00420          * NAB: COULDN'T THESE TESTS BE COMBINED AS BELOW
00421          * (Vacc_splineAccAtom)? */
00422         else if ((VABS(dist - (arad - win)) < VSMALL) ||
00423             (VABS(dist - (arad + win)) < VSMALL)) return;
00424         /* If we're inside the smoothing window */
00425         else {

```

```

00426         sm = dist - arad + win;
00427         sm2 = VSQR(sm);
00428         mychi = 0.75*sm2*w2i - 0.25*sm*sm2*w3i;
00429         mygrad = 1.5*sm*w2i - 0.75*sm2*w3i;
00430     }
00431     /* Now assemble the grad vector */
00432     VASSERT(mychi > 0.0);
00433     for (i=0; i<VAPBS_DIM; i++)
00434         grad[i] = -(mygrad)*((center[i] - apos[i])/dist);
00435     }
00436 }
00437
00438 VPUBLIC double Vacc_splineAccAtom(Vacc *thee,
00439                                   double center[VAPBS_DIM],
00440                                   double win,
00441                                   double infrad,
00442                                   Vatom *atom
00443                                   ) {
00444
00445     double dist,
00446           *apos,
00447           arad,
00448           sm,
00449           sm2,
00450           w2i, /* Inverse of win squared */
00451           w3i, /* Inverse of win cubed */
00452           value,
00453           stot,
00454           sctot;
00455
00456     VASSERT(thee != NULL);
00457
00458     /* Inverse squared window parameter */
00459     w2i = 1.0/(win*win);
00460     w3i = 1.0/(win*win*win);
00461
00462     apos = Vatom_getPosition(atom);
00463     /* Zero-radius atoms don't contribute */
00464     if (Vatom_getRadius(atom) > 0.0) {
00465         arad = Vatom_getRadius(atom) + infrad;
00466         stot = arad + win;
00467         sctot = VMAX2(0, (arad - win));
00468         dist = VSQRT(VSQR(apos[0]-center[0]) + VSQR(apos[1]-center[1])
00469                     + VSQR(apos[2]-center[2]));
00470         /* If we're inside an atom, the entire characteristic function
00471          * will be zero */
00472         if ((dist < sctot) || (VABS(dist - sctot) < VSMALL)){
00473             value = 0.0;
00474         }
00475         /* We're outside the smoothing window */
00476         } else if ((dist > stot) || (VABS(dist - stot) < VSMALL)) {
00477             value = 1.0;
00478         }
00479         /* We're inside the smoothing window */
00480         } else {
00481             sm = dist - arad + win;
00482             sm2 = VSQR(sm);
00483             value = 0.75*sm2*w2i - 0.25*sm*sm2*w3i;
00484         }
00485     } else value = 1.0;
00486     return value;
00487 }
00488
00493 VPRIVATE double splineAcc(
00494     Vacc *thee,
00495     double center[VAPBS_DIM],
00496     double win,
00497     double infrad,
00498     VclistCell *cell
00499     ) {
00500
00501     int atomID, iatom;
00502     Vatom *atom;
00503     double value = 1.0;
00504
00505     VASSERT(thee != NULL);
00506
00507     /* Now loop through the atoms assembling the characteristic function */
00508     for (iatom=0; iatom<cell->natoms; iatom++) {
00509
00510         atom = cell->atoms[iatom];
00511         atomID = atom->id;

```

```

00513
00514     /* Check to see if we've counted this atom already */
00515     if ( !(thee->atomFlags[atomID]) ) {
00516
00517         thee->atomFlags[atomID] = 1;
00518         value *= Vacc_splineAccAtom(thee, center, win, infrad, atom);
00519
00520         if (value < VSMALL) return value;
00521     }
00522 }
00523
00524 return value;
00525 }
00526
00527
00528 VPUBLIC double Vacc_splineAcc(Vacc *thee, double center[VAPBS_DIM], double win,
00529     double infrad) {
00530
00531     VclistCell *cell;
00532     Vatom *atom;
00533     int iatom, atomID;
00534
00535
00536     VASSERT(thee != NULL);
00537
00538     if (Vclist_maxRadius(thee->clist) < (win + infrad)) {
00539         Vnm_print(2, "Vacc_splineAcc: Vclist has max_radius=%g;\n",
00540             Vclist_maxRadius(thee->clist));
00541         Vnm_print(2, "Vacc_splineAcc: Insufficient for win=%g, infrad=%g\n",
00542             win, infrad);
00543         VASSERT(0);
00544     }
00545
00546     /* Get a cell or VNULL; in the latter case return 1.0 */
00547     cell = Vclist_getCell(thee->clist, center);
00548     if (cell == VNULL) return 1.0;
00549
00550     /* First, reset the list of atom flags
00551      * NAB: THIS SEEMS VERY INEFFICIENT */
00552     for (iatom=0; iatom<cell->natoms; iatom++) {
00553         atom = cell->atoms[iatom];
00554         atomID = atom->id;
00555         thee->atomFlags[atomID] = 0;
00556     }
00557
00558     return splineAcc(thee, center, win, infrad, cell);
00559 }
00560
00561 VPUBLIC void Vacc_splineAccGrad(Vacc *thee, double center[VAPBS_DIM],
00562     double win, double infrad, double *grad) {
00563
00564     int iatom, i, atomID;
00565     double acc = 1.0;
00566     double tgrad[VAPBS_DIM];
00567     VclistCell *cell;
00568     Vatom *atom = VNULL;
00569
00570     VASSERT(thee != NULL);
00571
00572     if (Vclist_maxRadius(thee->clist) < (win + infrad)) {
00573         Vnm_print(2, "Vacc_splineAccGrad: Vclist max_radius=%g;\n",
00574             Vclist_maxRadius(thee->clist));
00575         Vnm_print(2, "Vacc_splineAccGrad: Insufficient for win=%g, infrad=%g\n",
00576             win, infrad);
00577         VASSERT(0);
00578     }
00579
00580     /* Reset the gradient */
00581     for (i=0; i<VAPBS_DIM; i++) grad[i] = 0.0;
00582
00583     /* Get the cell; check for nullity */
00584     cell = Vclist_getCell(thee->clist, center);
00585     if (cell == VNULL) return;
00586
00587     /* Reset the list of atom flags */
00588     for (iatom=0; iatom<cell->natoms; iatom++) {
00589         atom = cell->atoms[iatom];
00590         atomID = atom->id;
00591         thee->atomFlags[atomID] = 0;
00592     }
00593

```



```

00594      /* Get the local accessibility */
00595      acc = splineAcc(thee, center, win, infrad, cell);
00596
00597      /* Accumulate the gradient of all local atoms */
00598      if (acc > VSMALL) {
00599          for (iatom=0; iatom<cell->natoms; iatom++) {
00600              atom = cell->atoms[iatom];
00601              Vacc_splineAccGradAtomNorm(thee, center, win, infrad, atom, tgrad);
00602          }
00603          for (i=0; i<VAPBS_DIM; i++) grad[i] += tgrad[i];
00604      }
00605      for (i=0; i<VAPBS_DIM; i++) grad[i] *= -acc;
00606  }
00607
00608  VPUBLIC double Vacc_molAcc(Vacc *thee, double center[VAPBS_DIM],
00609      double radius) {
00610
00611      double rc;
00612
00613      /* ***** CHECK IF OUTSIDE ATOM+PROBE RADIUS SURFACE ***** */
00614      if (Vacc_ivdwAcc(thee, center, radius) == 1.0) {
00615
00616          /* Vnm_print(2, "DEBUG: ivdwAcc = 1.0\n"); */
00617          rc = 1.0;
00618
00619          /* ***** CHECK IF INSIDE ATOM RADIUS SURFACE ***** */
00620      } else if (Vacc_vdwAcc(thee, center) == 0.0) {
00621
00622          /* Vnm_print(2, "DEBUG: vdwAcc = 0.0\n"); */
00623          rc = 0.0;
00624
00625          /* ***** CHECK IF OUTSIDE MOLECULAR SURFACE ***** */
00626      } else {
00627
00628          /* Vnm_print(2, "DEBUG: calling fastMolAcc...\n"); */
00629          rc = Vacc_fastMolAcc(thee, center, radius);
00630      }
00631  }
00632
00633  return rc;
00634  }
00635  }
00636
00637  VPUBLIC double Vacc_fastMolAcc(Vacc *thee, double center[VAPBS_DIM],
00638      double radius) {
00639
00640      Vatom *atom;
00641      VaccSurf *surf;
00642      VclistCell *cell;
00643      int ipt, iatom, atomID;
00644      double dist2, rad2;
00645
00646      rad2 = radius*radius;
00647
00648      /* Check to see if the SAS has been defined */
00649      if (thee->surf == VNULL) Vacc_SASA(thee, radius);
00650
00651      /* Get the cell associated with this point */
00652      cell = Vclist_getCell(thee->clist, center);
00653      if (cell == VNULL) {
00654          Vnm_print(2, "Vacc_fastMolAcc: unexpected VNULL VclistCell!\n");
00655          return 1.0;
00656      }
00657
00658      /* Loop through all the atoms in the cell */
00659      for (iatom=0; iatom<cell->natoms; iatom++) {
00660          atom = cell->atoms[iatom];
00661          atomID = Vatom_getAtomID(atom);
00662          surf = thee->surf[atomID];
00663          /* Loop through all SAS points associated with this atom */
00664          for (ipt=0; ipt<surf->npts; ipt++) {
00665              /* See if we're within a probe radius of the point */
00666              dist2 = VSQR(center[0]-(surf->xpts[ipt]))
00667                  + VSQR(center[1]-(surf->ypts[ipt]))
00668                  + VSQR(center[2]-(surf->zpts[ipt]));
00669              if (dist2 < rad2) return 1.0;
00670          }
00671      }
00672
00673      /* If all else failed, we are not inside the molecular surface */
00674      return 0.0;

```

```

00675 }
00676
00677
00678 #if defined(HAVE_MC_H)
00679 VPUBLIC void Vacc_writeGMV(Vacc *thee, double radius, int meth, Gem *gm,
00680   char *iodev, char *iofmt, char *iohost, char *iofile) {
00681     double *accVals[MAXV], coord[3];
00682     Vio *sock;
00683     int ivert, icoord;
00684
00685     for (ivert=0; ivert<MAXV; ivert++) accVals[ivert] = VNULL;
00686     accVals[0] = (void *)Vmem_malloc(thee->mem, Gem_numVV(gm), sizeof(double));
00687     accVals[1] = (void *)Vmem_malloc(thee->mem, Gem_numVV(gm), sizeof(double));
00688     for (ivert=0; ivert<Gem_numVV(gm); ivert++) {
00689         for (icoord=0; icoord<3; icoord++)
00690             coord[icoord] = VV_coord(Gem_VV(gm, ivert), icoord);
00691         if (meth == 0) {
00692             accVals[0][ivert] = Vacc_molAcc(thee, coord, radius);
00693             accVals[1][ivert] = Vacc_molAcc(thee, coord, radius);
00694         } else if (meth == 1) {
00695             accVals[0][ivert] = Vacc_ivdwAcc(thee, coord, radius);
00696             accVals[1][ivert] = Vacc_ivdwAcc(thee, coord, radius);
00697         } else if (meth == 2) {
00698             accVals[0][ivert] = Vacc_vdwAcc(thee, coord);
00699             accVals[1][ivert] = Vacc_vdwAcc(thee, coord);
00700         } else VASSERT(0);
00701     }
00702     sock = Vio_ctor(iodev, iofmt, iohost, iofile, "w");
00703     Gem_writeGMV(gm, sock, 1, accVals);
00704     Vio_dtor(&sock);
00705     Vmem_free(thee->mem, Gem_numVV(gm), sizeof(double),
00706       (void *)&(accVals[0]));
00707     Vmem_free(thee->mem, Gem_numVV(gm), sizeof(double),
00708       (void *)&(accVals[1]));
00709 }
00710 #endif /* defined(HAVE_MC_H) */
00711
00712 VPUBLIC double Vacc_SASA(Vacc *thee,
00713   double radius
00714   ) {
00715     int i,
00716       natom;
00717     double area;
00718     /*apos; // gcc says unused
00719     Vatom *atom;
00720     VaccSurf *asurf;
00721
00722     time_t ts; // PCE: temp
00723     ts = clock();
00724
00725     //unsigned long long mbeg; // gcc says unused
00726
00727     natom = Valist_getNumberAtoms(thee->alist);
00728
00729     /* Check to see if we need to build the surface */
00730     if (thee->surf == VNULL) {
00731         thee->surf = Vmem_malloc(thee->mem, natom, sizeof(VaccSurf *));
00732
00733         #if defined(DEBUG_MAC_OSX_OCL) || defined(DEBUG_MAC_OSX_STANDARD)
00734         #include "mach_chud.h"
00735         machm_(&mbeg);
00736         #pragma omp parallel for private(i,atom)
00737         #endif
00738         for (i=0; i<natom; i++) {
00739             atom = Valist_getAtom(thee->alist, i);
00740             /* NOTE: RIGHT NOW WE DO THIS FOR THE ENTIRE MOLECULE WHICH IS
00741              * INCREDIBLY INEFFICIENT, PARTICULARLY DURING FOCUSING!!! */
00742             thee->surf[i] = Vacc_atomSurf(thee, atom, thee->refSphere,
00743               radius);
00744         }
00745     }
00746
00747     /* Calculate the area */
00748     area = 0.0;
00749     for (i=0; i<natom; i++) {
00750         atom = Valist_getAtom(thee->alist, i);
00751         asurf = thee->surf[i];
00752         /* See if this surface needs to be rebuilt */
00753         if (asurf->probe_radius != radius) {

```

```

00756         Vnm_print(2, "Vacc_SASA: Warning -- probe radius changed from %g to %g!\n",
00757                     asurf->probe_radius, radius);
00758         VaccSurf_dtor2(asurf);
00759         thee->surf[i] = Vacc_atomSurf(thee, atom, thee->refSphere, radius);
00760         asurf = thee->surf[i];
00761     }
00762     area += (asurf->area);
00763 }
00764
00765 #if defined(DEBUG_MAC_OSX_OCL) || defined(DEBUG_MAC_OSX_STANDARD)
00766     mets_(&mbeg, "Vacc_SASA - Parallel");
00767 #endif
00768
00769     Vnm_print(0, "Vacc_SASA: Time elapsed: %f\n", ((double)clock() - ts) / CLOCKS_PER_SEC);
00770     return area;
00771 }
00772
00773
00774 VPUBLIC double Vacc_totalSASA(Vacc *thee, double radius) {
00775
00776     return Vacc_SASA(thee, radius);
00777 }
00778
00779
00780 VPUBLIC double Vacc_atomSASA(Vacc *thee, double radius, Vatom *atom) {
00781
00782     VaccSurf *asurf;
00783     int id;
00784
00785     if (thee->surf == VNULL) Vacc_SASA(thee, radius);
00786
00787     id = Vatom_getAtomID(atom);
00788     asurf = thee->surf[id];
00789
00790     /* See if this surface needs to be rebuilt */
00791     if (asurf->probe_radius != radius) {
00792         Vnm_print(2, "Vacc_SASA: Warning -- probe radius changed from %g to %g!\n",
00793                     asurf->probe_radius, radius);
00794         VaccSurf_dtor2(asurf);
00795         thee->surf[id] = Vacc_atomSurf(thee, atom, thee->refSphere, radius);
00796         asurf = thee->surf[id];
00797     }
00798
00799     return asurf->area;
00800 }
00801
00802
00803 VPUBLIC VaccSurf* VaccSurf_ctor(Vmem *mem, double probe_radius, int nsphere) {
00804     VaccSurf *thee;
00805
00806     //thee = Vmem_malloc(mem, 1, sizeof(Vacc) );
00807     thee = (VaccSurf*)calloc(1, sizeof(Vacc));
00808     VASSERT( VaccSurf_ctor2(thee, mem, probe_radius, nsphere) );
00809
00810     return thee;
00811 }
00812
00813 VPUBLIC int VaccSurf_ctor2(VaccSurf *thee, Vmem *mem, double probe_radius,
00814     int nsphere) {
00815
00816     if (thee == VNULL)
00817         return 0;
00818
00819     thee->mem = mem;
00820     thee->npts = nsphere;
00821     thee->probe_radius = probe_radius;
00822     thee->area = 0.0;
00823
00824     if (thee->npts > 0) {
00825         thee->xpts = Vmem_malloc(thee->mem, thee->npts, sizeof(double));
00826         thee->ypts = Vmem_malloc(thee->mem, thee->npts, sizeof(double));
00827         thee->zpts = Vmem_malloc(thee->mem, thee->npts, sizeof(double));
00828         thee->bpts = Vmem_malloc(thee->mem, thee->npts, sizeof(char));
00829     } else {
00830         thee->xpts = VNULL;
00831         thee->ypts = VNULL;
00832         thee->zpts = VNULL;
00833         thee->bpts = VNULL;
00834     }
00835
00836     return 1;

```

```

00837 }
00838
00839 VPUBLIC void VaccSurf_dtor(VaccSurf **thee) {
00840     Vmem *mem;
00841
00842     if ((*thee) != VNULL) {
00843         mem = (*thee)->mem;
00844         VaccSurf_dtor2(*thee);
00845         //Vmem_free(mem, 1, sizeof(VaccSurf), (void **)thee);
00846         free(*thee);
00847         (*thee) = VNULL;
00848     }
00849 }
00850
00851 }
00852
00853 VPUBLIC void VaccSurf_dtor2(VaccSurf *thee) {
00854
00855     if (thee->npts > 0) {
00856         Vmem_free(thee->mem, thee->npts, sizeof(double),
00857             (void **)&(thee->xpts));
00858         Vmem_free(thee->mem, thee->npts, sizeof(double),
00859             (void **)&(thee->ypts));
00860         Vmem_free(thee->mem, thee->npts, sizeof(double),
00861             (void **)&(thee->zpts));
00862         Vmem_free(thee->mem, thee->npts, sizeof(char),
00863             (void **)&(thee->bpts));
00864     }
00865 }
00866 }
00867
00868 VPUBLIC VaccSurf* Vacc_atomSurf(Vacc *thee, Vatom *atom,
00869     VaccSurf *ref, double prad) {
00870
00871     VaccSurf *surf;
00872     size_t i, j, npts;
00873     int atomID;
00874     double arad, rad, pos[3], *apos;
00875
00876     /* Get atom information */
00877     arad = Vatom_getRadius(atom);
00878     apos = Vatom_getPosition(atom);
00879     atomID = Vatom_getAtomID(atom);
00880
00881     if (arad < VSMALL) {
00882         return VaccSurf_ctor(thee->mem, prad, 0);
00883     }
00884
00885     rad = arad + prad;
00886
00887     /* Determine which points will contribute */
00888     npts = 0;
00889     for (i=0; i<ref->npts; i++) {
00890         /* Reset point flag: zero-radius atoms do not contribute */
00891         pos[0] = rad*(ref->xpts[i]) + apos[0];
00892         pos[1] = rad*(ref->ypts[i]) + apos[1];
00893         pos[2] = rad*(ref->zpts[i]) + apos[2];
00894         if (ivdwAccExclus(thee, pos, prad, atomID)) {
00895             npts++;
00896             ref->bpts[i] = (ref->bpts[i] << 1) + 1;
00897         } else {
00898             ref->bpts[i] <= 1;
00899         }
00900     }
00901
00902     /* Allocate space for the points */
00903     surf = VaccSurf_ctor(thee->mem, prad, npts);
00904
00905     /* Assign the points */
00906     j = 0;
00907     for (i=0; i<ref->npts; i++) {
00908         char flag = ref->bpts[i] & 1;
00909         ref->bpts[i] >= 1;
00910         if (flag) {
00911             surf->bpts[j] = 1;
00912             surf->xpts[j] = rad*(ref->xpts[i]) + apos[0];
00913             surf->ypts[j] = rad*(ref->ypts[i]) + apos[1];
00914             surf->zpts[j] = rad*(ref->zpts[i]) + apos[2];
00915             j++;
00916         }
00917     }

```

```

00918
00919     /* Assign the area */
00920     surf->area = 4.0*VPI*rad*rad*((double) (surf->npts))/((double) (ref->npts));
00921
00922     return surf;
00923
00924 }
00925
00926 VPUBLIC VaccSurf* VaccSurf_refSphere(Vmem *mem, int npts) {
00927     VaccSurf *surf;
00928     int nactual, i, itheta, ntheta, iphi, nphimax, nphi;
00929     double frac;
00930     double sintheta, costheta, theta, dtheta;
00931     double sinphi, cosphi, phi, dphi;
00932
00933     /* Setup "constants" */
00934     frac = ((double) (npts))/4.0;
00935     ntheta = VRINT(VSQRT(Vunit_pi*frac));
00936     dtheta = Vunit_pi/((double) (ntheta));
00937     nphimax = 2*ntheta;
00938
00939     /* Count the actual number of points to be used */
00940     nactual = 0;
00941     for (itheta=0; itheta<ntheta; itheta++) {
00942         theta = dtheta*((double) (itheta));
00943         sintheta = VSIN(theta);
00944         costheta = VCOS(theta);
00945         nphi = VRINT(sintheta*nphimax);
00946         nactual += nphi;
00947     }
00948
00949     /* Allocate space for the points */
00950     surf = VaccSurf_ctor(mem, 1.0, nactual);
00951
00952     /* Clear out the boolean array */
00953     for (i=0; i<nactual; i++) surf->bpts[i] = 1;
00954
00955     /* Assign the points */
00956     nactual = 0;
00957     for (itheta=0; itheta<ntheta; itheta++) {
00958         theta = dtheta*((double) (itheta));
00959         sintheta = VSIN(theta);
00960         costheta = VCOS(theta);
00961         nphi = VRINT(sintheta*nphimax);
00962         if (nphi != 0) {
00963             dphi = 2*Vunit_pi/((double) (nphi));
00964             for (iphi=0; iphi<nphi; iphi++) {
00965                 phi = dphi*((double) (iphi));
00966                 sinphi = VSIN(phi);
00967                 cosphi = VCOS(phi);
00968                 surf->xpts[nactual] = cosphi * sintheta;
00969                 surf->ypts[nactual] = sinphi * sintheta;
00970                 surf->zpts[nactual] = costheta;
00971                 nactual++;
00972             }
00973         }
00974     }
00975
00976     surf->npts = nactual;
00977
00978     return surf;
00979 }
00980
00981 VPUBLIC VaccSurf* Vacc_atomSASPoints(Vacc *thee, double radius,
00982     Vatom *atom) {
00983     VaccSurf *asurf = VNULL;
00984     int id;
00985
00986     if (thee->surf == VNULL) Vacc_SASA(thee, radius);
00987     id = Vatom_getAtomID(atom);
00988
00989     asurf = thee->surf[id];
00990
00991     /* See if this surface needs to be rebuilt */
00992     if (asurf->probe_radius != radius) {
00993         Vnm_print(2, "Vacc_SASA: Warning -- probe radius changed from %g to %g!\n",
00994             asurf->probe_radius, radius);
00995         VaccSurf_dtor2(asurf);
00996         thee->surf[id] = Vacc_atomSurf(thee, atom, thee->refSphere, radius);
00997     }
00998 }

```

```

00999     asurf = thee->surf[id];
01000 }
01001
01002     return asurf;
01003
01004 }
01005
01006 VPUBLIC void Vacc_splineAccGradAtomNorm4(Vacc *thee, double center[VAPBS_DIM],
01007     double win, double infrad, Vatom *atom, double *grad) {
01008
01009     int i;
01010     double dist, *apos, arad, sm, sm2, sm3, sm4, sm5, sm6, sm7;
01011     double e, e2, e3, e4, e5, e6, e7;
01012     double b, b2, b3, b4, b5, b6, b7;
01013     double c0, c1, c2, c3, c4, c5, c6, c7;
01014     double denom, mygrad;
01015     double mychi = 1.0;          /* Char. func. value for given atom */
01016
01017     VASSERT(thee != NULL);
01018
01019     /* The grad is zero by default */
01020     for (i=0; i<VAPBS_DIM; i++) grad[i] = 0.0;
01021
01022     /* *** CALCULATE THE CHARACTERISTIC FUNCTION VALUE FOR THIS ATOM AND THE
01023      * *** MAGNITUDE OF THE FORCE *** */
01024     apos = Vatom_getPosition(atom);
01025     /* Zero-radius atoms don't contribute */
01026     if (Vatom_getRadius(atom) > 0.0) {
01027
01028         arad = Vatom_getRadius(atom);
01029         arad = arad + infrad;
01030         b = arad - win;
01031         e = arad + win;
01032
01033         e2 = e * e;
01034         e3 = e2 * e;
01035         e4 = e3 * e;
01036         e5 = e4 * e;
01037         e6 = e5 * e;
01038         e7 = e6 * e;
01039         b2 = b * b;
01040         b3 = b2 * b;
01041         b4 = b3 * b;
01042         b5 = b4 * b;
01043         b6 = b5 * b;
01044         b7 = b6 * b;
01045
01046         denom = e7 - 7.0*b*e6 + 21.0*b2*e5 - 35.0*e4*b3
01047             + 35.0*e3*b4 - 21.0*b5*e2 + 7.0*e*b6 - b7;
01048         c0 = b4*(35.0*e3 - 21.0*b*e2 + 7*e*b2 - b3)/denom;
01049         c1 = -140.0*b3*e3/denom;
01050         c2 = 210.0*e2*b2*(e + b)/denom;
01051         c3 = -140.0*e*b*(e2 + 3.0*b*e + b2)/denom;
01052         c4 = 35.0*(e3 + 9.0*b*e2 + 9.0*e*b2 + b3)/denom;
01053         c5 = -84.0*(e2 + 3.0*b*e + b2)/denom;
01054         c6 = 70.0*(e + b)/denom;
01055         c7 = -20.0/denom;
01056
01057         dist = VSQR(VSQR(apos[0]-center[0]) + VSQR(apos[1]-center[1])
01058             + VSQR(apos[2]-center[2]));
01059
01060         /* If we're inside an atom, the entire characteristic function
01061          * will be zero and the grad will be zero, so we can stop */
01062         if (dist < (arad - win)) return;
01063         /* Likewise, if we're outside the smoothing window, the characteristic
01064          * function is unity and the grad will be zero, so we can stop */
01065         else if (dist > (arad + win)) return;
01066         /* Account for floating point error at the border
01067          * NAB: COULDN'T THESE TESTS BE COMBINED AS BELOW
01068          * (Vacc_splineAccAtom)? */
01069         else if ((VABS(dist - (arad - win)) < VSMALL) ||
01070             (VABS(dist - (arad + win)) < VSMALL)) return;
01071         /* If we're inside the smoothing window */
01072         else {
01073             sm = dist;
01074             sm2 = sm * sm;
01075             sm3 = sm2 * sm;
01076             sm4 = sm3 * sm;
01077             sm5 = sm4 * sm;
01078             sm6 = sm5 * sm;
01079             sm7 = sm6 * sm;

```

```

01080         mychi = c0 + c1*sm + c2*sm2 + c3*sm3
01081             + c4*sm4 + c5*sm5 + c6*sm6 + c7*sm7;
01082         mygrad = c1 + 2.0*c2*sm + 3.0*c3*sm2 + 4.0*c4*sm3
01083             + 5.0*c5*sm4 + 6.0*c6*sm5 + 7.0*c7*sm6;
01084         if (mychi <= 0.0) {
01085             /* Avoid numerical round off errors */
01086             return;
01087         } else if (mychi > 1.0) {
01088             /* Avoid numerical round off errors */
01089             mychi = 1.0;
01090         }
01091     }
01092     /* Now assemble the grad vector */
01093     VASSERT(mychi > 0.0);
01094     for (i=0; i<VAPBS_DIM; i++)
01095         grad[i] = -(mygrad/mychi)*((center[i] - apos[i])/dist);
01096     }
01097 }
01098
01099 VPUBLIC void Vacc_splineAccGradAtomNorm3(Vacc *thee, double center[VAPBS_DIM],
01100                                         double win, double infrad, Vatom *atom, double *grad) {
01101     int i;
01102     double dist, *apos, arad, sm, sm2, sm3, sm4, sm5;
01103     double e, e2, e3, e4, e5;
01104     double b, b2, b3, b4, b5;
01105     double c0, c1, c2, c3, c4, c5;
01106     double denom, mygrad;
01107     double mychi = 1.0;          /* Char. func. value for given atom */
01108
01109     VASSERT(thee != NULL);
01110
01111     /* The grad is zero by default */
01112     for (i=0; i<VAPBS_DIM; i++) grad[i] = 0.0;
01113
01114     /* *** CALCULATE THE CHARACTERISTIC FUNCTION VALUE FOR THIS ATOM AND THE
01115      * *** MAGNITUDE OF THE FORCE *** */
01116     apos = Vatom_getPosition(atom);
01117     /* Zero-radius atoms don't contribute */
01118     if (Vatom_getRadius(atom) > 0.0) {
01119         arad = Vatom_getRadius(atom);
01120         arad = arad + infrad;
01121         b = arad - win;
01122         e = arad + win;
01123
01124         e2 = e * e;
01125         e3 = e2 * e;
01126         e4 = e3 * e;
01127         e5 = e4 * e;
01128         b2 = b * b;
01129         b3 = b2 * b;
01130         b4 = b3 * b;
01131         b5 = b4 * b;
01132
01133         denom = pow((e - b), 5.0);
01134         c0 = -10.0*e2*b3 + 5.0*e*b4 - b5;
01135         c1 = 30.0*e2*b2;
01136         c2 = -30.0*(e2*b + e*b2);
01137         c3 = 10.0*(e2 + 4.0*e*b + b2);
01138         c4 = -15.0*(e + b);
01139         c5 = 6;
01140         c0 = c0/denom;
01141         c1 = c1/denom;
01142         c2 = c2/denom;
01143         c3 = c3/denom;
01144         c4 = c4/denom;
01145         c5 = c5/denom;
01146
01147         dist = VSQRT(VSQR(apos[0]-center[0]) + VSQR(apos[1]-center[1])
01148             + VSQR(apos[2]-center[2]));
01149
01150         /* If we're inside an atom, the entire characteristic function
01151          * will be zero and the grad will be zero, so we can stop */
01152         if (dist < (arad - win)) return;
01153         /* Likewise, if we're outside the smoothing window, the characteristic
01154          * function is unity and the grad will be zero, so we can stop */
01155         else if (dist > (arad + win)) return;
01156         /* Account for floating point error at the border
01157          * NAB: COULDN'T THESE TESTS BE COMBINED AS BELOW
01158          * (Vacc_splineAccAtom)? */
01159     }
01160 }

```

```

01161     else if ((VABS(dist - (arad - win)) < VSMALL) ||
01162             (VABS(dist - (arad + win)) < VSMALL)) return;
01163     /* If we're inside the smoothing window */
01164     else {
01165         sm = dist;
01166         sm2 = sm * sm;
01167         sm3 = sm2 * sm;
01168         sm4 = sm3 * sm;
01169         sm5 = sm4 * sm;
01170         mychi = c0 + c1*sm + c2*sm2 + c3*sm3
01171               + c4*sm4 + c5*sm5;
01172         mygrad = c1 + 2.0*c2*sm + 3.0*c3*sm2 + 4.0*c4*sm3
01173               + 5.0*c5*sm4;
01174         if (mychi <= 0.0) {
01175             /* Avoid numerical round off errors */
01176             return;
01177         } else if (mychi > 1.0) {
01178             /* Avoid numerical round off errors */
01179             mychi = 1.0;
01180         }
01181     }
01182     /* Now assemble the grad vector */
01183     VASSERT(mychi > 0.0);
01184     for (i=0; i<VAPBS_DIM; i++)
01185         grad[i] = -(mygrad/mychi)*((center[i] - apos[i])/dist);
01186 }
01187 }
01188
01189 /* =====
01190 // Routine:  Vacc_atomdSAV
01191 //
01192 // Purpose:  Calculates the vector valued atomic derivative of volume
01193 //
01194 // Args:     radius  The radius of the solvent probe in Angstroms
01195 //           iatom   Index of the atom in thee->alist
01196 //
01197 // Author:   Jason Wagoner
01198 //           Nathan Baker (original FORTRAN routine from UHBD by Brock Luty)
01200 VPUBLIC void Vacc_atomdSAV(Vacc *thee,
01201                          double srad,
01202                          Vatom *atom,
01203                          double *dSA
01204                          ) {
01205
01206     int ipt, iatom;
01207
01208     double area;
01209     double *tPos, tRad, vec[3];
01210     double dx,dy,dz;
01211     VaccSurf *ref;
01212     dx = 0.0;
01213     dy = 0.0;
01214     dz = 0.0;
01215     /* Get the atom information */
01216     ref = thee->refSphere;
01217     iatom = Vatom_getAtomID(atom);
01218
01219     dSA[0] = 0.0;
01220     dSA[1] = 0.0;
01221     dSA[2] = 0.0;
01222
01223     tPos = Vatom_getPosition(atom);
01224     tRad = Vatom_getRadius(atom);
01225
01226     if(tRad == 0.0) return;
01227
01228     area = 4.0*VPI*(tRad+srad)*(tRad+srad)/((double)(ref->npts));
01229     for (ipt=0; ipt<ref->npts; ipt++) {
01230         vec[0] = (tRad+srad)*ref->xpts[ipt] + tPos[0];
01231         vec[1] = (tRad+srad)*ref->ypts[ipt] + tPos[1];
01232         vec[2] = (tRad+srad)*ref->zpts[ipt] + tPos[2];
01233         if (ivdwAccExclus(thee, vec, srad, iatom)) {
01234             dx = dx+vec[0]-tPos[0];
01235             dy = dy+vec[1]-tPos[1];
01236             dz = dz+vec[2]-tPos[2];
01237         }
01238     }
01239
01240     if ((tRad+srad) != 0){
01241         dSA[0] = dx*area/(tRad+srad);
01242         dSA[1] = dy*area/(tRad+srad);

```



```

01243         dSA[2] = dz*area/(tRad+srad);
01244     }
01245
01246 }
01247
01248 /* Note: This is purely test code to make certain that the dSASA code is
01249         behaving properly. This function should NEVER be called by anyone
01250         other than an APBS developer at Wash U.
01251 */
01252 VPRIVATE double Vacc_SASAPos(Vacc *thee, double radius) {
01253     int i, natom;
01254     double area;
01255     Vatom *atom;
01256     VaccSurf *asurf;
01257
01258     natom = Valist_getNumberAtoms(thee->alist);
01259
01260     /* Calculate the area */
01261     area = 0.0;
01262     for (i=0; i<natom; i++) {
01263         atom = Valist_getAtom(thee->alist, i);
01264         asurf = thee->surf[i];
01265
01266         VaccSurf_dtor2(asurf);
01267         thee->surf[i] = Vacc_atomSurf(thee, atom, thee->refSphere, radius);
01268         asurf = thee->surf[i];
01269         area += (asurf->area);
01270     }
01271
01272     return area;
01273 }
01274
01275 }
01276
01277 VPRIVATE double Vacc_atomSASAPos(Vacc *thee,
01278                                 double radius,
01279                                 Vatom *atom, /* The atom being manipulated */
01280                                 int mode
01281                                 ) {
01282     VaccSurf *asurf;
01283     int id;
01284     static int warned = 0;
01285
01286     if ((thee->surf == VNULL) || (mode == 1)){
01287         if(!warned){
01288             Vnm_print(2, "WARNING: Recalculating entire surface!!!!\n");
01289             warned = 1;
01290         }
01291         Vacc_SASAPos(thee, radius); // reinitialize before we can do anything about doing a calculation on
01292         a repositioned atom
01293     }
01294
01295     id = Vatom_getAtomID(atom);
01296     asurf = thee->surf[id];
01297
01298     VaccSurf_dtor(&asurf);
01299     thee->surf[id] = Vacc_atomSurf(thee, atom, thee->refSphere, radius);
01300     asurf = thee->surf[id];
01301
01302     //printf("%s: Time elapsed: %f\n", __func__, ((double)clock() - ts) / CLOCKS_PER_SEC);
01303
01304     return asurf->area;
01305 }
01306
01307 /* ////////////////////////////////////////
01308 // Routine: Vacc_atomdSASA
01309 //
01310 // Purpose: Calculates the derivative of surface area with respect to atomic
01311 //           displacement using finite difference methods.
01312 //
01313 // Args:    radius The radius of the solvent probe in Angstroms
01314 //           iatom  Index of the atom in thee->alist
01315 //
01316 // Author:   Jason Wagoner
01317 //           David Gohara
01318 //           Nathan Baker (original FORTRAN routine from UHBD by Brock Luty)
01320 VPUBLIC void Vacc_atomdSASA(Vacc *thee,
01321                             double dpos,
01322                             double srad,
01323                             Vatom *atom,

```

```

01324             double *dSA
01325         ) {
01326
01327         double *temp_Pos,
01328             tPos[3],
01329             axbl,
01330             axtl,
01331             aybl,
01332             aytl,
01333             azbl,
01334             aztl;
01335         VaccSurf *ref;
01336
01337         //printf("%s: entering\n", __func__);
01338         time_t ts;
01339         ts = clock();
01340
01341         /* Get the atom information */
01342         ref = thee->refSphere;
01343         temp_Pos = Vatom_getPosition(atom); // Get a pointer to the position object. You actually manipulate
the atom doing this...
01344
01345         tPos[0] = temp_Pos[0];
01346         tPos[1] = temp_Pos[1];
01347         tPos[2] = temp_Pos[2];
01348
01349         /* Shift by pos +/- on x */
01350         temp_Pos[0] -= dpos;
01351         axbl = Vacc_atomSASAPos(thee, srاد, atom, 0);
01352         temp_Pos[0] = tPos[0];
01353
01354         temp_Pos[0] += dpos;
01355         axtl = Vacc_atomSASAPos(thee, srاد, atom, 0);
01356         temp_Pos[0] = tPos[0];
01357
01358         /* Shift by pos +/- on y */
01359         temp_Pos[1] -= dpos;
01360         aybl = Vacc_atomSASAPos(thee, srاد, atom, 0);
01361         temp_Pos[1] = tPos[1];
01362
01363         temp_Pos[1] += dpos;
01364         aytl = Vacc_atomSASAPos(thee, srاد, atom, 0);
01365         temp_Pos[1] = tPos[1];
01366
01367         /* Shift by pos +/- on z */
01368         temp_Pos[2] -= dpos;
01369         azbl = Vacc_atomSASAPos(thee, srاد, atom, 0);
01370         temp_Pos[2] = tPos[2];
01371
01372         temp_Pos[2] += dpos;
01373         aztl = Vacc_atomSASAPos(thee, srاد, atom, 0);
01374         temp_Pos[2] = tPos[2];
01375
01376         /* Reset the atom SASA to zero displacement */
01377         Vacc_atomSASAPos(thee, srاد, atom, 0);
01378
01379         /* Calculate the final value */
01380         dSA[0] = (axtl-axbl)/(2.0 * dpos);
01381         dSA[1] = (aytl-aybl)/(2.0 * dpos);
01382         dSA[2] = (aztl-azbl)/(2.0 * dpos);
01383     }
01384
01385     /* Note: This is purely test code to make certain that the dSASA code is
01386        behaving properly. This function should NEVER be called by anyone
01387        other than an APBS developer at Wash U.
01388    */
01389     VPUBLIC void Vacc_totalAtomdSASA(Vacc *thee, double dpos, double srاد, Vatom *atom, double *dSA) {
01390
01391         int iatom;
01392         double *temp_Pos, tRad;
01393         double tPos[3];
01394         double axbl, axtl, aybl, aytl, azbl, aztl;
01395         VaccSurf *ref;
01396
01397         /* Get the atom information */
01398         ref = thee->refSphere;
01399         temp_Pos = Vatom_getPosition(atom);
01400         tRad = Vatom_getRadius(atom);
01401         iatom = Vatom_getAtomID(atom);
01402
01403         dSA[0] = 0.0;

```

```

01404     dSA[1] = 0.0;
01405     dSA[2] = 0.0;
01406
01407     tPos[0] = temp_Pos[0];
01408     tPos[1] = temp_Pos[1];
01409     tPos[2] = temp_Pos[2];
01410
01411     /* Shift by pos +/- on x */
01412     temp_Pos[0] -= dpos;
01413     axb1 = Vacc_atomSASAPos(thee, srاد, atom, 1);
01414     temp_Pos[0] = tPos[0];
01415
01416     temp_Pos[0] += dpos;
01417     axt1 = Vacc_atomSASAPos(thee, srاد, atom, 1);
01418     temp_Pos[0] = tPos[0];
01419
01420     /* Shift by pos +/- on y */
01421     temp_Pos[1] -= dpos;
01422     ayb1 = Vacc_atomSASAPos(thee, srاد, atom, 1);
01423     temp_Pos[1] = tPos[1];
01424
01425     temp_Pos[1] += dpos;
01426     ayt1 = Vacc_atomSASAPos(thee, srاد, atom, 1);
01427     temp_Pos[1] = tPos[1];
01428
01429     /* Shift by pos +/- on z */
01430     temp_Pos[2] -= dpos;
01431     azb1 = Vacc_atomSASAPos(thee, srاد, atom, 1);
01432     temp_Pos[2] = tPos[2];
01433
01434     temp_Pos[2] += dpos;
01435     azt1 = Vacc_atomSASAPos(thee, srاد, atom, 1);
01436     temp_Pos[2] = tPos[2];
01437
01438     /* Calculate the final value */
01439     dSA[0] = (axt1-axb1)/(2.0 * dpos);
01440     dSA[1] = (ayt1-ayb1)/(2.0 * dpos);
01441     dSA[2] = (azt1-azb1)/(2.0 * dpos);
01442 }
01443
01444 /* Note: This is purely test code to make certain that the dSASA code is
01445         behaving properly. This function should NEVER be called by anyone
01446         other than an APBS developer at Wash U.
01447 */
01448 VPUBLIC void Vacc_totalAtomdSAV(Vacc *thee, double dpos, double srاد, Vatom *atom, double *dSA, Vclist
    *clist) {
01449
01450     int iatom;
01451     double *temp_Pos, tRad;
01452     double tPos[3];
01453     double axb1,axt1,ayb1,ayt1,azb1,azt1;
01454     VaccSurf *ref;
01455
01456     /* Get the atom information */
01457     ref = thee->refSphere;
01458     temp_Pos = Vatom_getPosition(atom);
01459     tRad = Vatom_getRadius(atom);
01460     iatom = Vatom_getAtomID(atom);
01461
01462     dSA[0] = 0.0;
01463     dSA[1] = 0.0;
01464     dSA[2] = 0.0;
01465
01466     tPos[0] = temp_Pos[0];
01467     tPos[1] = temp_Pos[1];
01468     tPos[2] = temp_Pos[2];
01469
01470     /* Shift by pos +/- on x */
01471     temp_Pos[0] -= dpos;
01472     axb1 = Vacc_totalSAV(thee,clist, VNULL, srاد);
01473     temp_Pos[0] = tPos[0];
01474
01475     temp_Pos[0] += dpos;
01476     axt1 = Vacc_totalSAV(thee,clist, VNULL, srاد);
01477     temp_Pos[0] = tPos[0];
01478
01479     /* Shift by pos +/- on y */
01480     temp_Pos[1] -= dpos;
01481     ayb1 = Vacc_totalSAV(thee,clist, VNULL, srاد);
01482     temp_Pos[1] = tPos[1];
01483

```

```

01484     temp_Pos[1] += dpos;
01485     ayt1 = Vacc_totalSAV(thee,clist, VNULL, srاد);
01486     temp_Pos[1] = tPos[1];
01487
01488     /* Shift by pos +/- on z */
01489     temp_Pos[2] -= dpos;
01490     azb1 = Vacc_totalSAV(thee,clist, VNULL, srاد);
01491     temp_Pos[2] = tPos[2];
01492
01493     temp_Pos[2] += dpos;
01494     azt1 = Vacc_totalSAV(thee,clist, VNULL, srاد);
01495     temp_Pos[2] = tPos[2];
01496
01497     /* Calculate the final value */
01498     dSA[0] = (axt1-axb1)/(2.0 * dpos);
01499     dSA[1] = (ayt1-ayb1)/(2.0 * dpos);
01500     dSA[2] = (azt1-azb1)/(2.0 * dpos);
01501 }
01502
01503 VPUBLIC double Vacc_totalSAV(Vacc *thee, Vclist *clist, APOLparm *apolparm, double radius) {
01504
01505     int i;
01506     int npts[3];
01507
01508     double spacs[3], vec[3];
01509     double w, wx, wy, wz, len, fn, x, y, z, vol;
01510     double vol_density,sav;
01511     double *lower_corner, *upper_corner;
01512
01513     sav = 0.0;
01514     vol = 1.0;
01515     vol_density = 2.0;
01516
01517     lower_corner = clist->lower_corner;
01518     upper_corner = clist->upper_corner;
01519
01520     for (i=0; i<3; i++) {
01521         len = upper_corner[i] - lower_corner[i];
01522         vol *= len;
01523         fn = len*vol_density + 1;
01524         npts[i] = (int)ceil(fn);
01525         spacs[i] = len/((double)(npts[i])-1.0);
01526         if (apolparm != VNULL) {
01527             if (apolparm->setgrid) {
01528                 if (apolparm->grid[i] > spacs[i]) {
01529                     Vnm_print(2, "Vacc_totalSAV: Warning, your GRID value (%g) is larger than the
recommended value (%g)!\n",
                                apolparm->grid[i], spacs[i]);
01530                 }
01531                 spacs[i] = apolparm->grid[i];
01532             }
01533         }
01534     }
01535 }
01536
01537
01538     for (x=lower_corner[0]; x<=upper_corner[0]; x=x+spacs[0]) {
01539         if ( VABS(x - lower_corner[0]) < VSMALL) {
01540             wx = 0.5;
01541         } else if ( VABS(x - upper_corner[0]) < VSMALL) {
01542             wx = 0.5;
01543         } else {
01544             wx = 1.0;
01545         }
01546         vec[0] = x;
01547         for (y=lower_corner[1]; y<=upper_corner[1]; y=y+spacs[1]) {
01548             if ( VABS(y - lower_corner[1]) < VSMALL) {
01549                 wy = 0.5;
01550             } else if ( VABS(y - upper_corner[1]) < VSMALL) {
01551                 wy = 0.5;
01552             } else {
01553                 wy = 1.0;
01554             }
01555             vec[1] = y;
01556             for (z=lower_corner[2]; z<=upper_corner[2]; z=z+spacs[2]) {
01557                 if ( VABS(z - lower_corner[2]) < VSMALL) {
01558                     wz = 0.5;
01559                 } else if ( VABS(z - upper_corner[2]) < VSMALL) {
01560                     wz = 0.5;
01561                 } else {
01562                     wz = 1.0;
01563                 }

```

```

01564         vec[2] = z;
01565
01566         w = wx*wy*wz;
01567
01568         sav += (w*(1.0-Vacc_ivdwAcc(thee, vec, radius)));
01569
01570     } /* z loop */
01571 } /* y loop */
01572 } /* x loop */
01573
01574 w = spacs[0]*spacs[1]*spacs[2];
01575 sav *= w;
01576
01577 return sav;
01578 }
01579
01580 int Vacc_wcaEnergyAtom(Vacc *thee, APOLparm *apolparm, Valist *alist,
01581                       Vclist *clist, int iatom, double *value) {
01582
01583     int i;
01584     int npts[3];
01585     int pad = 14;
01586
01587     int xmin, ymin, zmin;
01588     int xmax, ymax, zmax;
01589
01590     double sigma6, sigma12;
01591
01592     double spacs[3], vec[3];
01593     double w, wx, wy, wz, len, fn, x, y, z, vol;
01594     double x2,y2,z2,r;
01595     double vol_density, energy, rho, srad;
01596     double psig, epsilon, watepsilon, sigma, watsigma, eni, chi;
01597
01598     double *pos;
01599     double *lower_corner, *upper_corner;
01600
01601     Vatom *atom = VNULL;
01602     VASSERT(apolparm != VNULL);
01603
01604     energy = 0.0;
01605     vol = 1.0;
01606     vol_density = 2.0;
01607
01608     lower_corner = clist->lower_corner;
01609     upper_corner = clist->upper_corner;
01610
01611     atom = Valist_getAtom(alist, iatom);
01612     pos = Vatom_getPosition(atom);
01613
01614     /* Note: these are the original temporary water parameters... they have been
01615        replaced by entries in a parameter file:
01616     watsigma = 1.7683;
01617     watepsilon = 0.1521;
01618     watepsilon = watepsilon*4.184;
01619     */
01620
01621     srad = apolparm->srad;
01622     rho = apolparm->bconc;
01623     watsigma = apolparm->watsigma;
01624     watepsilon = apolparm->watepsilon;
01625     psig = atom->radius;
01626     epsilon = atom->epsilon;
01627     sigma = psig + watsigma;
01628     epsilon = VSQRT((epsilon * watepsilon));
01629
01630     /* parameters */
01631     sigma6 = VPOW(sigma,6);
01632     sigma12 = VPOW(sigma,12);
01633     /* OPLS-style radius: double sigmar = sigma*VPOW(2, (1.0/6.0)); */
01634
01635     xmin = pos[0] - pad;
01636     xmax = pos[0] + pad;
01637     ymin = pos[1] - pad;
01638     ymax = pos[1] + pad;
01639     zmin = pos[2] - pad;
01640     zmax = pos[2] + pad;
01641
01642     for (i=0; i<3; i++) {
01643         len = (upper_corner[i] + pad) - (lower_corner[i] - pad);
01644         vol *= len;

```

```

01645         fn = len*vol_density + 1;
01646         npts[i] = (int)ceil(fn);
01647         spacs[i] = 0.5;
01648         if (apolparm->setgrid) {
01649             if (apolparm->grid[i] > spacs[i]) {
01650                 Vnm_print(2, "Vacc_totalSAV: Warning, your GRID value (%g) is larger than the recommended
value (%g)!\n",
01651                     apolparm->grid[i], spacs[i]);
01652             }
01653             spacs[i] = apolparm->grid[i];
01654         }
01655     }
01656     for (x=xmin; x<=xmax; x=x+spacs[0]) {
01657         if ( VABS(x - xmin) < VSMALL) {
01658             wx = 0.5;
01659         } else if ( VABS(x - xmax) < VSMALL) {
01660             wx = 0.5;
01661         } else {
01662             wx = 1.0;
01663         }
01664     }
01665     vec[0] = x;
01666     for (y=ymin; y<=ymax; y=y+spacs[1]) {
01667         if ( VABS(y - ymin) < VSMALL) {
01668             wy = 0.5;
01669         } else if ( VABS(y - ymax) < VSMALL) {
01670             wy = 0.5;
01671         } else {
01672             wy = 1.0;
01673         }
01674     }
01675     vec[1] = y;
01676     for (z=zmin; z<=zmax; z=z+spacs[2]) {
01677         if ( VABS(z - zmin) < VSMALL) {
01678             wz = 0.5;
01679         } else if ( VABS(z - zmax) < VSMALL) {
01680             wz = 0.5;
01681         } else {
01682             wz = 1.0;
01683         }
01684     }
01685     vec[2] = z;
01686     w = wx*wy*wz;
01687     chi = Vacc_ivdwAcc(thee, vec, srads);
01688     if (VABS(chi) > VSMALL) {
01689         x2 = VSQR(vec[0]-pos[0]);
01690         y2 = VSQR(vec[1]-pos[1]);
01691         z2 = VSQR(vec[2]-pos[2]);
01692         r = VSQRT(x2+y2+z2);
01693         if (r <= 14 && r >= sigma) {
01694             eni = chi*rho*epsilon*(-2.0*sigma6/VPOW(r,6)+sigma12/VPOW(r,12));
01695         } else if (r <= 14){
01696             eni = -1.0*epsilon*chi*rho;
01697         } else{
01698             eni = 0.0;
01699         }
01700     } else{
01701         eni = 0.0;
01702     }
01703     energy += eni*w;
01704     } /* z loop */
01705     } /* y loop */
01706     } /* x loop */
01707     w = spacs[0]*spacs[1]*spacs[2];
01708     energy *= w;
01709     *value = energy;
01710     return VRC_SUCCESS;
01711 }
01712
01721 VPUBLIC int Vacc_wcaEnergy(Vacc *acc, APOLparm *apolparm, Valist *alist,
01722                           Vclist *clist){
01723     int iatom;

```

```

01725     int rc = 0;
01726
01727     double energy = 0.0;
01728     double tenergy = 0.0;
01729     double rho = apolparm->bconc;
01730
01731     /* Do a sanity check to make sure that watepsilon and watsigma are set
01732      * If not, return with an error. */
01733     if (apolparm->setwat == 0) {
01734         Vnm_print(2, "Vacc_wcaEnergy: Error. No value was set for watsigma and watepsilon.\n");
01735         return VRC_FAILURE;
01736     }
01737
01738     if (VABS(rho) < VSMALL) {
01739         apolparm->wcaEnergy = tenergy;
01740         return 1;
01741     }
01742
01743     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++){
01744         rc = Vacc_wcaEnergyAtom(acc, apolparm, alist, clist, iatom, &energy);
01745         if(rc == 0) return 0;
01746
01747         tenergy += energy;
01748     }
01749
01750     apolparm->wcaEnergy = tenergy;
01751
01752     return VRC_SUCCESS;
01753 }
01754 }
01755
01756 VPUBLIC int Vacc_wcaForceAtom(Vacc *thee,
01757                             APOLparm *apolparm,
01758                             Vclist *clist,
01759                             Vatom *atom,
01760                             double *force
01761 ) {
01762     int i,
01763         si,
01764         npts[3],
01765         pad = 14,
01766         xmin,
01767         ymin,
01768         zmin,
01769         xmax,
01770         ymax,
01771         zmax;
01772
01773     double sigma6,
01774         sigma12,
01775         spacs[3],
01776         vec[3],
01777         fpt[3],
01778         w,
01779         wx,
01780         wy,
01781         wz,
01782         len,
01783         fn,
01784         x,
01785         y,
01786         z,
01787         vol,
01788         x2,
01789         y2,
01790         z2,
01791         r,
01792         vol_density,
01793         fo,
01794         rho,
01795         srاد,
01796         psig,
01797         epsilon,
01798         watepsilon,
01799         sigma,
01800         watsigma,
01801         chi,
01802         *pos,
01803         *lower_corner,
01804         *upper_corner;
01805

```

```

01806      /* Allocate needed variables now that we've asserted required conditions. */
01807      time_t ts;
01808      ts = clock();
01809
01810      VASSERT(apolparm != VNULL);
01811
01812      /* Do a sanity check to make sure that watepsilon and watsigma are set
01813       * If not, return with an error. */
01814      if(apolparm->setwat == 0){
01815          Vnm_print(2,"Vacc_wcaEnergy: Error. No value was set for watsigma and watepsilon.\n");
01816          return VRC_FAILURE;
01817      }
01818
01819      vol = 1.0;
01820      vol_density = 2.0;
01821
01822      lower_corner = clist->lower_corner;
01823      upper_corner = clist->upper_corner;
01824
01825      pos = Vatom_getPosition(atom);
01826
01827      srad = apolparm->srad;
01828      rho = apolparm->bconc;
01829      watsigma = apolparm->watsigma;
01830      watepsilon = apolparm->watepsilon;
01831
01832      psig = atom->radius;
01833      epsilon = atom->epsilon;
01834      sigma = psig + watsigma;
01835      epsilon = VSQRT((epsilon * watepsilon));
01836
01837      /* parameters */
01838      sigma6 = VPOW(sigma,6);
01839      sigma12 = VPOW(sigma,12);
01840      /* OPLS-style radius: double sigmar = sigma*VPOW(2, (1.0/6.0)); */
01841
01842      for (i=0; i<3; i++) {
01843          len = (upper_corner[i] + pad) - (lower_corner[i] - pad);
01844          vol *= len;
01845          fn = len*vol_density + 1;
01846          npts[i] = (int)ceil(fn);
01847          spacs[i] = 0.5;
01848          force[i] = 0.0;
01849          if (apolparm->setgrid) {
01850              if (apolparm->grid[i] > spacs[i]) {
01851                  Vnm_print(2, "Vacc_totalsAV: Warning, your GRID value (%g) is larger than the recommended
value (%g)!\n",
01852                      apolparm->grid[i], spacs[i]);
01853              }
01854              spacs[i] = apolparm->grid[i];
01855          }
01856      }
01857
01858      xmin = pos[0] - pad;
01859      xmax = pos[0] + pad;
01860      ymin = pos[1] - pad;
01861      ymax = pos[1] + pad;
01862      zmin = pos[2] - pad;
01863      zmax = pos[2] + pad;
01864
01865      for (x=xmin; x<=xmax; x=x+spacs[0]) {
01866          if ( VABS(x - xmin) < VSMALL) {
01867              wx = 0.5;
01868          } else if ( VABS(x - xmax) < VSMALL) {
01869              wx = 0.5;
01870          } else {
01871              wx = 1.0;
01872          }
01873          vec[0] = x;
01874          for (y=ymin; y<=ymax; y=y+spacs[1]) {
01875              if ( VABS(y - ymin) < VSMALL) {
01876                  wy = 0.5;
01877              } else if ( VABS(y - ymax) < VSMALL) {
01878                  wy = 0.5;
01879              } else {
01880                  wy = 1.0;
01881              }
01882              vec[1] = y;
01883              for (z=zmin; z<=zmax; z=z+spacs[2]) {
01884                  if ( VABS(z - zmin) < VSMALL) {
01885                      wz = 0.5;

```



```

01886         } else if ( VABS(z - zmax) < VSMALL) {
01887             wz = 0.5;
01888         } else {
01889             wz = 1.0;
01890         }
01891         vec[2] = z;
01892
01893         w = wx*wy*wz;
01894
01895         chi = Vacc_ivdwAcc(thee, vec, srad);
01896
01897         if (chi != 0.0) {
01898
01899             x2 = VSQR(vec[0]-pos[0]);
01900             y2 = VSQR(vec[1]-pos[1]);
01901             z2 = VSQR(vec[2]-pos[2]);
01902             r = VSQRT(x2+y2+z2);
01903
01904             if (r <= 14 && r >= sigma){
01905
01906                 fo = 12.0*chi*rho*epsilon*(sigma6/VPOW(r,7)-sigma12/VPOW(r,13));
01907
01908                 fpt[0] = -1.0*(pos[0]-vec[0])*fo/r;
01909                 fpt[1] = -1.0*(pos[1]-vec[1])*fo/r;
01910                 fpt[2] = -1.0*(pos[2]-vec[2])*fo/r;
01911
01912                 }else {
01913                     for (si=0; si < 3; si++) fpt[si] = 0.0;
01914                 }
01915             }else {
01916                 for (si=0; si < 3; si++) fpt[si] = 0.0;
01917             }
01918
01919             for(i=0;i<3;i++){
01920                 force[i] += (w*fpt[i]);
01921             }
01922
01923             } /* z loop */
01924         } /* y loop */
01925     } /* x loop */
01926
01927     w = spacs[0]*spacs[1]*spacs[2];
01928     for(i=0;i<3;i++) force[i] *= w;
01929
01930     return VRC_SUCCESS;
01931 }

```

9.52 src/generic/vacc.h File Reference

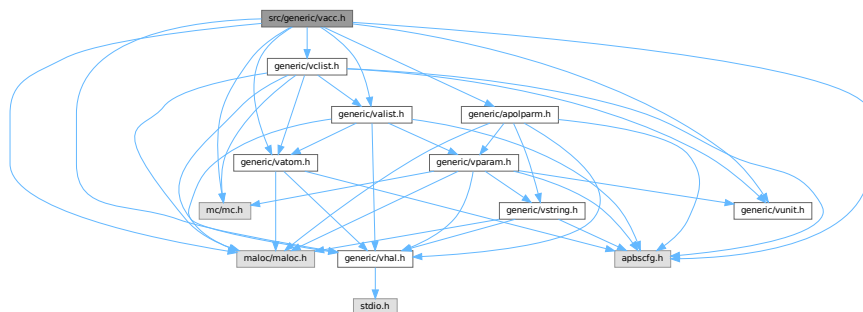
Contains declarations for class Vacc.

```

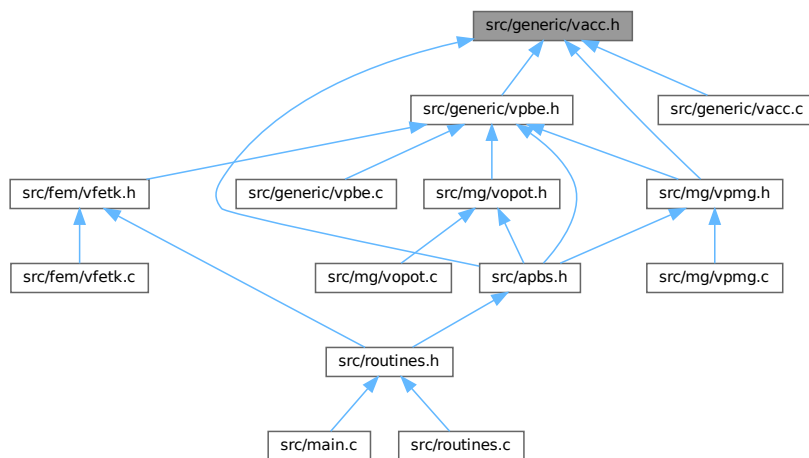
#include "apbscfg.h"
#include "malloc/malloc.h"
#include "mc/mc.h"
#include "generic/vhal.h"
#include "generic/valist.h"
#include "generic/vclist.h"
#include "generic/vatom.h"
#include "generic/vunit.h"
#include "generic/apolparm.h"

```

Include dependency graph for vacc.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVaccSurf](#)
Surface object list of per-atom surface points.
- struct [sVacc](#)
Oracle for solvent- and ion-accessibility around a biomolecule.

Typedefs

- typedef struct [sVaccSurf](#) [VaccSurf](#)
Declaration of the VaccSurf class as the VaccSurf structure.
- typedef struct [sVacc](#) [Vacc](#)
Declaration of the Vacc class as the Vacc structure.

Functions

- VEXTERNC unsigned long int [Vacc_memChk](#) ([Vacc](#) *thee)
Get number of bytes in this object and its members.
- VEXTERNC [VaccSurf](#) * [VaccSurf_ctor](#) ([Vmem](#) *mem, double probe_radius, int nsphere)
Allocate and construct the surface object; do not assign surface points to positions.
- VEXTERNC int [VaccSurf_ctor2](#) ([VaccSurf](#) *thee, [Vmem](#) *mem, double probe_radius, int nsphere)
Construct the surface object using previously allocated memory; do not assign surface points to positions.
- VEXTERNC void [VaccSurf_dtor](#) ([VaccSurf](#) **thee)
Destroy the surface object and free its memory.
- VEXTERNC void [VaccSurf_dtor2](#) ([VaccSurf](#) *thee)
Destroy the surface object.
- VEXTERNC [VaccSurf](#) * [VaccSurf_refSphere](#) ([Vmem](#) *mem, int npts)
Set up an array of points for a reference sphere of unit radius.
- VEXTERNC [VaccSurf](#) * [Vacc_atomSurf](#) ([Vacc](#) *thee, [Vatom](#) *atom, [VaccSurf](#) *ref, double probe_radius)
Set up an array of points corresponding to the SAS due to a particular atom.
- VEXTERNC [Vacc](#) * [Vacc_ctor](#) ([Valist](#) *alist, [Vclist](#) *clist, double surf_density)
Construct the accessibility object.
- VEXTERNC int [Vacc_ctor2](#) ([Vacc](#) *thee, [Valist](#) *alist, [Vclist](#) *clist, double surf_density)
FORTTRAN stub to construct the accessibility object.
- VEXTERNC void [Vacc_dtor](#) ([Vacc](#) **thee)
Destroy object.
- VEXTERNC void [Vacc_dtor2](#) ([Vacc](#) *thee)
FORTTRAN stub to destroy object.
- VEXTERNC double [Vacc_vdwAcc](#) ([Vacc](#) *thee, double center[[VAPBS_DIM](#)])
Report van der Waals accessibility.
- VEXTERNC double [Vacc_ivdwAcc](#) ([Vacc](#) *thee, double center[[VAPBS_DIM](#)], double radius)
Report inflated van der Waals accessibility.
- VEXTERNC double [Vacc_molAcc](#) ([Vacc](#) *thee, double center[[VAPBS_DIM](#)], double radius)
Report molecular accessibility.
- VEXTERNC double [Vacc_fastMolAcc](#) ([Vacc](#) *thee, double center[[VAPBS_DIM](#)], double radius)
Report molecular accessibility quickly.
- VEXTERNC double [Vacc_splineAcc](#) ([Vacc](#) *thee, double center[[VAPBS_DIM](#)], double win, double infrad)
Report spline-based accessibility.
- VEXTERNC void [Vacc_splineAccGrad](#) ([Vacc](#) *thee, double center[[VAPBS_DIM](#)], double win, double infrad, double *grad)
Report gradient of spline-based accessibility.
- VEXTERNC double [Vacc_splineAccAtom](#) ([Vacc](#) *thee, double center[[VAPBS_DIM](#)], double win, double infrad, [Vatom](#) *atom)
Report spline-based accessibility for a given atom.
- VEXTERNC void [Vacc_splineAccGradAtomUnnorm](#) ([Vacc](#) *thee, double center[[VAPBS_DIM](#)], double win, double infrad, [Vatom](#) *atom, double *force)
Report gradient of spline-based accessibility with respect to a particular atom (see [Vpmsg_splineAccAtom](#))
- VEXTERNC void [Vacc_splineAccGradAtomNorm](#) ([Vacc](#) *thee, double center[[VAPBS_DIM](#)], double win, double infrad, [Vatom](#) *atom, double *force)
Report gradient of spline-based accessibility with respect to a particular atom normalized by the accessibility value due to that atom at that point (see [Vpmsg_splineAccAtom](#))
- VEXTERNC void [Vacc_splineAccGradAtomNorm4](#) ([Vacc](#) *thee, double center[[VAPBS_DIM](#)], double win, double infrad, [Vatom](#) *atom, double *force)

Report gradient of spline-based accessibility with respect to a particular atom normalized by a 4th order accessibility value due to that atom at that point (see Vpmg_splineAccAtom)

- VEXTERNC void `Vacc_splineAccGradAtomNorm3` (`Vacc` *thee, double center[VAPBS_DIM], double win, double infrad, `Vatom` *atom, double *force)

Report gradient of spline-based accessibility with respect to a particular atom normalized by a 3rd order accessibility value due to that atom at that point (see Vpmg_splineAccAtom)

- VEXTERNC double `Vacc_SASA` (`Vacc` *thee, double radius)

Build the solvent accessible surface (SAS) and calculate the solvent accessible surface area.

- VEXTERNC double `Vacc_totalSASA` (`Vacc` *thee, double radius)

Return the total solvent accessible surface area (SASA)

- VEXTERNC double `Vacc_atomSASA` (`Vacc` *thee, double radius, `Vatom` *atom)

Return the atomic solvent accessible surface area (SASA)

- VEXTERNC `VaccSurf` * `Vacc_atomSASPoints` (`Vacc` *thee, double radius, `Vatom` *atom)

Get the set of points for this atom's solvent-accessible surface.

- VEXTERNC void `Vacc_atomdSAV` (`Vacc` *thee, double radius, `Vatom` *atom, double *dSA)

Get the derivatve of solvent accessible volume.

- VEXTERNC void `Vacc_atomdSASA` (`Vacc` *thee, double dpos, double radius, `Vatom` *atom, double *dSA)

Get the derivatve of solvent accessible area.

- VEXTERNC void `Vacc_totalAtomdSASA` (`Vacc` *thee, double dpos, double radius, `Vatom` *atom, double *dSA)

Testing purposes only.

- VEXTERNC void `Vacc_totalAtomdSAV` (`Vacc` *thee, double dpos, double radius, `Vatom` *atom, double *dSA, `Vclist` *clist)

Total solvent accessible volume.

- VEXTERNC double `Vacc_totalSAV` (`Vacc` *thee, `Vclist` *clist, `APOLparm` *apolparm, double radius)

Return the total solvent accessible volume (SAV)

- VEXTERNC int `Vacc_wcaEnergy` (`Vacc` *thee, `APOLparm` *apolparm, `Valist` *alist, `Vclist` *clist)

Return the WCA integral energy.

- VEXTERNC int `Vacc_wcaForceAtom` (`Vacc` *thee, `APOLparm` *apolparm, `Vclist` *clist, `Vatom` *atom, double *force)

Return the WCA integral force.

- VEXTERNC int `Vacc_wcaEnergyAtom` (`Vacc` *thee, `APOLparm` *apolparm, `Valist` *alist, `Vclist` *clist, int iatom, double *value)

Calculate the WCA energy for an atom.

9.52.1 Detailed Description

Contains declarations for class Vacc.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```

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*
*

```

Definition in file [vacc.h](#).

9.53 vacc.h

[Go to the documentation of this file.](#)

```

00001
00062 #ifndef _VACC_H_
00063 #define _VACC_H_
00064
00065 #include "apbscfg.h"
00066
00067 #include "malloc/malloc.h"
00068 #if defined(HAVE_MC_H)
00069 #include "mc/mc.h"
00070 #endif
00071
00072 #include "generic/vhal.h"
00073 #include "generic/valist.h"
00074 #include "generic/vclist.h"
00075 #include "generic/vatom.h"

```

```

00076 #include "generic/vunit.h"
00077 #include "generic/apolparm.h"
00078
00084 struct sVaccSurf {
00085     Vmem *mem;
00086     double *xpts;
00087     double *ypts;
00088     double *zpts;
00089     char *bpts;
00091     double area;
00092     int npts;
00093     double probe_radius;
00095 };
00096
00101 typedef struct sVaccSurf VaccSurf;
00102
00108 struct sVacc {
00109
00110     Vmem *mem;
00111     Valist *alist;
00112     Vclist *clist;
00113     int *atomFlags;
00116     VaccSurf *refSphere;
00117     VaccSurf **surf;
00120     Vset acc;
00122     double surf_density;
00125 };
00126
00131 typedef struct sVacc Vacc;
00132
00133 #if !defined(VINLINE_VACC)
00134
00140     VEXTERNC unsigned long int Vacc_memChk(
00141         Vacc *thee
00142     );
00143
00144 #else /* if defined(VINLINE_VACC) */
00145
00146 #    define Vacc_memChk(thee) (Vmem_bytes((thee)->mem))
00147
00148 #endif /* if !defined(VINLINE_VACC) */
00149
00157 VEXTERNC VaccSurf* VaccSurf_ctor(
00158     Vmem *mem,
00159     double probe_radius,
00160     int nsphere
00161 );
00162
00170 VEXTERNC int VaccSurf_ctor2(
00171     VaccSurf *thee,
00172     Vmem *mem,
00173     double probe_radius,
00174     int nsphere
00175 );
00176
00182 VEXTERNC void VaccSurf_dtor(
00183     VaccSurf **thee
00184 );
00185
00191 VEXTERNC void VaccSurf_dtor2(
00192     VaccSurf *thee
00193 );
00194
00209 VEXTERNC VaccSurf* VaccSurf_refSphere(
00210     Vmem *mem,
00211     int npts
00212 );
00213
00221 VEXTERNC VaccSurf* Vacc_atomSurf(
00222     Vacc *thee,
00223     Vatom *atom,
00224     VaccSurf *ref,
00226     double probe_radius
00227 );
00228
00233 VEXTERNC Vacc* Vacc_ctor(
00234     Valist *alist,
00235     Vclist *clist,
00237     double surf_density
00239 );
00240

```

```
00245 VEXTERNC int Vacc_ctor2(  
00246     Vacc *thee,  
00247     Valist *alist,  
00248     Vclist *clist,  
00250     double surf_density  
00252 );  
00253  
00258 VEXTERNC void Vacc_dtor(  
00259     Vacc **thee  
00260 );  
00261  
00266 VEXTERNC void Vacc_dtor2(  
00267     Vacc *thee  
00268 );  
00269  
00280 VEXTERNC double Vacc_vdwAcc(  
00281     Vacc *thee,  
00282     double center[VAPBS_DIM]  
00283 );  
00284  
00296 VEXTERNC double Vacc_ivdwAcc(  
00297     Vacc *thee,  
00298     double center[VAPBS_DIM],  
00299     double radius  
00300 );  
00301  
00316 VEXTERNC double Vacc_molAcc(  
00317     Vacc *thee,  
00318     double center[VAPBS_DIM],  
00319     double radius  
00320 );  
00321  
00340 VEXTERNC double Vacc_fastMolAcc(  
00341     Vacc *thee,  
00342     double center[VAPBS_DIM],  
00343     double radius  
00344 );  
00345  
00357 VEXTERNC double Vacc_splineAcc(  
00358     Vacc *thee,  
00359     double center[VAPBS_DIM],  
00360     double win,  
00361     double infrad  
00362 );  
00363  
00369 VEXTERNC void Vacc_splineAccGrad(  
00370     Vacc *thee,  
00371     double center[VAPBS_DIM],  
00372     double win,  
00373     double infrad,  
00374     double *grad  
00375 );  
00376  
00388 VEXTERNC double Vacc_splineAccAtom(  
00389     Vacc *thee,  
00390     double center[VAPBS_DIM],  
00391     double win,  
00392     double infrad,  
00393     Vatom *atom  
00394 );  
00395  
00406 VEXTERNC void Vacc_splineAccGradAtomUnnorm(  
00407     Vacc *thee,  
00408     double center[VAPBS_DIM],  
00409     double win,  
00410     double infrad,  
00411     Vatom *atom,  
00412     double *force  
00413 );  
00414  
00426 VEXTERNC void Vacc_splineAccGradAtomNorm(  
00427     Vacc *thee,  
00428     double center[VAPBS_DIM],  
00429     double win,  
00430     double infrad,  
00431     Vatom *atom,  
00432     double *force  
00433 );  
00434  
00442 VEXTERNC void Vacc_splineAccGradAtomNorm4(  
00443     Vacc *thee,
```

```
00444         double center[VAPBS_DIM],
00445         double win,
00446         double infrad,
00447         Vatom *atom,
00448         double *force
00449     );
00450
00458 VEXTERNC void Vacc_splineAccGradAtomNorm3(
00459     Vacc *thee,
00460     double center[VAPBS_DIM],
00461     double win,
00462     double infrad,
00463     Vatom *atom,
00464     double *force
00465 );
00466
00467
00477 VEXTERNC double Vacc_SASA(
00478     Vacc *thee,
00479     double radius
00480 );
00481
00489 VEXTERNC double Vacc_totalSASA(
00490     Vacc *thee,
00491     double radius
00492 );
00493
00501 VEXTERNC double Vacc_atomSASA(
00502     Vacc *thee,
00503     double radius,
00504     Vatom *atom
00505 );
00506
00513 VEXTERNC VaccSurf* Vacc_atomSASPoints(
00514     Vacc *thee,
00515     double radius,
00516     Vatom *atom
00517 );
00518
00524 VEXTERNC void Vacc_atomdSAV(
00525     Vacc *thee,
00526     double radius,
00527     Vatom *atom,
00528     double *dSA
00529 );
00530
00536 VEXTERNC void Vacc_atomdSASA(
00537     Vacc *thee,
00538     double dpos,
00539     double radius,
00540     Vatom *atom,
00541     double *dSA
00542 );
00543
00549 VEXTERNC void Vacc_totalAtomdSASA(
00550     Vacc *thee,
00551     double dpos,
00552     double radius,
00553     Vatom *atom,
00554     double *dSA
00555 );
00556
00562 VEXTERNC void Vacc_totalAtomdSAV(
00563     Vacc *thee,
00564     double dpos,
00565     double radius,
00566     Vatom *atom,
00567     double *dSA,
00568     Vclist *clist
00569 );
00570
00578 VEXTERNC double Vacc_totalSAV(
00579     Vacc *thee,
00580     Vclist *clist,
00581     APOLparm *apolparm,
00583     double radius
00584 );
00585
00592 VEXTERNC int Vacc_wcaEnergy(
00593     Vacc *thee,
00594     APOLparm *apolparm,
```



```

00595             Valist *alist,
00596             Vclist *clist
00597         );
00604 VEXTERNC int Vacc_wcaForceAtom(Vacc *thee,
00605                                APOLparm *apolparm,
00606                                Vclist *clist,
00607                                Vatom *atom,
00608                                double *force
00609        );
00610
00616 VEXTERNC int Vacc_wcaEnergyAtom(
00617     Vacc *thee,
00618     APOLparm *apolparm,
00619     Valist *alist,
00620     Vclist *clist,
00621     int iatom,
00622     double *value
00623 );
00624
00625 #endif /* ifndef _VACC_H_ */

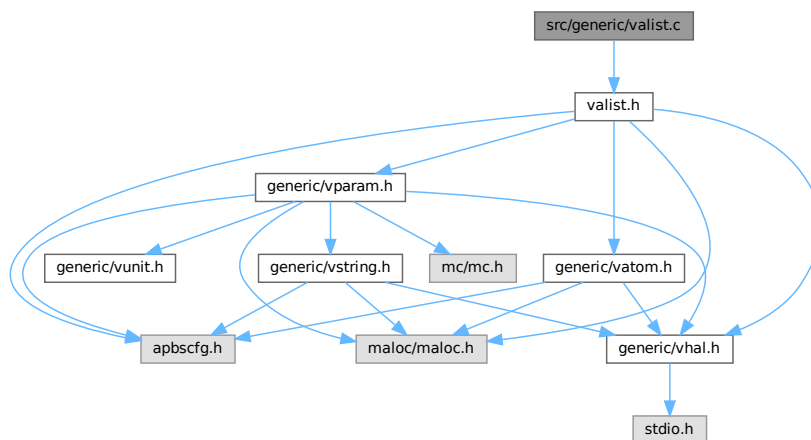
```

9.54 src/generic/valist.c File Reference

Class Valist methods.

```
#include "valist.h"
```

Include dependency graph for valist.c:



Functions

- VPUBLIC double [Valist_getCenterX](#) (Valist *thee)
Get x-coordinate of molecule center.
- VPUBLIC double [Valist_getCenterY](#) (Valist *thee)
Get y-coordinate of molecule center.
- VPUBLIC double [Valist_getCenterZ](#) (Valist *thee)
Get z-coordinate of molecule center.
- VPUBLIC Vatom * [Valist_getAtomList](#) (Valist *thee)
Get actual array of atom objects from the list.
- VPUBLIC int [Valist_getNumberAtoms](#) (Valist *thee)
Get number of atoms in the list.

- VPUBLIC Vatom * Valist_getAtom (Valist *thee, int i)
Get pointer to particular atom in list.
- VPUBLIC unsigned long int Valist_memChk (Valist *thee)
Get total memory allocated for this object and its members.
- VPUBLIC Valist * Valist_ctor ()
Construct the atom list object.
- VPUBLIC Vrc_Codes Valist_ctor2 (Valist *thee)
FORTTRAN stub to construct the atom list object.
- VPUBLIC void Valist_dtor (Valist **thee)
Destroys atom list object.
- VPUBLIC void Valist_dtor2 (Valist *thee)
FORTTRAN stub to destroy atom list object.
- VPRIVATE Vrc_Codes Valist_readPDBSerial (Valist *thee, Vio *sock, int *serial)
- VPRIVATE Vrc_Codes Valist_readPDBAtomName (Valist *thee, Vio *sock, char atomName[VMAX_ARGLEN])
- VPRIVATE Vrc_Codes Valist_readPDBResidueName (Valist *thee, Vio *sock, char resName[VMAX_ARGLEN])
- VPRIVATE Vrc_Codes Valist_readPDBResidueNumber (Valist *thee, Vio *sock, int *resSeq)
- VPRIVATE Vrc_Codes Valist_readPDBAtomCoord (Valist *thee, Vio *sock, double *coord)
- VPRIVATE Vrc_Codes Valist_readPDBChargeRadius (Valist *thee, Vio *sock, double *charge, double *radius)
- VPRIVATE Vrc_Codes Valist_readPDB_throughXYZ (Valist *thee, Vio *sock, int *serial, char atomName[VMAX_ARGLEN], char resName[VMAX_ARGLEN], int *resSeq, double *x, double *y, double *z)
- VPRIVATE Vatom * Valist_getAtomStorage (Valist *thee, Vatom **plist, int *pnlist, int *pnatoms)
- VPRIVATE Vrc_Codes Valist_setAtomArray (Valist *thee, Vatom **plist, int nlist, int natoms)
- VPUBLIC Vrc_Codes Valist_readPDB (Valist *thee, Vparam *param, Vio *sock)
Fill atom list with information from a PDB file.
- VPUBLIC Vrc_Codes Valist_readPQR (Valist *thee, Vparam *params, Vio *sock)
Fill atom list with information from a PQR file.
- VPUBLIC Vrc_Codes Valist_readXML (Valist *thee, Vparam *params, Vio *sock)
Fill atom list with information from an XML file.
- VPUBLIC Vrc_Codes Valist_getStatistics (Valist *thee)
Load up Valist with various statistics.

Variables

- VPRIVATE char * Valist_whiteChars = "\t\r\n"
- VPRIVATE char * Valist_commChars = "#%"
- VPRIVATE char * Valist_xmlwhiteChars = "\t\r\n<>"

9.54.1 Detailed Description

Class Valist methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```

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*
*

```

Definition in file [valist.c](#).

9.54.2 Function Documentation

9.54.2.1 Valist_getAtomStorage()

```

VPRIVATE Vatom * Valist_getAtomStorage (
    Valist * thee,
    Vatom ** plist,
    int * pnlst,
    int * pnatoms )

```

Definition at line 424 of file [valist.c](#).

9.54.2.2 Valist_readPDB_throughXYZ()

```
VPRIVATE Vrc_Codes Valist_readPDB_throughXYZ (
    Valist * thee,
    Vio * sock,
    int * serial,
    char atomName[VMAX_ARGLLEN],
    char resName[VMAX_ARGLLEN],
    int * resSeq,
    double * x,
    double * y,
    double * z )
```

Definition at line 344 of file [valist.c](#).

9.54.2.3 Valist_readPDBAtomCoord()

```
VPRIVATE Vrc_Codes Valist_readPDBAtomCoord (
    Valist * thee,
    Vio * sock,
    double * coord )
```

Definition at line 298 of file [valist.c](#).

9.54.2.4 Valist_readPDBAtomName()

```
VPRIVATE Vrc_Codes Valist_readPDBAtomName (
    Valist * thee,
    Vio * sock,
    char atomName[VMAX_ARGLLEN] )
```

Definition at line 206 of file [valist.c](#).

9.54.2.5 Valist_readPDBChargeRadius()

```
VPRIVATE Vrc_Codes Valist_readPDBChargeRadius (
    Valist * thee,
    Vio * sock,
    double * charge,
    double * radius )
```

Definition at line 316 of file [valist.c](#).

9.54.2.6 Valist_readPDBResidueName()

```
VPRIVATE Vrc_Codes Valist_readPDBResidueName (
    Valist * thee,
    Vio * sock,
    char resName[VMAX_ARGLLEN] )
```

Definition at line 224 of file [valist.c](#).

9.54.2.7 Valist_readPDBResidueNumber()

```
VPRIVATE Vrc_Codes Valist_readPDBResidueNumber (
    Valist * thee,
```

```
Vio * sock,
int * resSeq )
```

Definition at line 242 of file `valist.c`.

9.54.2.8 `Valist_readPDBSerial()`

```
VPRIVATE Vrc_Codes Valist_readPDBSerial (
    Valist * thee,
    Vio * sock,
    int * serial )
```

Definition at line 186 of file `valist.c`.

9.54.2.9 `Valist_setAtomArray()`

```
VPRIVATE Vrc_Codes Valist_setAtomArray (
    Valist * thee,
    Vatom ** plist,
    int nlist,
    int natoms )
```

Definition at line 480 of file `valist.c`.

9.54.3 Variable Documentation

9.54.3.1 `Valist_commChars`

```
VPRIVATE char* Valist_commChars = "#%"
```

Definition at line 61 of file `valist.c`.

9.54.3.2 `Valist_whiteChars`

```
VPRIVATE char* Valist_whiteChars = " \t\r\n"
```

Definition at line 60 of file `valist.c`.

9.54.3.3 `Valist_xmlwhiteChars`

```
VPRIVATE char* Valist_xmlwhiteChars = " \t\r\n<>"
```

Definition at line 62 of file `valist.c`.

9.55 `valist.c`

[Go to the documentation of this file.](#)

```
00001
00056 #include "valist.h"
00057
00058 VEMBED(rcsid="$Id$")
00059
00060 VPRIVATE char *Valist_whiteChars = " \t\r\n";
00061 VPRIVATE char *Valist_commChars = "#%";
00062 VPRIVATE char *Valist_xmlwhiteChars = " \t\r\n<>";
00063
00064 #if !defined(VINLINE_VATOM)
00065
```

```

00066 VPUBLIC double Valist_getCenterX(Valist *thee) {
00067
00068     if (thee == NULL) {
00069         Vnm_print(2, "Valist_getCenterX: Found null pointer when getting the center of X coordinate!\n");
00070         VASSERT(0);
00071     }
00072     return thee->center[0];
00073
00074 }
00075
00076 VPUBLIC double Valist_getCenterY(Valist *thee) {
00077
00078     if (thee == NULL) {
00079         Vnm_print(2, "Valist_getCenterY: Found null pointer when getting the center of Y coordinate!\n");
00080         VASSERT(0);
00081     }
00082     return thee->center[1];
00083
00084 }
00085 VPUBLIC double Valist_getCenterZ(Valist *thee) {
00086
00087     if (thee == NULL) {
00088         Vnm_print(2, "Valist_getCenterZ: Found null pointer when getting the center of Z coordinate!\n");
00089         VASSERT(0);
00090     }
00091     return thee->center[2];
00092
00093 }
00094
00095 VPUBLIC Vatom* Valist_getAtomList(Valist *thee) {
00096
00097     if (thee == NULL) {
00098         Vnm_print(2, "Valist_getAtomList: Found null pointer when getting the atom list!\n");
00099         VASSERT(0);
00100     }
00101     return thee->atoms;
00102
00103 }
00104
00105 VPUBLIC int Valist_getNumberAtoms(Valist *thee) {
00106
00107     if (thee == NULL) {
00108         Vnm_print(2, "Valist_getNumberAtoms: Found null pointer when getting the number of atoms!\n");
00109         VASSERT(0);
00110     }
00111     return thee->number;
00112
00113 }
00114
00115 VPUBLIC Vatom* Valist_getAtom(Valist *thee, int i) {
00116
00117     if (thee == NULL) {
00118         Vnm_print(2, "Valist_getAtom: Found null pointer when getting atoms!\n");
00119         VASSERT(0);
00120     }
00121     if (i >= thee->number) {
00122         Vnm_print(2, "Valist_getAtom: Requested atom number (%d) outside of atom list range (%d)!\n", i,
00123             thee->number);
00124         VASSERT(0);
00125     }
00126     return &(thee->atoms[i]);
00127
00128 }
00129 VPUBLIC unsigned long int Valist_memChk(Valist *thee) {
00130
00131     if (thee == NULL) return 0;
00132     return Vmem_bytes(thee->vmem);
00133
00134 }
00135
00136 #endif /* if !defined(VINLINE_VATOM) */
00137
00138 VPUBLIC Valist* Valist_ctor() {
00139
00140     /* Set up the structure */
00141     Valist *thee = VNULL;
00142     thee = (Valist*)Vmem_malloc(VNULL, 1, sizeof(Valist));
00143     if (thee == VNULL) {
00144         Vnm_print(2, "Valist_ctor: Got NULL pointer when constructing the atom list object!\n");
00145         VASSERT(0);

```

```

00146     }
00147     if ( Valist_ctor2(thee) != VRC_SUCCESS) {
00148         Vnm_print(2, "Valist_ctor: Error in constructing the atom list object!\n");
00149         VASSERT(0);
00150     }
00151
00152     return thee;
00153 }
00154
00155 VPUBLIC Vrc_Codes Valist_ctor2(Valist *thee) {
00156     thee->atoms = VNULL;
00157     thee->number = 0;
00158
00159     /* Initialize the memory management object */
00160     thee->vmem = Vmem_ctor("APBS:VALIST");
00161
00162     return VRC_SUCCESS;
00163 }
00164
00165 }
00166
00167 VPUBLIC void Valist_dtor(Valist **thee)
00168 {
00169     if ((*thee) != VNULL) {
00170         Valist_dtor2(*thee);
00171         Vmem_free(VNULL, 1, sizeof(Valist), (void **)thee);
00172         (*thee) = VNULL;
00173     }
00174 }
00175
00176 VPUBLIC void Valist_dtor2(Valist *thee) {
00177     Vmem_free(thee->vmem, thee->number, sizeof(Vatom), (void **)&(thee->atoms));
00178     thee->atoms = VNULL;
00179     thee->number = 0;
00180
00181     Vmem_dtor(&(thee->vmem));
00182 }
00183
00184 /* Read serial number from PDB ATOM/HETATM field */
00185 VPRIVATE Vrc_Codes Valist_readPDBSerial(Valist *thee, Vio *sock, int *serial) {
00186     char tok[VMAX_BUFSIZE];
00187     int ti = 0;
00188
00189     if (Vio_scanf(sock, "%s", tok) != 1) {
00190         Vnm_print(2, "Valist_readPDB: Ran out of tokens while parsing serial!\n");
00191         return VRC_FAILURE;
00192     }
00193     if (sscanf(tok, "%d", &ti) != 1) {
00194         Vnm_print(2, "Valist_readPDB: Unable to parse serial token (%s) as int!\n",
00195             tok);
00196         return VRC_FAILURE;
00197     }
00198     *serial = ti;
00199
00200     return VRC_SUCCESS;
00201 }
00202
00203 /* Read atom name from PDB ATOM/HETATM field */
00204 VPRIVATE Vrc_Codes Valist_readPDBAtomName(Valist *thee, Vio *sock,
00205     char atomName[VMAX_ARGLEN]) {
00206     char tok[VMAX_BUFSIZE];
00207
00208     if (Vio_scanf(sock, "%s", tok) != 1) {
00209         Vnm_print(2, "Valist_readPDB: Ran out of tokens while parsing atom name!\n");
00210         return VRC_FAILURE;
00211     }
00212     if (strlen(tok) < VMAX_ARGLEN) strcpy(atomName, tok);
00213     else {
00214         Vnm_print(2, "Valist_readPDB: Atom name (%s) too long!\n", tok);
00215         return VRC_FAILURE;
00216     }
00217     return VRC_SUCCESS;
00218 }
00219
00220 /* Read residue name from PDB ATOM/HETATM field */
00221 VPRIVATE Vrc_Codes Valist_readPDBResidueName(Valist *thee, Vio *sock,
00222     char resName[VMAX_ARGLEN]) {
00223

```

```

00227     char tok[VMAX_BUFSIZE];
00228
00229     if (Vio_scanf(sock, "%s", tok) != 1) {
00230         Vnm_print(2, "Valist_readPDB: Ran out of tokens while parsing residue name!\n");
00231         return VRC_FAILURE;
00232     }
00233     if (strlen(tok) < VMAX_ARGLEN) strcpy(resName, tok);
00234     else {
00235         Vnm_print(2, "Valist_readPDB: Residue name (%s) too long!\n", tok);
00236         return VRC_FAILURE;
00237     }
00238     return VRC_SUCCESS;
00239 }
00240
00241 /* Read residue number from PDB ATOM/HETATM field */
00242 VPRIVATE Vrc_Codes Valist_readPDBResidueNumber(
00243     Valist *thee, Vio *sock, int *resSeq) {
00244
00245     char tok[VMAX_BUFSIZE];
00246     char *resstring;
00247     int ti = 0;
00248
00249     if (Vio_scanf(sock, "%s", tok) != 1) {
00250         Vnm_print(2, "Valist_readPDB: Ran out of tokens while parsing resSeq!\n");
00251         return VRC_FAILURE;
00252     }
00253     if (sscanf(tok, "%d", &ti) != 1) {
00254
00255         /* One of three things can happen here:
00256            1) There is a chainID in the line:   THR A   1
00257            2) The chainID is merged with resSeq: THR A1001
00258            3) An actual error:                 THR foo
00259
00260         */
00261
00262         if (strlen(tok) == 1) {
00263             /* Case 1: Chain ID Present
00264                Read the next field and hope its a float */
00265
00266             if (Vio_scanf(sock, "%s", tok) != 1) {
00267                 Vnm_print(2, "Valist_readPDB: Ran out of tokens while parsing resSeq!\n");
00268                 return VRC_FAILURE;
00269             }
00270             if (sscanf(tok, "%d", &ti) != 1) {
00271                 Vnm_print(2, "Valist_readPDB: Unable to parse resSeq token (%s) as int!\n",
00272                     tok);
00273                 return VRC_FAILURE;
00274             }
00275
00276         } else {
00277             /* Case 2: Chain ID, merged string.
00278                Move pointer forward past the chainID and check
00279
00280             */
00281             //strcpy(resstring, tok);
00282             resstring = tok;
00283             resstring++;
00284
00285             if (sscanf(resstring, "%d", &ti) != 1) {
00286                 /* Case 3: More than one non-numeral char is present. Error.*/
00287                 Vnm_print(2, "Valist_readPDB: Unable to parse resSeq token (%s) as int!\n",
00288                     resstring);
00289                 return VRC_FAILURE;
00290             }
00291         }
00292         *resSeq = ti;
00293
00294         return VRC_SUCCESS;
00295     }
00296
00297 /* Read atom coordinate from PDB ATOM/HETATM field */
00298 VPRIVATE Vrc_Codes Valist_readPDBAtomCoord(Valist *thee, Vio *sock, double *coord) {
00299
00300     char tok[VMAX_BUFSIZE];
00301     double tf = 0;
00302
00303     if (Vio_scanf(sock, "%s", tok) != 1) {
00304         Vnm_print(2, "Valist_readPDB: Ran out of tokens while parsing atom coordinate!\n");
00305         return VRC_FAILURE;
00306     }
00307     if (sscanf(tok, "%lf", &tf) != 1) {

```



```
00308         return VRC_FAILURE;
00309     }
00310     *coord = tf;
00311
00312     return VRC_SUCCESS;
00313 }
00314
00315 /* Read charge and radius from PQR ATOM/HETATM field */
00316 VPRIVATE Vrc_Codes Valist_readPDBChargeRadius(Valist *thee, Vio *sock,
00317     double *charge, double *radius) {
00318
00319     char tok[VMAX_BUFSIZE];
00320     double tf = 0;
00321
00322     if (Vio_scanf(sock, "%s", tok) != 1) {
00323         Vnm_print(2, "Valist_readPQR: Ran out of tokens while parsing charge!\n");
00324         return VRC_FAILURE;
00325     }
00326     if (sscanf(tok, "%lf", &tf) != 1) {
00327         return VRC_FAILURE;
00328     }
00329     *charge = tf;
00330
00331     if (Vio_scanf(sock, "%s", tok) != 1) {
00332         Vnm_print(2, "Valist_readPQR: Ran out of tokens while parsing radius!\n");
00333         return VRC_FAILURE;
00334     }
00335     if (sscanf(tok, "%lf", &tf) != 1) {
00336         return VRC_FAILURE;
00337     }
00338     *radius = tf;
00339
00340     return VRC_SUCCESS;
00341 }
00342
00343 /* Read ATOM/HETATM field of PDB through the X/Y/Z fields */
00344 VPRIVATE Vrc_Codes Valist_readPDB_throughXYZ(
00345     Valist *thee,
00346     Vio *sock, /* Socket ready for reading */
00347     int *serial, /* Set to atom number */
00348     char atomName[VMAX_ARGLEN], /* Set to atom name */
00349     char resName[VMAX_ARGLEN], /* Set to residue name */
00350     int *resSeq, /* Set to residue number */
00351     double *x, /* Set to x-coordinate */
00352     double *y, /* Set to y-coordinate */
00353     double *z /* Set to z-coordinate */
00354 ) {
00355
00356     int i, njunk, gotit;
00357
00358     /* Grab serial */
00359     if (Valist_readPDBSerial(thee, sock, serial) == VRC_FAILURE) {
00360         Vnm_print(2, "Valist_readPDB: Error while parsing serial!\n");
00361     }
00362
00363     /* Grab atom name */
00364     if (Valist_readPDBAtomName(thee, sock, atomName) == VRC_FAILURE) {
00365         Vnm_print(2, "Valist_readPDB: Error while parsing atom name!\n");
00366         return VRC_FAILURE;
00367     }
00368
00369     /* Grab residue name */
00370     if (Valist_readPDBResidueName(thee, sock, resName) == VRC_FAILURE) {
00371         Vnm_print(2, "Valist_readPDB: Error while parsing residue name!\n");
00372         return VRC_FAILURE;
00373     }
00374
00375     /* Grab residue number */
00376     if (Valist_readPDBResidueNumber(thee, sock, resSeq) == VRC_FAILURE) {
00377         Vnm_print(2, "Valist_readPDB: Error while parsing residue number!\n");
00378         return VRC_FAILURE;
00379     }
00380
00381     /* Read tokens until we find one that can be parsed as an atom
00382     * x-coordinate. We will allow njunk=1 intervening field that
00383     * cannot be parsed as a coordinate */
00384     njunk = 1;
00385     gotit = 0;
```

```

00389     for (i=0; i<(njunk+1); i++) {
00390         if (Valist_readPDBAtomCoord(thee, sock, x) == VRC_SUCCESS) {
00391             gotit = 1;
00392             break;
00393         }
00394     }
00395     if (!gotit) {
00396         Vnm_print(2, "Valist_readPDB: Can't find x!\n");
00397         return VRC_FAILURE;
00398     }
00399     /* Read y-coordinate */
00400     if (Valist_readPDBAtomCoord(thee, sock, y) == VRC_FAILURE) {
00401         Vnm_print(2, "Valist_readPDB: Can't find y!\n");
00402         return VRC_FAILURE;
00403     }
00404     /* Read z-coordinate */
00405     if (Valist_readPDBAtomCoord(thee, sock, z) == VRC_FAILURE) {
00406         Vnm_print(2, "Valist_readPDB: Can't find z!\n");
00407         return VRC_FAILURE;
00408     }
00409
00410     #if 0 /* Set to 1 if you want to debug */
00411         Vnm_print(1, "Valist_readPDB: serial = %d\n", *serial);
00412         Vnm_print(1, "Valist_readPDB: atomName = %s\n", atomName);
00413         Vnm_print(1, "Valist_readPDB: resName = %s\n", resName);
00414         Vnm_print(1, "Valist_readPDB: resSeq = %d\n", *resSeq);
00415         Vnm_print(1, "Valist_readPDB: pos = (%g, %g, %g)\n",
00416                 *x, *y, *z);
00417     #endif
00418
00419     return VRC_SUCCESS;
00420 }
00421
00422 /* Get a the next available atom storage location, increasing the storage
00423  * space if necessary. Return VNULL if something goes wrong. */
00424 VPRIVATE Vatom* Valist_getAtomStorage(
00425     Valist *thee,
00426     Vatom **plist, /* Pointer to existing list of atoms */
00427     int *pnlist, /* Size of existing list, may be changed */
00428     int *pnatoms /* Existing number of atoms in list; incremented
00429                  before exit */
00430 ) {
00431
00432     Vatom *oldList, *newList, *theList;
00433     Vatom *oldAtom, *newAtom;
00434     int iatom, inext, oldLength, newLength, natoms;
00435
00436     newList = VNULL;
00437
00438     /* See if we need more space */
00439     if (*pnatoms >= *pnlist) {
00440
00441         /* Double the storage space */
00442         oldLength = *pnlist;
00443         newLength = 2*oldLength;
00444         newList = (Vatom*)Vmem_malloc(thee->vmem, newLength, sizeof(Vatom));
00445         oldList = *plist;
00446
00447         /* Check the allocation */
00448         if (newList == VNULL) {
00449             Vnm_print(2, "Valist_readPDB: failed to allocate space for %d (Vatom)s!\n", newLength);
00450             return VNULL;
00451         }
00452
00453         /* Copy the atoms over */
00454         natoms = *pnatoms;
00455         for (iatom=0; iatom<natoms; iatom++) {
00456             oldAtom = &(oldList[iatom]);
00457             newAtom = &(newList[iatom]);
00458             Vatom_copyTo(oldAtom, newAtom);
00459             Vatom_dtor2(oldAtom);
00460         }
00461
00462         /* Free the old list */
00463         Vmem_free(thee->vmem, oldLength, sizeof(Vatom), (void **)plist);
00464
00465         /* Copy new list to plist */
00466         *plist = newList;
00467         *pnlist = newLength;
00468     }
00469

```

```

00470     theList = *plist;
00471     inext = *pnatoms;
00472
00473     /* Get the next available spot and increment counters */
00474     newAtom = &(theList[inext]);
00475     *pnatoms = inext + 1;
00476
00477     return newAtom;
00478 }
00479
00480 VPRIVATE Vrc_Codes Valist_setAtomArray(Valist *thee,
00481     Vatom **plist, /* Pointer to list of atoms to store */
00482     int nlist, /* Length of list */
00483     int natoms /* Number of real atom entries in list */
00484     ) {
00485
00486     Vatom *list, *newAtom, *oldAtom;
00487     int i;
00488
00489     list = *plist;
00490
00491     /* Allocate necessary space */
00492     thee->number = 0;
00493     thee->atoms = (Vatom*)Vmem_malloc(thee->vmem, natoms, sizeof(Vatom));
00494     if (thee->atoms == VNULL) {
00495         Vnm_print(2, "Valist_readPDB: Unable to allocate space for %d (Vatom)s!\n",
00496             natoms);
00497         return VRC_FAILURE;
00498     }
00499     thee->number = natoms;
00500
00501     /* Copy over data */
00502     for (i=0; i<thee->number; i++) {
00503         newAtom = &(thee->atoms[i]);
00504         oldAtom = &(list[i]);
00505         Vatom_copyTo(oldAtom, newAtom);
00506         Vatom_dtor2(oldAtom);
00507     }
00508
00509     /* Free old array */
00510     Vmem_free(thee->vmem, nlist, sizeof(Vatom), (void **)plist);
00511
00512     return VRC_SUCCESS;
00513 }
00514
00515 VPUBLIC Vrc_Codes Valist_readPDB(Valist *thee, Vparam *param, Vio *sock) {
00516
00517     /* WE DO NOT DIRECTLY CONFORM TO PDB STANDARDS -- TO ALLOW LARGER FILES, WE
00518      * REQUIRE ALL FIELDS TO BE WHITESPACE DELIMITED */
00519
00520     Vatom *atoms = VNULL;
00521     Vatom *nextAtom = VNULL;
00522     Vparam_AtomData *atomData = VNULL;
00523
00524     char tok[VMAX_BUFSIZE];
00525     char atomName[VMAX_ARGLEN], resName[VMAX_ARGLEN];
00526
00527     int nlist, natoms, serial, resSeq;
00528
00529     double x, y, z, charge, radius, epsilon;
00530     double pos[3];
00531
00532     if (thee == VNULL) {
00533         Vnm_print(2, "Valist_readPDB: Got NULL pointer when reading PDB file!\n");
00534         VASSERT(0);
00535     }
00536     thee->number = 0;
00537
00538     Vio_setWhiteChars(sock, Valist_whiteChars);
00539     Vio_setCommChars(sock, Valist_commChars);
00540
00541     /* Allocate some initial space for the atoms */
00542     nlist = 200;
00543     atoms = (Vatom*)Vmem_malloc(thee->vmem, nlist, sizeof(Vatom));
00544
00545     natoms = 0;
00546     /* Read until we run out of lines */
00547     while (Vio_scanf(sock, "%s", tok) == 1) {
00548
00549         /* Parse only ATOM/HETATOM fields */
00550         if ((Vstring_strcasecmp(tok, "ATOM") == 0) ||

```

```

00551         (Vstring_strcasecmp(tok, "HETATM") == 0)) {
00552
00553         /* Read ATOM/HETATM field of PDB through the X/Y/Z fields */
00554         if (Valist_readPDB_throughXYZ(thee, sock, &serial, atomName,
00555             resName, &resSeq, &x, &y, &z) == VRC_FAILURE) {
00556             Vnm_print(2, "Valist_readPDB: Error parsing atom %d!\n",
00557                 serial);
00558             return VRC_FAILURE;
00559         }
00560
00561         /* Try to find the parameters. */
00562         atomData = Vparam_getAtomData(param, resName, atomName);
00563         if (atomData == VNULL) {
00564             Vnm_print(2, "Valist_readPDB: Couldn't find parameters for \
00565 atom = %s, residue = %s\n", atomName, resName);
00566             return VRC_FAILURE;
00567         }
00568         charge = atomData->charge;
00569         radius = atomData->radius;
00570         epsilon = atomData->epsilon;
00571
00572         /* Get pointer to next available atom position */
00573         nextAtom = Valist_getAtomStorage(thee, &atoms, &nlist, &natoms);
00574         if (nextAtom == VNULL) {
00575             Vnm_print(2, "Valist_readPDB: Error in allocating spacing for atoms!\n");
00576             return VRC_FAILURE;
00577         }
00578
00579         /* Store the information */
00580         pos[0] = x; pos[1] = y; pos[2] = z;
00581         Vatom_setPosition(nextAtom, pos);
00582         Vatom_setCharge(nextAtom, charge);
00583         Vatom_setRadius(nextAtom, radius);
00584         Vatom_setEpsilon(nextAtom, epsilon);
00585         Vatom_setAtomID(nextAtom, natoms-1);
00586         Vatom_setResName(nextAtom, resName);
00587         Vatom_setAtomName(nextAtom, atomName);
00588
00589     } /* if ATOM or HETATM */
00590 } /* while we haven't run out of tokens */
00591
00592 Vnm_print(0, "Valist_readPDB: Counted %d atoms\n", natoms);
00593 fflush(stdout);
00594
00595 /* Store atoms internally */
00596 if (Valist_setAtomArray(thee, &atoms, nlist, natoms) == VRC_FAILURE) {
00597     Vnm_print(2, "Valist_readPDB: unable to store atoms!\n");
00598     return VRC_FAILURE;
00599 }
00600
00601 return Valist_getStatistics(thee);
00602
00603 }
00604 }
00605
00606 VPUBLIC Vrc_Codes Valist_readPQR(Valist *thee, Vparam *params, Vio *sock) {
00607
00608     /* WE DO NOT DIRECTLY CONFORM TO PDB STANDARDS -- TO ALLOW LARGER FILES, WE
00609      * REQUIRE ALL FIELDS TO BE WHITESPACE DELIMITED */
00610
00611
00612     Vatom *atoms = VNULL;
00613     Vatom *nextAtom = VNULL;
00614     Vparam_AtomData *atomData = VNULL;
00615
00616     char tok[VMAX_BUF_SIZE];
00617     char atomName[VMAX_ARGLEN], resName[VMAX_ARGLEN];
00618     char chs[VMAX_BUF_SIZE];
00619
00620     int use_params = 0;
00621     int nlist, natoms, serial, resSeq;
00622
00623     double x, y, z, charge, radius, epsilon;
00624     double pos[3];
00625
00626     epsilon = 0.0;
00627
00628     if (thee == VNULL) {
00629         Vnm_print(2, "Valist_readPQR: Got NULL pointer when reading PQR file!\n");
00630         VASSERT(0);
00631     }

```

```

00632     thee->number = 0;
00633
00634     Vio_setWhiteChars(sock, Valist_whiteChars);
00635     Vio_setCommChars(sock, Valist_commChars);
00636
00637     /* Allocate some initial space for the atoms */
00638     nlist = 200;
00639     atoms = (Vatom*)Vmem_malloc(thee->vmem, nlist, sizeof(Vatom));
00640
00641     /* Check if we are using a parameter file or not */
00642     if(params != VNULL) use_params = 1;
00643
00644     natoms = 0;
00645     /* Read until we run out of lines */
00646     while (Vio_scanf(sock, "%s", tok) == 1) {
00647
00648         /* Parse only ATOM/HETATOM fields */
00649         if ((Vstring_strcasecmp(tok, "ATOM") == 0) ||
00650             (Vstring_strcasecmp(tok, "HETATM") == 0)) {
00651
00652             /* Read ATOM/HETATM field of PDB through the X/Y/Z fields */
00653             if (Valist_readPDB_throughXYZ(thee, sock, &serial, atomName,
00654                 resName, &resSeq, &x, &y, &z) == VRC_FAILURE) {
00655                 Vnm_print(2, "Valist_readPQR: Error parsing atom %d!\n", serial);
00656                 Vnm_print(2, "Please double check this atom in the pqr file, e.g., make sure there are no
concatenated fields.\n");
00657                 return VRC_FAILURE;
00658             }
00659
00660             /* Read Q/R fields */
00661             if (Valist_readPDBChargeRadius(thee, sock, &charge, &radius) == VRC_FAILURE) {
00662                 Vnm_print(2, "Valist_readPQR: Error parsing atom %d!\n",
00663                     serial);
00664                 Vnm_print(2, "Please double check this atom in the pqr file, e.g., make sure there are no
concatenated fields.\n");
00665                 return VRC_FAILURE;
00666             }
00667
00668             if(use_params){
00669                 /* Try to find the parameters. */
00670                 atomData = Vparam_getAtomData(params, resName, atomName);
00671                 if (atomData == VNULL) {
00672                     Vnm_print(2, "Valist_readPDB: Couldn't find parameters for \
00673 atom = %s, residue = %s\n", atomName, resName);
00674                     return VRC_FAILURE;
00675                 }
00676                 charge = atomData->charge;
00677                 radius = atomData->radius;
00678                 epsilon = atomData->epsilon;
00679             }
00680
00681             /* Get pointer to next available atom position */
00682             nextAtom = Valist_getAtomStorage(thee, &atoms, &nlist, &natoms);
00683             if (nextAtom == VNULL) {
00684                 Vnm_print(2, "Valist_readPQR: Error in allocating spacing for atoms!\n");
00685                 return VRC_FAILURE;
00686             }
00687
00688             /* Store the information */
00689             pos[0] = x; pos[1] = y; pos[2] = z;
00690             Vatom_setPosition(nextAtom, pos);
00691             Vatom_setCharge(nextAtom, charge);
00692             Vatom_setRadius(nextAtom, radius);
00693             Vatom_setEpsilon(nextAtom, epsilon);
00694             Vatom_setAtomID(nextAtom, natoms-1);
00695             Vatom_setResName(nextAtom, resName);
00696             Vatom_setAtomName(nextAtom, atomName);
00697
00698             } /* if ATOM or HETATM */
00699         else {
00700             /*
00701              * nop
00702              * Note that if we find a line that starts with something that's not
00703              * ATOM or HETATM we'll just keep parsing strings until we find one
00704              * of the acceptable keywords.
00705              * Extraordinary measures are not necessary, and only add to the
00706              * befuddlement.
00707              */
00708         }
00709     } /* while we haven't run out of tokens */
00710

```

```

00711     Vnm_print(0, "Valist_readPQR: Counted %d atoms\n", natoms);
00712     fflush(stdout);
00713
00714     /* Store atoms internally */
00715     if (Valist_setAtomArray(thee, &atoms, nlist, natoms) == VRC_FAILURE) {
00716         Vnm_print(2, "Valist_readPDB: unable to store atoms!\n");
00717         return VRC_FAILURE;
00718     }
00719
00720     return Valist_getStatistics(thee);
00721
00722 }
00723
00724
00725 VPUBLIC Vrc_Codes Valist_readXML(Valist *thee, Vparam *params, Vio *sock) {
00726     Vatom *atoms = VNULL;
00727     Vatom *nextAtom = VNULL;
00728
00729     char tok[VMAX_BUFSIZE];
00730     char endtag[VMAX_BUFSIZE];
00731
00732     int nlist, natoms;
00733     int xset, yset, zset, chgset, radset;
00734
00735     double x, y, z, charge, radius, dtmp;
00736     double pos[3];
00737
00738     if (thee == VNULL) {
00739         Vnm_print(2, "Valist_readXML: Got NULL pointer when reading XML file!\n");
00740         VASSERT(0);
00741     }
00742     thee->number = 0;
00743
00744     Vio_setWhiteChars(sock, Valist_xmlwhiteChars);
00745     Vio_setCommChars(sock, Valist_commChars);
00746
00747     /* Allocate some initial space for the atoms */
00748     nlist = 200;
00749     atoms = (Vatom*)Vmem_malloc(thee->vmem, nlist, sizeof(Vatom));
00750
00751     /* Initialize some variables */
00752     natoms = 0;
00753     xset = 0;
00754     yset = 0;
00755     zset = 0;
00756     chgset = 0;
00757     radset = 0;
00758     strcpy(endtag, "/");
00759
00760     if (params == VNULL) {
00761         Vnm_print(1, "\nValist_readXML: Warning Warning Warning Warning\n");
00762         Vnm_print(1, "Valist_readXML: The use of XML input files with parameter\n");
00763         Vnm_print(1, "Valist_readXML: files is currently not supported.\n");
00764         Vnm_print(1, "Valist_readXML: Warning Warning Warning Warning\n\n");
00765     }
00766
00767     /* Read until we run out of lines */
00768     while (Vio_scanf(sock, "%s", tok) == 1) {
00769
00770         /* The first tag taken is the start tag - save it to detect end */
00771         if (Vstring_strcasecmp(endtag, "/") == 0) strcat(endtag, tok);
00772
00773         if (Vstring_strcasecmp(tok, "x") == 0) {
00774             Vio_scanf(sock, "%s", tok);
00775             if (sscanf(tok, "%lf", &dtmp) != 1) {
00776                 Vnm_print(2, "Valist_readXML: Unexpected token (%s) while \
00777 reading x!\n", tok);
00778                 return VRC_FAILURE;
00779             }
00780             x = dtmp;
00781             xset = 1;
00782         } else if (Vstring_strcasecmp(tok, "y") == 0) {
00783             Vio_scanf(sock, "%s", tok);
00784             if (sscanf(tok, "%lf", &dtmp) != 1) {
00785                 Vnm_print(2, "Valist_readXML: Unexpected token (%s) while \
00786 reading y!\n", tok);
00787                 return VRC_FAILURE;
00788             }
00789             y = dtmp;
00790             yset = 1;
00791

```

```

00792     } else if (Vstring_strcasecmp(tok, "z") == 0) {
00793         Vio_scanf(sock, "%s", tok);
00794         if (sscanf(tok, "%lf", &dtmp) != 1) {
00795             Vnm_print(2, "Valist_readXML: Unexpected token (%s) while \
00796 reading z!\n", tok);
00797             return VRC_FAILURE;
00798         }
00799         z = dtmp;
00800         zset = 1;
00801     } else if (Vstring_strcasecmp(tok, "charge") == 0) {
00802         Vio_scanf(sock, "%s", tok);
00803         if (sscanf(tok, "%lf", &dtmp) != 1) {
00804             Vnm_print(2, "Valist_readXML: Unexpected token (%s) while \
00805 reading charge!\n", tok);
00806             return VRC_FAILURE;
00807         }
00808         charge = dtmp;
00809         chgset = 1;
00810     } else if (Vstring_strcasecmp(tok, "radius") == 0) {
00811         Vio_scanf(sock, "%s", tok);
00812         if (sscanf(tok, "%lf", &dtmp) != 1) {
00813             Vnm_print(2, "Valist_readXML: Unexpected token (%s) while \
00814 reading radius!\n", tok);
00815             return VRC_FAILURE;
00816         }
00817         radius = dtmp;
00818         radset = 1;
00819     } else if (Vstring_strcasecmp(tok, "/atom") == 0) {
00820
00821         /* Get pointer to next available atom position */
00822         nextAtom = Valist_getAtomStorage(thee, &atoms, &nlist, &natoms);
00823         if (nextAtom == VNULL) {
00824             Vnm_print(2, "Valist_readXML: Error in allocating spacing for atoms!\n");
00825             return VRC_FAILURE;
00826         }
00827
00828         if (xset && yset && zset && chgset && radset){
00829
00830             /* Store the information */
00831             pos[0] = x; pos[1] = y; pos[2] = z;
00832             Vatom_setPosition(nextAtom, pos);
00833             Vatom_setCharge(nextAtom, charge);
00834             Vatom_setRadius(nextAtom, radius);
00835             Vatom_setAtomID(nextAtom, natoms-1);
00836
00837             /* Reset the necessary flags */
00838             xset = 0;
00839             yset = 0;
00840             zset = 0;
00841             chgset = 0;
00842             radset = 0;
00843         } else {
00844             Vnm_print(2, "Valist_readXML: Missing field(s) in atom tag:\n");
00845             if (!xset) Vnm_print(2, "\tx value not set!\n");
00846             if (!yset) Vnm_print(2, "\ty value not set!\n");
00847             if (!zset) Vnm_print(2, "\tz value not set!\n");
00848             if (!chgset) Vnm_print(2, "\tcharge value not set!\n");
00849             if (!radset) Vnm_print(2, "\tradius value not set!\n");
00850             return VRC_FAILURE;
00851         }
00852     } else if (Vstring_strcasecmp(tok, endtag) == 0) break;
00853 }
00854
00855 Vnm_print(0, "Valist_readXML: Counted %d atoms\n", natoms);
00856 fflush(stdout);
00857
00858 /* Store atoms internally */
00859 if (Valist_setAtomArray(thee, &atoms, nlist, natoms) == VRC_FAILURE) {
00860     Vnm_print(2, "Valist_readXML: unable to store atoms!\n");
00861     return VRC_FAILURE;
00862 }
00863
00864 return Valist_getStatistics(thee);
00865
00866 }
00867
00868 /* Load up Valist with various statistics */
00869 VPUBLIC Vrc_Codes Valist_getStatistics(Valist *thee) {
00870
00871     Vatom *atom;
00872     int i, j;

```

```

00873
00874     if (thee == VNULL) {
00875         Vnm_print(2, "Valist_getStatistics: Got NULL pointer when loading up Valist with various
statistics!\n");
00876         VASSERT(0);
00877     }
00878
00879     thee->center[0] = 0.;
00880     thee->center[1] = 0.;
00881     thee->center[2] = 0.;
00882     thee->maxrad = 0.;
00883     thee->charge = 0.;
00884
00885     if (thee->number == 0) return VRC_FAILURE;
00886
00887     /* Reset stat variables */
00888     atom = &(thee->atoms[0]);
00889     for (i=0; i<3; i++) {
00890         thee->maxcrd[i] = thee->mincrd[i] = atom->position[i];
00891     }
00892     thee->maxrad = atom->radius;
00893     thee->charge = 0.0;
00894
00895     for (i=0; i<thee->number; i++) {
00896         atom = &(thee->atoms[i]);
00897         for (j=0; j<3; j++) {
00898             if (atom->position[j] < thee->mincrd[j])
00899                 thee->mincrd[j] = atom->position[j];
00900             if (atom->position[j] > thee->maxcrd[j])
00901                 thee->maxcrd[j] = atom->position[j];
00902         }
00903         if (atom->radius > thee->maxrad) thee->maxrad = atom->radius;
00904         thee->charge = thee->charge + atom->charge;
00905     }
00906
00907     thee->center[0] = 0.5*(thee->maxcrd[0] + thee->mincrd[0]);
00908     thee->center[1] = 0.5*(thee->maxcrd[1] + thee->mincrd[1]);
00909     thee->center[2] = 0.5*(thee->maxcrd[2] + thee->mincrd[2]);
00910
00911     Vnm_print(0, "Valist_getStatistics: Max atom coordinate: (%g, %g, %g)\n",
00912               thee->maxcrd[0], thee->maxcrd[1], thee->maxcrd[2]);
00913     Vnm_print(0, "Valist_getStatistics: Min atom coordinate: (%g, %g, %g)\n",
00914               thee->mincrd[0], thee->mincrd[1], thee->mincrd[2]);
00915     Vnm_print(0, "Valist_getStatistics: Molecule center: (%g, %g, %g)\n",
00916               thee->center[0], thee->center[1], thee->center[2]);
00917
00918     return VRC_SUCCESS;
00919 }
00920 }

```

9.56 src/generic/valist.h File Reference

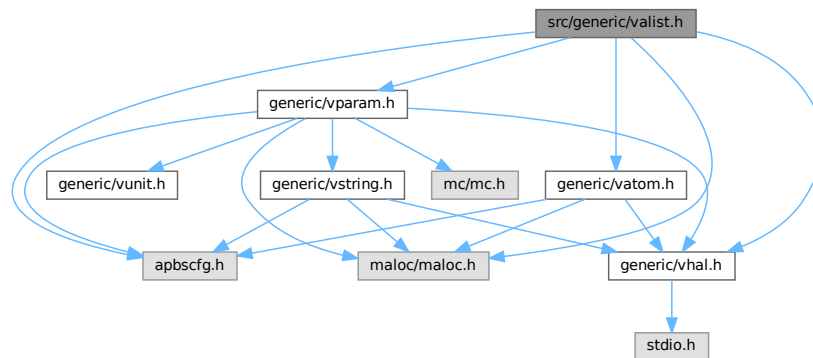
Contains declarations for class Valist.

```

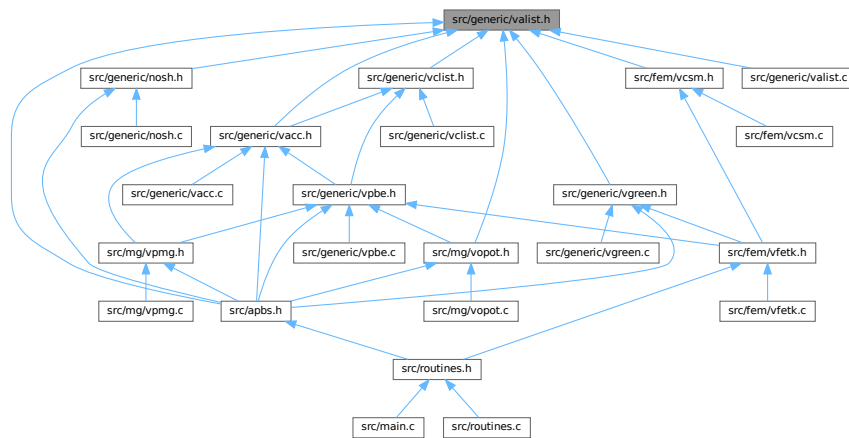
#include "apbscfg.h"
#include "malloc/malloc.h"
#include "generic/vhal.h"
#include "generic/vatom.h"
#include "generic/vparam.h"

```


Include dependency graph for valist.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sValist](#)
Container class for list of atom objects.

Typedefs

- typedef struct [sValist](#) [Valist](#)
Declaration of the Valist class as the Valist structure.

Functions

- VEXTERNC [Vatom](#) * [Valist_getAtomList](#) ([Valist](#) *thee)
Get actual array of atom objects from the list.
- VEXTERNC double [Valist_getCenterX](#) ([Valist](#) *thee)

- Get x-coordinate of molecule center.*
- VEXTERNC double [Valist_getCenterY](#) ([Valist](#) *thee)
- Get y-coordinate of molecule center.*
- VEXTERNC double [Valist_getCenterZ](#) ([Valist](#) *thee)
- Get z-coordinate of molecule center.*
- VEXTERNC int [Valist_getNumberAtoms](#) ([Valist](#) *thee)
- Get number of atoms in the list.*
- VEXTERNC [Vatom](#) * [Valist_getAtom](#) ([Valist](#) *thee, int i)
- Get pointer to particular atom in list.*
- VEXTERNC unsigned long int [Valist_memChk](#) ([Valist](#) *thee)
- Get total memory allocated for this object and its members.*
- VEXTERNC [Valist](#) * [Valist_ctor](#) ()
- Construct the atom list object.*
- VEXTERNC [Vrc_Codes](#) [Valist_ctor2](#) ([Valist](#) *thee)
- FORTTRAN stub to construct the atom list object.*
- VEXTERNC void [Valist_dtor](#) ([Valist](#) **thee)
- Destroys atom list object.*
- VEXTERNC void [Valist_dtor2](#) ([Valist](#) *thee)
- FORTTRAN stub to destroy atom list object.*
- VEXTERNC [Vrc_Codes](#) [Valist_readPQR](#) ([Valist](#) *thee, [Vparam](#) *param, [Vio](#) *sock)
- Fill atom list with information from a PQR file.*
- VEXTERNC [Vrc_Codes](#) [Valist_readPDB](#) ([Valist](#) *thee, [Vparam](#) *param, [Vio](#) *sock)
- Fill atom list with information from a PDB file.*
- VEXTERNC [Vrc_Codes](#) [Valist_readXML](#) ([Valist](#) *thee, [Vparam](#) *param, [Vio](#) *sock)
- Fill atom list with information from an XML file.*
- VEXTERNC [Vrc_Codes](#) [Valist_getStatistics](#) ([Valist](#) *thee)
- Load up Valist with various statistics.*

9.56.1 Detailed Description

Contains declarations for class Valist.

Version

\$Id\$

Author

Nathan A. Baker

Attention

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* Pacific Northwest National Laboratory
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*
```

```

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*
*

```

Definition in file [valist.h](#).

9.57 valist.h

[Go to the documentation of this file.](#)

```

00001
00062 #ifndef _VALIST_H_
00063 #define _VALIST_H_
00064
00065 #include "apbscfg.h"
00066
00067 #include "malloc/malloc.h"
00068
00069 #include "generic/vhal.h"
00070 #include "generic/vatom.h"
00071 #include "generic/vparam.h"
00072
00078 struct sValist {
00079
00080     int number;
00081     double center[3];
00082     double mincrd[3];
00083     double maxcrd[3];
00084     double maxrad;
00085     double charge;
00086     Vatom *atoms;
00087     Vmem *vmem;
00089 };
00090
00095 typedef struct sValist Valist;
00096
00097 #if !defined(VINLINE_VATOM)
00098
00105 VEXTERNC Vatom* Valist_getAtomList(
00106     Valist *thee
00107 );

```

```

00108
00114 VEXTERNC double Valist_getCenterX(
00115     Valist *thee
00116 );
00117
00123 VEXTERNC double Valist_getCenterY(
00124     Valist *thee
00125 );
00126
00132 VEXTERNC double Valist_getCenterZ(
00133     Valist *thee
00134 );
00135
00141 VEXTERNC int Valist_getNumberAtoms(
00142     Valist *thee
00143 );
00144
00150 VEXTERNC Vatom* Valist_getAtom(
00151     Valist *thee,
00152     int i
00153 );
00154
00160 VEXTERNC unsigned long int Valist_memChk(
00161     Valist *thee
00162 );
00163
00164 #else /* if defined(VINLINE_VATOM) */
00165 #   define Valist_getAtomList(thee) ((thee)->atoms)
00166 #   define Valist_getNumberAtoms(thee) ((thee)->number)
00167 #   define Valist_getAtom(thee, i) (&((thee)->atoms[i]))
00168 #   define Valist_memChk(thee) (Vmem_bytes((thee)->vmem))
00169 #   define Valist_getCenterX(thee) ((thee)->center[0])
00170 #   define Valist_getCenterY(thee) ((thee)->center[1])
00171 #   define Valist_getCenterZ(thee) ((thee)->center[2])
00172 #endif /* if !defined(VINLINE_VATOM) */
00173
00179 VEXTERNC Valist* Valist_ctor();
00180
00186 VEXTERNC Vrc_Codes Valist_ctor2(
00187     Valist *thee
00188 );
00189
00194 VEXTERNC void Valist_dtor(
00195     Valist **thee
00196 );
00197
00202 VEXTERNC void Valist_dtor2(
00203     Valist *thee
00204 );
00205
00217 VEXTERNC Vrc_Codes Valist_readPQR(
00218     Valist *thee,
00219     Vparam *param,
00220     Vio *sock
00221 );
00222
00232 VEXTERNC Vrc_Codes Valist_readPDB(
00233     Valist *thee,
00234     Vparam *param,
00235     Vio *sock
00236 );
00237
00247 VEXTERNC Vrc_Codes Valist_readXML(
00248     Valist *thee,
00249     Vparam *param,
00250     Vio *sock
00251 );
00252
00259 VEXTERNC Vrc_Codes Valist_getStatistics(Valist *thee);
00260
00261
00262 #endif /* ifndef _VALIST_H_ */

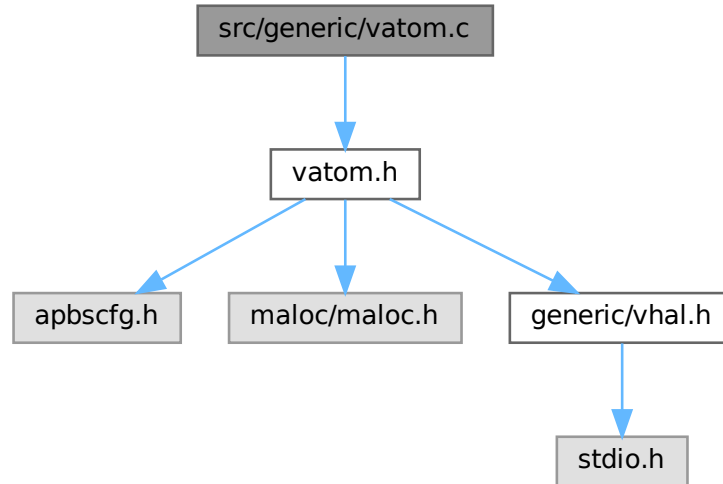
```

9.58 src/generic/vatom.c File Reference

Class Vatom methods.

```
#include "vatom.h"
```

Include dependency graph for vatom.c:



Functions

- VPUBLIC double * [Vatom_getPosition](#) ([Vatom](#) *thee)
Get atomic position.
- VPUBLIC double [Vatom_getPartID](#) ([Vatom](#) *thee)
Get partition ID.
- VPUBLIC void [Vatom_setPartID](#) ([Vatom](#) *thee, int partID)
Set partition ID.
- VPUBLIC double [Vatom_getAtomID](#) ([Vatom](#) *thee)
Get atom ID.
- VPUBLIC void [Vatom_setAtomID](#) ([Vatom](#) *thee, int atomID)
Set atom ID.
- VPUBLIC void [Vatom_setRadius](#) ([Vatom](#) *thee, double radius)
Set atomic radius.
- VPUBLIC double [Vatom_getRadius](#) ([Vatom](#) *thee)
Get atomic position.
- VPUBLIC void [Vatom_setCharge](#) ([Vatom](#) *thee, double charge)
Set atomic charge.
- VPUBLIC double [Vatom_getCharge](#) ([Vatom](#) *thee)
Get atomic charge.
- VPUBLIC void [Vatom_setEpsilon](#) ([Vatom](#) *thee, double epsilon)
Set atomic epsilon.
- VPUBLIC double [Vatom_getEpsilon](#) ([Vatom](#) *thee)
Get atomic epsilon.

- VPUBLIC unsigned long int [Vatom_memChk](#) ([Vatom](#) *thee)
Return the memory used by this structure (and its contents) in bytes.
- VPUBLIC [Vatom](#) * [Vatom_ctor](#) ()
Constructor for the Vatom class.
- VPUBLIC int [Vatom_ctor2](#) ([Vatom](#) *thee)
FORTTRAN stub constructor for the Vatom class.
- VPUBLIC void [Vatom_dtor](#) ([Vatom](#) **thee)
Object destructor.
- VPUBLIC void [Vatom_dtor2](#) ([Vatom](#) *thee)
FORTTRAN stub object destructor.
- VPUBLIC void [Vatom_setPosition](#) ([Vatom](#) *thee, double position[3])
Set the atomic position.
- VPUBLIC void [Vatom_copyTo](#) ([Vatom](#) *thee, [Vatom](#) *dest)
Copy information to another atom.
- VPUBLIC void [Vatom_copyFrom](#) ([Vatom](#) *thee, [Vatom](#) *src)
Copy information to another atom.
- VPUBLIC void [Vatom_setResName](#) ([Vatom](#) *thee, char resName[VMAX_RECLEN])
Set residue name.
- VPUBLIC void [Vatom_getResName](#) ([Vatom](#) *thee, char resName[VMAX_RECLEN])
Retrieve residue name.
- VPUBLIC void [Vatom_setAtomName](#) ([Vatom](#) *thee, char atomName[VMAX_RECLEN])
Set atom name.
- VPUBLIC void [Vatom_getAtomName](#) ([Vatom](#) *thee, char atomName[VMAX_RECLEN])
Retrieve atom name.

9.58.1 Detailed Description

Class Vatom methods.

Author

Nathan Baker

Version

\$Id\$

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*
*

```

Definition in file [vatom.c](#).

9.59 vatom.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "vatom.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 #if !defined(VINLINE_VATOM)
00062
00063 VPUBLIC double *Vatom_getPosition(Vatom *thee) {
00064
00065     VASSERT(thee != VNULL);
00066     return thee->position;
00067 }
00068
00069
00070 VPUBLIC double Vatom_getPartID(Vatom *thee) {
00071
00072     VASSERT(thee != VNULL);
00073     return thee->partID;
00074 }
00075
00076
00077 VPUBLIC void Vatom_setPartID(Vatom *thee, int partID) {
00078
00079     VASSERT(thee != VNULL);
00080     thee->partID = (double)partID;
00081 }
00082
00083
00084 VPUBLIC double Vatom_getAtomID(Vatom *thee) {
00085
00086     VASSERT(thee != VNULL);
00087     return thee->id;
00088 }
00089
00090
00091 VPUBLIC void Vatom_setAtomID(Vatom *thee, int atomID) {

```

```

00092
00093     VASSERT(thee != VNULL);
00094     thee->id = atomID;
00095
00096 }
00097
00098 VPUBLIC void Vatom_setRadius(Vatom *thee, double radius) {
00099
00100     VASSERT(thee != VNULL);
00101     thee->radius = radius;
00102
00103 }
00104
00105 VPUBLIC double Vatom_getRadius(Vatom *thee) {
00106
00107     VASSERT(thee != VNULL);
00108     return thee->radius;
00109
00110 }
00111
00112 VPUBLIC void Vatom_setCharge(Vatom *thee, double charge) {
00113
00114     VASSERT(thee != VNULL);
00115     thee->charge = charge;
00116
00117 }
00118
00119 VPUBLIC double Vatom_getCharge(Vatom *thee) {
00120
00121     VASSERT(thee != VNULL);
00122     return thee->charge;
00123
00124 }
00125
00126 VPUBLIC void Vatom_setEpsilon(Vatom *thee, double epsilon) {
00127
00128     VASSERT(thee != VNULL);
00129     thee->epsilon = epsilon;
00130
00131 }
00132 VPUBLIC double Vatom_getEpsilon(Vatom *thee) {
00133
00134     VASSERT(thee != VNULL);
00135     return thee->epsilon;
00136
00137 }
00138 VPUBLIC unsigned long int Vatom_memChk(Vatom *thee) { return sizeof(Vatom); }
00139
00140 #endif /* if !defined(VINLINE_VATOM) */
00141
00142 VPUBLIC Vatom* Vatom_ctor() {
00143
00144     /* Set up the structure */
00145     Vatom *thee = VNULL;
00146     thee = (Vatom *)Vmem_malloc( VNULL, 1, sizeof(Vatom) );
00147     VASSERT( thee != VNULL);
00148     VASSERT( Vatom_ctor2(thee));
00149
00150     return thee;
00151 }
00152
00153 VPUBLIC int Vatom_ctor2(Vatom *thee) {
00154     thee->partID = -1;
00155     return 1;
00156 }
00157
00158 VPUBLIC void Vatom_dtor(Vatom **thee) {
00159     if ((*thee) != VNULL) {
00160         Vatom_dtor2(*thee);
00161         Vmem_free(VNULL, 1, sizeof(Vatom), (void **)thee);
00162         (*thee) = VNULL;
00163     }
00164 }
00165
00166 VPUBLIC void Vatom_dtor2(Vatom *thee) { ; }
00167
00168 VPUBLIC void Vatom_setPosition(Vatom *thee, double position[3]) {
00169
00170     VASSERT(thee != VNULL);
00171     (thee->position)[0] = position[0];
00172     (thee->position)[1] = position[1];

```



```
00173     (thee->position)[2] = position[2];
00174
00175 }
00176
00177 VPUBLIC void Vatom_copyTo(Vatom *thee, Vatom *dest) {
00178
00179     VASSERT(thee != VNULL);
00180     VASSERT(dest != VNULL);
00181
00182     memcpy(dest, thee, sizeof(Vatom));
00183
00184 }
00185
00186 VPUBLIC void Vatom_copyFrom(Vatom *thee, Vatom *src) {
00187
00188     Vatom_copyTo(src, thee);
00189
00190 }
00191
00192 VPUBLIC void Vatom_setResName(Vatom *thee, char resName[VMAX_RECLEN]) {
00193
00194     VASSERT(thee != VNULL);
00195     strcpy(thee->resName, resName);
00196
00197 }
00198
00199 VPUBLIC void Vatom_getResName(Vatom *thee, char resName[VMAX_RECLEN]) {
00200
00201     VASSERT(thee != VNULL);
00202     strcpy(resName, thee->resName);
00203
00204 }
00205
00206
00207 VPUBLIC void Vatom_setAtomName(Vatom *thee, char atomName[VMAX_RECLEN]) {
00208
00209     VASSERT(thee != VNULL);
00210     strcpy(thee->atomName, atomName);
00211
00212 }
00213
00214 VPUBLIC void Vatom_getAtomName(Vatom *thee, char atomName[VMAX_RECLEN]) {
00215
00216     VASSERT(thee != VNULL);
00217     strcpy(atomName, thee->atomName);
00218
00219 }
00220
00221 #if defined(WITH_TINKER)
00222
00223 VPUBLIC void Vatom_setDipole(Vatom *thee, double dipole[3]) {
00224
00225     VASSERT(thee != VNULL);
00226     (thee->dipole)[0] = dipole[0];
00227     (thee->dipole)[1] = dipole[1];
00228     (thee->dipole)[2] = dipole[2];
00229
00230 }
00231
00232 VPUBLIC void Vatom_setQuadrupole(Vatom *thee, double quadrupole[9]) {
00233
00234     int i;
00235     VASSERT(thee != VNULL);
00236     for (i=0; i<9; i++) (thee->quadrupole)[i] = quadrupole[i];
00237 }
00238
00239 VPUBLIC void Vatom_setInducedDipole(Vatom *thee, double dipole[3]) {
00240
00241     VASSERT(thee != VNULL);
00242     (thee->inducedDipole)[0] = dipole[0];
00243     (thee->inducedDipole)[1] = dipole[1];
00244     (thee->inducedDipole)[2] = dipole[2];
00245 }
00246
00247 VPUBLIC void Vatom_setNLInducedDipole(Vatom *thee, double dipole[3]) {
00248
00249     VASSERT(thee != VNULL);
00250     (thee->nlInducedDipole)[0] = dipole[0];
00251     (thee->nlInducedDipole)[1] = dipole[1];
00252     (thee->nlInducedDipole)[2] = dipole[2];
00253 }
```

```

00254 }
00255
00256 VPUBLIC double *Vatom_getDipole(Vatom *thee) {
00257
00258     VASSERT(thee != VNULL);
00259     return thee->dipole;
00260 }
00261 }
00262
00263 VPUBLIC double *Vatom_getQuadrupole(Vatom *thee) {
00264
00265     VASSERT(thee != VNULL);
00266     return thee->quadrupole;
00267 }
00268 }
00269
00270 VPUBLIC double *Vatom_getInducedDipole(Vatom *thee) {
00271
00272     VASSERT(thee != VNULL);
00273     return thee->inducedDipole;
00274 }
00275 }
00276
00277 VPUBLIC double *Vatom_getNLInducedDipole(Vatom *thee) {
00278
00279     VASSERT(thee != VNULL);
00280     return thee->nlInducedDipole;
00281 }
00282 }
00283
00284 #endif /* if defined(WITH_TINKER) */

```

9.60 src/generic/vatom.h File Reference

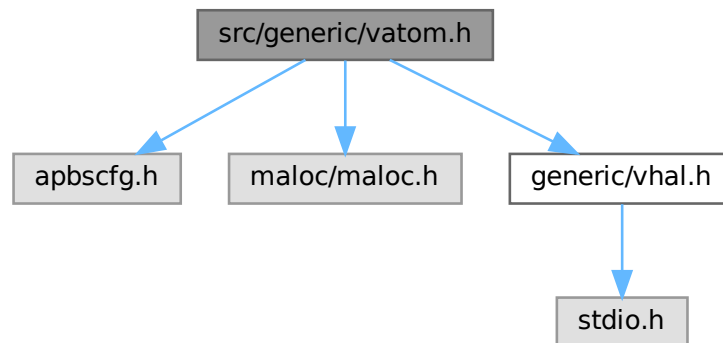
Contains declarations for class Vatom.

```
#include "apbscfg.h"
```

```
#include "malloc/malloc.h"
```

```
#include "generic/vhal.h"
```

Include dependency graph for vatom.h:



- Get atomic charge.*
- VEXTERNC void [Vatom_setEpsilon](#) ([Vatom](#) *thee, double epsilon)
- Set atomic epsilon.*
- VEXTERNC double [Vatom_getEpsilon](#) ([Vatom](#) *thee)
- Get atomic epsilon.*
- VEXTERNC unsigned long int [Vatom_memChk](#) ([Vatom](#) *thee)
- Return the memory used by this structure (and its contents) in bytes.*
- VEXTERNC void [Vatom_setResName](#) ([Vatom](#) *thee, char resName[VMAX_RECLEN])
- Set residue name.*
- VEXTERNC void [Vatom_setAtomName](#) ([Vatom](#) *thee, char atomName[VMAX_RECLEN])
- Set atom name.*
- VEXTERNC void [Vatom_getResName](#) ([Vatom](#) *thee, char resName[VMAX_RECLEN])
- Retrieve residue name.*
- VEXTERNC void [Vatom_getAtomName](#) ([Vatom](#) *thee, char atomName[VMAX_RECLEN])
- Retrieve atom name.*
- VEXTERNC [Vatom](#) * [Vatom_ctor](#) ()
- Constructor for the Vatom class.*
- VEXTERNC int [Vatom_ctor2](#) ([Vatom](#) *thee)
- FORTTRAN stub constructor for the Vatom class.*
- VEXTERNC void [Vatom_dtor](#) ([Vatom](#) **thee)
- Object destructor.*
- VEXTERNC void [Vatom_dtor2](#) ([Vatom](#) *thee)
- FORTTRAN stub object destructor.*
- VEXTERNC void [Vatom_setPosition](#) ([Vatom](#) *thee, double position[3])
- Set the atomic position.*
- VEXTERNC void [Vatom_copyTo](#) ([Vatom](#) *thee, [Vatom](#) *dest)
- Copy information to another atom.*
- VEXTERNC void [Vatom_copyFrom](#) ([Vatom](#) *thee, [Vatom](#) *src)
- Copy information to another atom.*

9.60.1 Detailed Description

Contains declarations for class Vatom.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```

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*
*

```

Definition in file [vatom.h](#).

9.61 vatom.h

[Go to the documentation of this file.](#)

```

00001
00062 #ifndef _VATOM_H_
00063 #define _VATOM_H_
00064
00065 #include "apbscfg.h"
00066
00067 #include "maloc/maloc.h"
00068
00069 #include "generic/vhal.h"
00070
00077 #define VMAX_RECLEN      64
00078
00084 struct sVatom {
00085
00086     double position[3];

```

```

00087     double radius;
00088     double charge;
00089     double partID;
00091     double epsilon;
00093     int id;
00097     char resName[VMAX_RECLEN];
00098     char atomName[VMAX_RECLEN];
00100 #if defined(WITH_TINKER)
00101
00102     double dipole[3];
00103     double quadrupole[9];
00104     double inducedDipole[3];
00105     double nlInducedDipole[3];
00107 #endif /* if defined(WITH_TINKER) */
00108 };
00109
00114 typedef struct sVatom Vatom;
00115
00116 #if !defined(VINLINE_VATOM)
00117
00124     VEXTERNC double* Vatom_getPosition(Vatom *thee);
00125
00132     VEXTERNC void Vatom_setRadius(Vatom *thee, double radius);
00133
00140     VEXTERNC double Vatom_getRadius(Vatom *thee);
00141
00149     VEXTERNC void Vatom_setPartID(Vatom *thee, int partID);
00150
00158     VEXTERNC double Vatom_getPartID(Vatom *thee);
00159
00166     VEXTERNC void Vatom_setAtomID(Vatom *thee, int id);
00167
00174     VEXTERNC double Vatom_getAtomID(Vatom *thee);
00175
00182     VEXTERNC void Vatom_setCharge(Vatom *thee, double charge);
00183
00190     VEXTERNC double Vatom_getCharge(Vatom *thee);
00191
00198     VEXTERNC void Vatom_setEpsilon(Vatom *thee, double epsilon);
00199
00206     VEXTERNC double Vatom_getEpsilon(Vatom *thee);
00207
00215     VEXTERNC unsigned long int Vatom_memChk(Vatom *thee);
00216
00217 #else /* if defined(VINLINE_VATOM) */
00218 # define Vatom_getPosition(thee) ((thee)->position)
00219 # define Vatom_setRadius(thee, tRadius) ((thee)->radius = (tRadius))
00220 # define Vatom_getRadius(thee) ((thee)->radius)
00221 # define Vatom_setPartID(thee, tpartID) ((thee)->partID = (double)(tpartID))
00222 # define Vatom_getPartID(thee) ((thee)->partID)
00223 # define Vatom_setAtomID(thee, tatomID) ((thee)->id = (tatomID))
00224 # define Vatom_getAtomID(thee) ((thee)->id)
00225 # define Vatom_setCharge(thee, tCharge) ((thee)->charge = (tCharge))
00226 # define Vatom_getCharge(thee) ((thee)->charge)
00227 # define Vatom_setEpsilon(thee, tEpsilon) ((thee)->epsilon = (tEpsilon))
00228 # define Vatom_getEpsilon(thee) ((thee)->epsilon)
00229 # define Vatom_memChk(thee) (sizeof(Vatom))
00230 #endif /* if !defined(VINLINE_VATOM) */
00231
00232 /* ////////////////////////////////////// */
00233 // Class Vatom: Non-Inlineable methods (vatom.c)
00235
00242 VEXTERNC void Vatom_setResName(Vatom *thee, char resName[VMAX_RECLEN]);
00243
00248 VEXTERNC void Vatom_setAtomName(
00249     Vatom *thee, /**< Vatom object */
00250     char atomName[VMAX_RECLEN]
00251 );
00252
00259 VEXTERNC void Vatom_getResName(Vatom *thee, char resName[VMAX_RECLEN]);
00260
00265 VEXTERNC void Vatom_getAtomName(
00266     Vatom *thee,
00267     char atomName[VMAX_RECLEN]
00268 );
00269
00275 VEXTERNC Vatom* Vatom_ctor();
00276
00283 VEXTERNC int Vatom_ctor2(Vatom *thee);
00284
00290 VEXTERNC void Vatom_dtor(Vatom **thee);

```

```

00291
00297 VEXTERNC void    Vatom_dtor2(Vatom *thee);
00298
00305 VEXTERNC void    Vatom_setPosition(Vatom *thee, double position[3]);
00306
00314 VEXTERNC void    Vatom_copyTo(Vatom *thee, Vatom *dest);
00315
00323 VEXTERNC void    Vatom_copyFrom(Vatom *thee, Vatom *src);
00324
00325 #if defined(WITH_TINKER)
00326
00333 VEXTERNC void    Vatom_setInducedDipole(Vatom *thee,
00334                                           double inducedDipole[3]);
00335
00342 VEXTERNC void    Vatom_setNLInducedDipole(Vatom *thee,
00343                                              double nlInducedDipole[3]);
00344
00351 VEXTERNC void    Vatom_setDipole(Vatom *thee, double dipole[3]);
00352
00359 VEXTERNC void    Vatom_setQuadrupole(Vatom *thee, double quadrupole[9]);
00360
00366 VEXTERNC double* Vatom_getDipole(Vatom *thee);
00367
00373 VEXTERNC double* Vatom_getQuadrupole(Vatom *thee);
00374
00380 VEXTERNC double* Vatom_getInducedDipole(Vatom *thee);
00381
00387 VEXTERNC double* Vatom_getNLInducedDipole(Vatom *thee);
00388 #endif /* if defined(WITH_TINKER) */
00389
00390 #endif /* ifndef _VATOM_H_ */

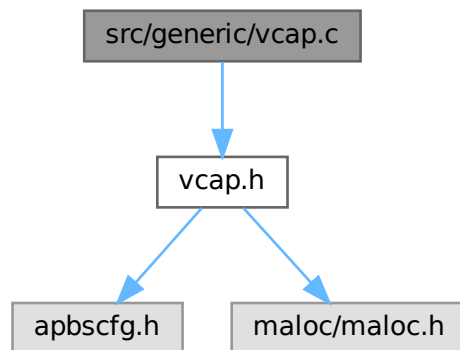
```

9.62 src/generic/vcap.c File Reference

Class Vcap methods.

```
#include "vcap.h"
```

Include dependency graph for vcap.c:



Functions

- VPUBLIC double [Vcap_exp](#) (double x, int *ichop)
Provide a capped exp() function.
- VPUBLIC double [Vcap_sinh](#) (double x, int *ichop)
Provide a capped sinh() function.

- VPUBLIC double [Vcap_cosh](#) (double x, int *ichop)

Provide a capped cosh() function.

9.62.1 Detailed Description

Class Vcap methods.

Author

Nathan Baker

Version

\$Id\$

Attention

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*
*
```

Definition in file [vcap.c](#).

9.63 vcap.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "vcap.h"
00058
00059 VPUBLIC double Vcap_exp(double x, int *ichop) {
00060
00061     /* The two chopped arguments */
00062     if (x > EXPMAX) {
00063         (*ichop) = 1;
00064         return VEXP(EXPMAX);
00065     } else if (x < EXPMIN) {
00066         (*ichop) = 1;
00067         return VEXP(EXPMIN);
00068     }
00069
00070     /* The normal EXP */
00071     (*ichop) = 0;
00072     return VEXP(x);
00073 }
00074
00075 VPUBLIC double Vcap_sinh(double x, int *ichop) {
00076
00077     /* The two chopped arguments */
00078     if (x > EXPMAX) {
00079         (*ichop) = 1;
00080         return VSINH(EXPMAX);
00081     } else if (x < EXPMIN) {
00082         (*ichop) = 1;
00083         return VSINH(EXPMIN);
00084     }
00085
00086     /* The normal SINH */
00087     (*ichop) = 0;
00088     return VSINH(x);
00089 }
00090
00091 VPUBLIC double Vcap_cosh(double x, int *ichop) {
00092
00093     /* The two chopped arguments */
00094     if (x > EXPMAX) {
00095         (*ichop) = 1;
00096         return VCOSH(EXPMAX);
00097     } else if (x < EXPMIN) {
00098         (*ichop) = 1;
00099         return VCOSH(EXPMIN);
00100     }
00101
00102     /* The normal COSH */
00103     (*ichop) = 0;
00104     return VCOSH(x);
00105 }

```

9.64 src/generic/vcap.h File Reference

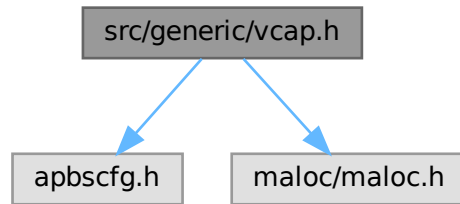
Contains declarations for class Vcap.

```

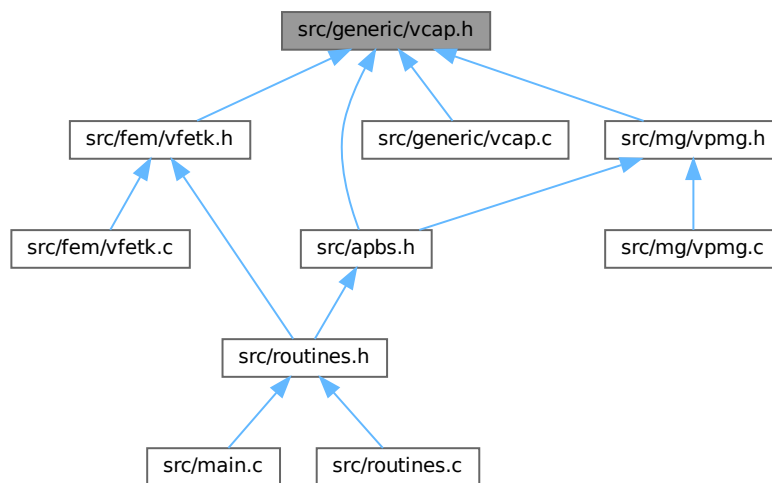
#include "apbscfg.h"
#include "malloc/malloc.h"

```

Include dependency graph for vcap.h:



This graph shows which files directly or indirectly include this file:



Macros

- #define **EXP_MAX** 85.00
Maximum argument for exp(), sinh(), or cosh()
- #define **EXP_MIN** -85.00
Minimum argument for exp(), sinh(), or cosh()

Functions

- VEXTERNC double **Vcap_exp** (double x, int *ichop)
Provide a capped exp() function.
- VEXTERNC double **Vcap_sinh** (double x, int *ichop)

Provide a capped sinh() function.

- VEXTERNC double [Vcap_cosh](#) (double x, int *ichop)

Provide a capped cosh() function.

9.64.1 Detailed Description

Contains declarations for class Vcap.

Version

\$Id\$

Author

Nathan A. Baker

Attention

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*
```

Definition in file [vcap.h](#).

9.65 vcap.h

[Go to the documentation of this file.](#)

```

00001
00064 #ifndef _VCAP_H_
00065 #define _VCAP_H_
00066
00067 #include "apbscfg.h"
00068
00072 #define EXPMAX 85.00
00073
00077 #define EXPMIN -85.00
00078
00079 #include "malloc/malloc.h"
00080
00099 VEXTERNC double Vcap_exp(
00100     double x,
00101     int *ichop
00102 );
00103
00104
00123 VEXTERNC double Vcap_sinh(
00124     double x,
00125     int *ichop
00126 );
00127
00146 VEXTERNC double Vcap_cosh(
00147     double x,
00148     int *ichop
00149 );
00150
00151 #endif /* ifndef _VCAP_H_ */

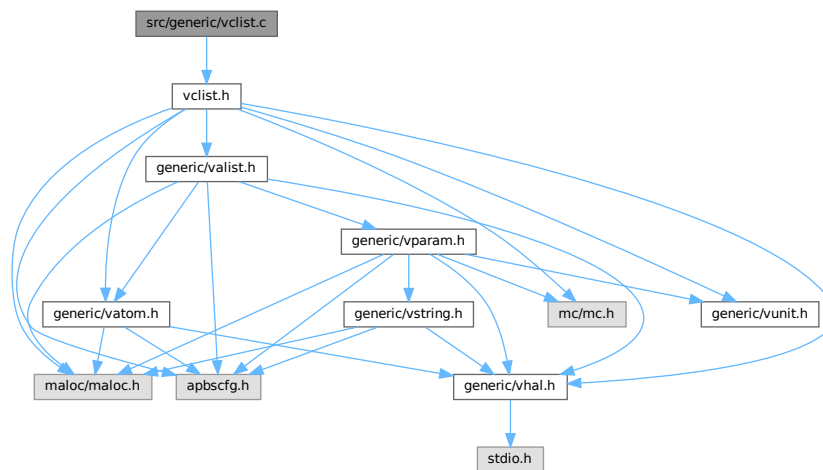
```

9.66 src/generic/vclist.c File Reference

Class Vclist methods.

```
#include "vclist.h"
```

Include dependency graph for vclist.c:



Macros

- `#define VCLIST_INFLATE 1.42`

Functions

- VPUBLIC unsigned long int `Vclist_memChk` (`Vclist *thee`)
Get number of bytes in this object and its members.
- VPUBLIC double `Vclist_maxRadius` (`Vclist *thee`)
Get the max probe radius value (in Å) the cell list was constructed with.
- VPUBLIC `Vclist *` `Vclist_ctor` (`Valist *alist`, double `max_radius`, int `npts[VAPBS_DIM]`, `Vclist_DomainMode` `mode`, double `lower_corner[VAPBS_DIM]`, double `upper_corner[VAPBS_DIM]`)
Construct the cell list object.
- VPRIVATE void `Vclist_getMolDims` (`Vclist *thee`, double `lower_corner[VAPBS_DIM]`, double `upper_↔corner[VAPBS_DIM]`, double `*r_max`)
- VPRIVATE `Vrc_Codes` `Vclist_setupGrid` (`Vclist *thee`)
- VPRIVATE `Vrc_Codes` `Vclist_storeParms` (`Vclist *thee`, `Valist *alist`, double `max_radius`, int `npts[VAPBS_DIM]`, `Vclist_DomainMode` `mode`, double `lower_corner[VAPBS_DIM]`, double `upper_corner[VAPBS_DIM]`)
- VPRIVATE void `Vclist_gridSpan` (`Vclist *thee`, `Vatom *atom`, int `imin[VAPBS_DIM]`, int `imax[VAPBS_DIM]`)
- VPRIVATE int `Vclist_arrayIndex` (`Vclist *thee`, int `i`, int `j`, int `k`)
- VPRIVATE `Vrc_Codes` `Vclist_assignAtoms` (`Vclist *thee`)
- VPUBLIC `Vrc_Codes` `Vclist_ctor2` (`Vclist *thee`, `Valist *alist`, double `max_radius`, int `npts[VAPBS_DIM]`, `Vclist_DomainMode` `mode`, double `lower_corner[VAPBS_DIM]`, double `upper_corner[VAPBS_DIM]`)
FORTTRAN stub to construct the cell list object.
- VPUBLIC void `Vclist_dtor` (`Vclist **thee`)
Destroy object.
- VPUBLIC void `Vclist_dtor2` (`Vclist *thee`)
FORTTRAN stub to destroy object.
- VPUBLIC `VclistCell *` `Vclist_getCell` (`Vclist *thee`, double `pos[VAPBS_DIM]`)
Return cell corresponding to specified position or return VNULL.
- VPUBLIC `VclistCell *` `VclistCell_ctor` (int `natoms`)
Allocate and construct a cell list cell object.
- VPUBLIC `Vrc_Codes` `VclistCell_ctor2` (`VclistCell *thee`, int `natoms`)
Construct a cell list object.
- VPUBLIC void `VclistCell_dtor` (`VclistCell **thee`)
Destroy object.
- VPUBLIC void `VclistCell_dtor2` (`VclistCell *thee`)
FORTTRAN stub to destroy object.

9.66.1 Detailed Description

Class Vclist methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```

*
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*
*

```

Definition in file [vclist.c](#).

9.66.2 Function Documentation

9.66.2.1 Vclist_arrayIndex()

```

VPRIVATE int Vclist_arrayIndex (
    Vclist * thee,
    int i,
    int j,
    int k )

```

Definition at line [262](#) of file [vclist.c](#).

9.66.2.2 Vclist_assignAtoms()

```
VPRIVATE Vrc_Codes Vclist_assignAtoms (
    Vclist * thee )
```

Definition at line 270 of file [vclist.c](#).

9.66.2.3 Vclist_getMolDims()

```
VPRIVATE void Vclist_getMolDims (
    Vclist * thee,
    double lower_corner[VAPBS_DIM],
    double upper_corner[VAPBS_DIM],
    double * r_max )
```

Definition at line 90 of file [vclist.c](#).

9.66.2.4 Vclist_gridSpan()

```
VPRIVATE void Vclist_gridSpan (
    Vclist * thee,
    Vatom * atom,
    int imin[VAPBS_DIM],
    int imax[VAPBS_DIM] )
```

Definition at line 231 of file [vclist.c](#).

9.66.2.5 Vclist_setupGrid()

```
VPRIVATE Vrc_Codes Vclist_setupGrid (
    Vclist * thee )
```

Definition at line 125 of file [vclist.c](#).

9.66.2.6 Vclist_storeParms()

```
VPRIVATE Vrc_Codes Vclist_storeParms (
    Vclist * thee,
    Valist * alist,
    double max_radius,
    int npts[VAPBS_DIM],
    Vclist_DomainMode mode,
    double lower_corner[VAPBS_DIM],
    double upper_corner[VAPBS_DIM] )
```

Definition at line 174 of file [vclist.c](#).

9.67 vclist.c

[Go to the documentation of this file.](#)

```
00001
00057 #include "vclist.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 #if !defined(VINLINE_VCLIST)
00062
00063 VPUBLIC unsigned long int Vclist_memChk(Vclist *thee) {
```

```

00064     if (thee == VNULL) return 0;
00065     return Vmem_bytes(thee->vmem);
00066 }
00067
00068 VPUBLIC double Vclist_maxRadius(Vclist *thee) {
00069     VASSERT(thee != VNULL);
00070     return thee->max_radius;
00071 }
00072
00073 #endif /* if !defined(VINLINE_VCLIST) */
00074
00075 VPUBLIC Vclist* Vclist_ctor(Valist *alist, double max_radius,
00076     int npts[VAPBS_DIM], Vclist_DomainMode mode,
00077     double lower_corner[VAPBS_DIM], double upper_corner[VAPBS_DIM]) {
00078
00079     Vclist *thee = VNULL;
00080
00081     /* Set up the structure */
00082     thee = (Vclist*)Vmem_malloc(VNULL, 1, sizeof(Vclist) );
00083     VASSERT( thee != VNULL);
00084     VASSERT( Vclist_ctor2(thee, alist, max_radius, npts, mode, lower_corner,
00085         upper_corner) == VRC_SUCCESS );
00086     return thee;
00087 }
00088
00089 /* Get the dimensions of the molecule stored in thee->alist */
00090 VPRIVATE void Vclist_getMolDims(
00091     Vclist *thee,
00092     double lower_corner[VAPBS_DIM], /* Set to lower corner of molecule */
00093     double upper_corner[VAPBS_DIM], /* Set to lower corner of molecule */
00094     double *r_max /* Set to max atom radius */
00095 ) {
00096
00097     int i, j;
00098     double pos;
00099     Valist *alist;
00100     Vatom *atom;
00101
00102     alist = thee->alist;
00103
00104     /* Initialize */
00105     for (i=0; i<VAPBS_DIM; i++) {
00106         lower_corner[i] = VLARGE;
00107         upper_corner[i] = -VLARGE;
00108     }
00109     *r_max = -1.0;
00110
00111     /* Check each atom */
00112     for (i=0; i<Valist_getNumberAtoms(alist); i++) {
00113         atom = Valist_getAtom(alist, i);
00114         for (j=0; j<VAPBS_DIM; j++) {
00115             pos = (Vatom_getPosition(atom))[j];
00116             if ( pos < lower_corner[j] ) lower_corner[j] = pos;
00117             if ( pos > upper_corner[j] ) upper_corner[j] = pos;
00118         }
00119         if (Vatom_getRadius(atom) > *r_max) *r_max = Vatom_getRadius(atom);
00120     }
00121
00122 }
00123
00124 /* Setup lookup grid */
00125 VPRIVATE Vrc_Codes Vclist_setupGrid(Vclist *thee) {
00126
00127     /* Inflation factor ~ sqrt(2)*/
00128     #define VCLIST_INFLATE 1.42
00129
00130     int i;
00131     double length[VAPBS_DIM], r_max;
00132
00133     /* Set up the grid corners */
00134     switch (thee->mode) {
00135     case CLIST_AUTO_DOMAIN:
00136         /* Get molecule dimensions */
00137         Vclist_getMolDims(thee, thee->lower_corner, thee->upper_corner,
00138             &r_max);
00139         /* Set up grid spacings */
00140         for (i=0; i<VAPBS_DIM; i++) {
00141             thee->upper_corner[i] = thee->upper_corner[i]
00142                 + VCLIST_INFLATE*(r_max+thee->max_radius);
00143             thee->lower_corner[i] = thee->lower_corner[i]
00144                 - VCLIST_INFLATE*(r_max+thee->max_radius);

```



```

00145         }
00146         break;
00147     case CLIST_MANUAL_DOMAIN:
00148         /* Grid corners established in constructor */
00149         break;
00150     default:
00151         Vnm_print(2, "Vclist_setupGrid: invalid setup mode (%d)!\n",
00152                 thee->mode);
00153         return VRC_FAILURE;
00154     }
00155
00156     /* Set up the grid lengths and spacings */
00157     for (i=0; i<VAPBS_DIM; i++) {
00158         length[i] = thee->upper_corner[i] - thee->lower_corner[i];
00159         thee->spacs[i] = length[i]/((double)(thee->npts[i] - 1));
00160     }
00161     Vnm_print(0, "Vclist_setupGrid: Grid lengths = (%g, %g, %g)\n",
00162             length[0], length[1], length[2]);
00163
00164     Vnm_print(0, "Vclist_setupGrid: Grid lower corner = (%g, %g, %g)\n",
00165             (thee->lower_corner)[0], (thee->lower_corner)[1],
00166             (thee->lower_corner)[2]);
00167
00168     return VRC_SUCCESS;
00169
00170     #undef VCLIST_INFLATE
00171 }
00172
00173 /* Check and store parameters passed to constructor */
00174 VPRIVATE Vrc_Codes Vclist_storeParms(Vclist *thee, Valist *alist,
00175         double max_radius, int npts[VAPBS_DIM], Vclist_DomainMode mode,
00176         double lower_corner[VAPBS_DIM], double upper_corner[VAPBS_DIM] ) {
00177
00178     int i = 0;
00179
00180     if (alist == VNULL) {
00181         Vnm_print(2, "Vclist_ctor2: Got NULL Valist!\n");
00182         return VRC_FAILURE;
00183     } else thee->alist = alist;
00184
00185     thee->n = 1;
00186     for (i=0; i<VAPBS_DIM; i++) {
00187         if (npts[i] < 3) {
00188             Vnm_print(2,
00189                     "Vclist_ctor2: n[%d] (%d) must be greater than 2!\n",
00190                     i, npts[i]);
00191             return VRC_FAILURE;
00192         }
00193         thee->npts[i] = npts[i];
00194         thee->n *= npts[i];
00195     }
00196     Vnm_print(0, "Vclist_ctor2: Using %d x %d x %d hash table\n",
00197             npts[0], npts[1], npts[2]);
00198
00199     thee->mode = mode;
00200     switch (thee->mode) {
00201     case CLIST_AUTO_DOMAIN:
00202         Vnm_print(0, "Vclist_ctor2: automatic domain setup.\n");
00203         break;
00204     case CLIST_MANUAL_DOMAIN:
00205         Vnm_print(0, "Vclist_ctor2: manual domain setup.\n");
00206         Vnm_print(0, "Vclist_ctor2: lower corner = [ \n");
00207         for (i=0; i<VAPBS_DIM; i++) {
00208             thee->lower_corner[i] = lower_corner[i];
00209             Vnm_print(0, "%g ", lower_corner[i]);
00210         }
00211         Vnm_print(0, "]\n");
00212         Vnm_print(0, "Vclist_ctor2: upper corner = [ \n");
00213         for (i=0; i<VAPBS_DIM; i++) {
00214             thee->upper_corner[i] = upper_corner[i];
00215             Vnm_print(0, "%g ", upper_corner[i]);
00216         }
00217         Vnm_print(0, "]\n");
00218         break;
00219     default:
00220         Vnm_print(2, "Vclist_ctor2: invalid setup mode (%d)!\n", mode);
00221         return VRC_FAILURE;
00222     }
00223
00224     thee->max_radius = max_radius;
00225     Vnm_print(0, "Vclist_ctor2: Using %g max radius\n", max_radius);

```

```

00226
00227     return VRC_SUCCESS;
00228 }
00229
00230 /* Calculate the gridpoints an atom spans */
00231 VPRIVATE void Vclist_gridSpan(Vclist *thee,
00232     Vatom *atom, /* Atom */
00233     int imin[VAPBS_DIM], /* Set to min grid indices */
00234     int imax[VAPBS_DIM] /* Set to max grid indices */
00235 ) {
00236
00237     int i;
00238     double *coord, dc, idc, rtot;
00239
00240     /* Get the position in the grid's frame of reference */
00241     coord = Vatom_getPosition(atom);
00242
00243     /* Get the range the atom radius + probe radius spans */
00244     rtot = Vatom_getRadius(atom) + thee->max_radius;
00245
00246     /* Calculate the range of grid points the inflated atom spans in the x
00247     * direction. */
00248     for (i=0; i<VAPBS_DIM; i++) {
00249         dc = coord[i] - (thee->lower_corner)[i];
00250         idc = (dc + rtot)/(thee->spacs[i]);
00251         imax[i] = (int)(ceil(idc));
00252         imax[i] = VMIN2(imax[i], thee->npts[i]-1);
00253         idc = (dc - rtot)/(thee->spacs[i]);
00254         imin[i] = (int)(floor(idc));
00255         imin[i] = VMAX2(imin[i], 0);
00256     }
00257 }
00258
00259 /* Get the array index for a particular cell based on its i,j,k
00260 * coordinates */
00261 VPRIVATE int Vclist_arrayIndex(Vclist *thee, int i, int j, int k) {
00262
00263     return (thee->npts[2])*(thee->npts[1])*i + (thee->npts[2])*j + k;
00264 }
00265
00266 /* Assign atoms to cells */
00267 VPRIVATE Vrc_Codes Vclist_assignAtoms(Vclist *thee) {
00268
00269     int iatom, i, j, k, ui, inext;
00270     int imax[VAPBS_DIM], imin[VAPBS_DIM];
00271     int totatoms;
00272     Vatom *atom;
00273     VclistCell *cell;
00274
00275     /* Find out how many atoms are associated with each grid point */
00276     totatoms = 0;
00277     for (iatom=0; iatom<Valist_getNumberAtoms(thee->alist); iatom++) {
00278
00279         /* Get grid span for atom */
00280         atom = Valist_getAtom(thee->alist, iatom);
00281         Vclist_gridSpan(thee, atom, imin, imax);
00282
00283         /* Now find and assign the grid points */
00284         VASSERT(VAPBS_DIM == 3);
00285         for (i = imin[0]; i <= imax[0]; i++) {
00286             for (j = imin[1]; j <= imax[1]; j++) {
00287                 for (k = imin[2]; k <= imax[2]; k++) {
00288                     /* Get index to array */
00289                     ui = Vclist_arrayIndex(thee, i, j, k);
00290                     /* Increment number of atoms for this grid point */
00291                     cell = &(thee->cells[ui]);
00292                     (cell->natoms)++;
00293                     totatoms++;
00294                 }
00295             }
00296         }
00297     }
00298
00299     Vnm_print(0, "Vclist_assignAtoms: Have %d atom entries\n", totatoms);
00300
00301     /* Allocate the space to store the pointers to the atoms */
00302     for (ui=0; ui<thee->n; ui++) {
00303         cell = &(thee->cells[ui]);
00304     }

```

```

00307         if ( VclistCell_ctor2(cell, cell->natoms) == VRC_FAILURE ) {
00308             Vnm_print(2, "Vclist_assignAtoms: cell error!\n");
00309             return VRC_FAILURE;
00310         }
00311         /* Clear the counter for later use */
00312         cell->natoms = 0;
00313     }
00314
00315     /* Assign the atoms to grid points */
00316     for (iatom=0; iatom<Valist_getNumberAtoms(thee->alist); iatom++) {
00317
00318         /* Get grid span for atom */
00319         atom = Valist_getAtom(thee->alist, iatom);
00320         Vclist_gridSpan(thee, atom, imin, imax);
00321
00322         /* Now find and assign the grid points */
00323         for (i = imin[0]; i <= imax[0]; i++) {
00324             for (j = imin[1]; j <= imax[1]; j++) {
00325                 for (k = imin[2]; k <= imax[2]; k++) {
00326                     /* Get index to array */
00327                     ui = Vclist_arrayIndex(thee, i, j, k);
00328                     cell = &(thee->cells[ui]);
00329                     /* Index of next available array location */
00330                     inext = cell->natoms;
00331                     cell->atoms[inext] = atom;
00332                     /* Increment number of atoms */
00333                     (cell->natoms)++;
00334                 }
00335             }
00336         }
00337     }
00338     return VRC_SUCCESS;
00339 }
00340
00341
00342 /* Main (FORTRAN stub) constructor */
00343 VPUBLIC Vrc_Codes Vclist_ctor2(Vclist *thee, Valist *alist, double max_radius,
00344     int npts[VAPBS_DIM], Vclist_DomainMode mode,
00345     double lower_corner[VAPBS_DIM], double upper_corner[VAPBS_DIM]) {
00346
00347     int i;
00348     VclistCell *cell;
00349
00350     /* Check and store parameters */
00351     if ( Vclist_storeParms(thee, alist, max_radius, npts, mode, lower_corner,
00352         upper_corner) == VRC_FAILURE ) {
00353         Vnm_print(2, "Vclist_ctor2: parameter check failed!\n");
00354         return VRC_FAILURE;
00355     }
00356
00357     /* Set up memory */
00358     thee->vmem = Vmem_ctor("APBS::VCLIST");
00359     if (thee->vmem == VNULL) {
00360         Vnm_print(2, "Vclist_ctor2: memory object setup failed!\n");
00361         return VRC_FAILURE;
00362     }
00363
00364     /* Set up cells */
00365     thee->cells = (VclistCell*)Vmem_malloc( thee->vmem, thee->n, sizeof(VclistCell) );
00366     if (thee->cells == VNULL) {
00367         Vnm_print(2,
00368             "Vclist_ctor2: Failed allocating %d VclistCell objects!\n",
00369             thee->n);
00370         return VRC_FAILURE;
00371     }
00372     for (i=0; i<thee->n; i++) {
00373         cell = &(thee->cells[i]);
00374         cell->natoms = 0;
00375     }
00376
00377     /* Set up the grid */
00378     if ( Vclist_setupGrid(thee) == VRC_FAILURE ) {
00379         Vnm_print(2, "Vclist_ctor2: grid setup failed!\n");
00380         return VRC_FAILURE;
00381     }
00382
00383     /* Assign atoms to grid cells */
00384     if (Vclist_assignAtoms(thee) == VRC_FAILURE) {
00385         Vnm_print(2, "Vclist_ctor2: atom assignment failed!\n");
00386         return VRC_FAILURE;
00387     }

```

```

00388
00389
00390
00391
00392
00393     return VRC_SUCCESS;
00394 }
00395
00396 /* Destructor */
00397 VPUBLIC void Vclist_dtor(Vclist **thee) {
00398
00399     if ((*thee) != VNULL) {
00400         Vclist_dtor2(*thee);
00401         Vmem_free(VNULL, 1, sizeof(Vclist), (void **)thee);
00402         (*thee) = VNULL;
00403     }
00404
00405 }
00406
00407 /* Main (stub) destructor */
00408 VPUBLIC void Vclist_dtor2(Vclist *thee) {
00409
00410     VclistCell *cell;
00411     int i;
00412
00413     for (i=0; i<thee->n; i++) {
00414         cell = &(thee->cells[i]);
00415         VclistCell_dtor2(cell);
00416     }
00417     Vmem_free(thee->vmem, thee->n, sizeof(VclistCell),
00418               (void **)&(thee->cells));
00419     Vmem_dtor(&(thee->vmem));
00420
00421 }
00422
00423 VPUBLIC VclistCell* Vclist_getCell(Vclist *thee,
00424                                   double pos[VAPBS_DIM]
00425                                   ) {
00426
00427     int i,
00428         ic[VAPBS_DIM],
00429         ui;
00430     double c[VAPBS_DIM];
00431
00432     /* Assert this before we do anything else, since its failure should fail the function */
00433     VASSERT(VAPBS_DIM == 3);
00434
00435     /* Convert to grid based coordinates */
00436     for (i=0; i<VAPBS_DIM; i++) {
00437         c[i] = pos[i] - (thee->lower_corner)[i];
00438         ic[i] = (int)(c[i]/thee->spacs[i]);
00439
00440         if (ic[i] < 0 || ic[i] >= thee->npts[i]) {
00441             return VNULL;
00442         }
00443     }
00444
00445     /* Get the array index */
00446     ui = Vclist_arrayIndex(thee, ic[0], ic[1], ic[2]);
00447
00448     return &(thee->cells[ui]);
00449
00450 }
00451
00452 VPUBLIC VclistCell* VclistCell_ctor(int natoms) {
00453
00454     VclistCell *thee = VNULL;
00455
00456     /* Set up the structure */
00457     thee = (VclistCell*)Vmem_malloc(VNULL, 1, sizeof(VclistCell));
00458     VASSERT(thee != VNULL);
00459     VASSERT(VclistCell_ctor2(thee, natoms) == VRC_SUCCESS);
00460
00461     return thee;
00462 }
00463
00464 VPUBLIC Vrc_Codes VclistCell_ctor2(VclistCell *thee, int natoms) {
00465
00466     if (thee == VNULL) {
00467         Vnm_print(2, "VclistCell_ctor2: NULL thee!\n");
00468         return VRC_FAILURE;

```

```

00469     }
00470
00471     thee->natoms = natoms;
00472     if (thee->natoms > 0) {
00473         thee->atoms = (Vatom**)Vmem_malloc(VNULL, natoms, sizeof(Vatom *));
00474         if (thee->atoms == VNULL) {
00475             Vnm_print(2,
00476                 "VclistCell_ctor2: unable to allocate space for %d atom pointers!\n",
00477                 natoms);
00478             return VRC_FAILURE;
00479         }
00480     }
00481
00482     return VRC_SUCCESS;
00483 }
00484
00485
00486 VPUBLIC void VclistCell_dtor(VclistCell **thee) {
00487
00488     if ((*thee) != VNULL) {
00489         VclistCell_dtor2(*thee);
00490         Vmem_free(VNULL, 1, sizeof(VclistCell), (void **)thee);
00491         (*thee) = VNULL;
00492     }
00493 }
00494
00495
00496 /* Main (stub) destructor */
00497 VPUBLIC void VclistCell_dtor2(VclistCell *thee) {
00498
00499     if (thee->natoms > 0) {
00500         Vmem_free(VNULL, thee->natoms, sizeof(Vatom *),
00501             (void **)&(thee->atoms));
00502     }
00503 }
00504 }

```

9.68 src/generic/vclist.h File Reference

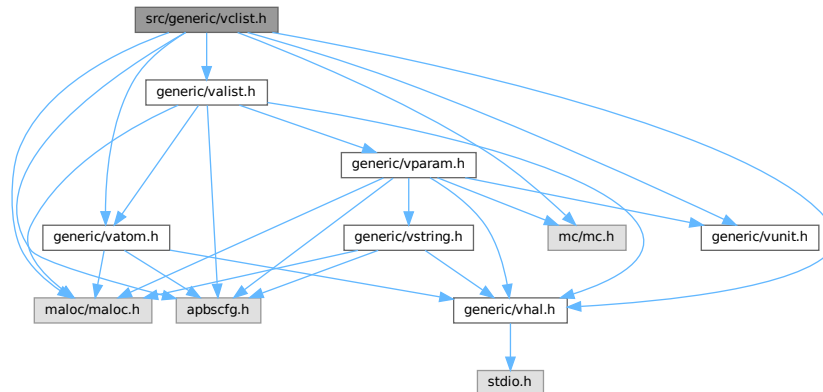
Contains declarations for class Vclist.

```

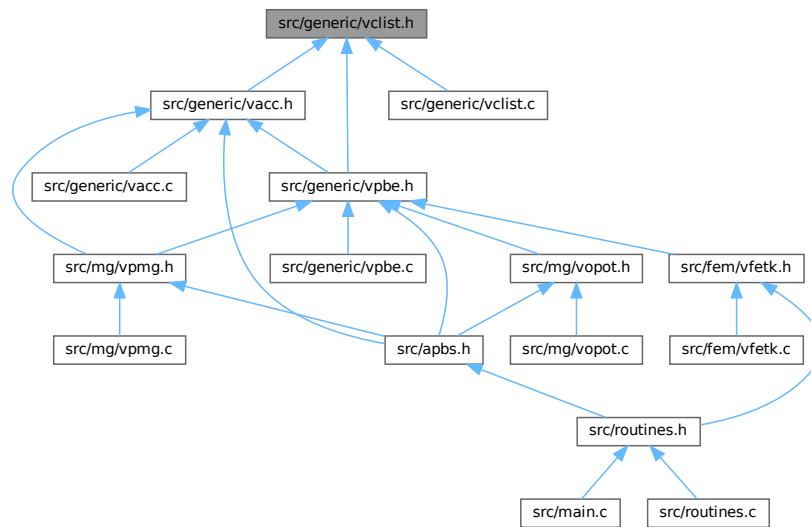
#include "apbscfg.h"
#include "maloc/maloc.h"
#include "mc/mc.h"
#include "generic/vhal.h"
#include "generic/valist.h"
#include "generic/vatom.h"
#include "generic/vunit.h"

```

Include dependency graph for vclist.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVclistCell](#)
Atom cell list cell.
- struct [sVclist](#)
Atom cell list.

Typedefs

- typedef enum [eVclist_DomainMode](#) [Vclist_DomainMode](#)
Declaration of Vclist_DomainMode enumeration type.
- typedef struct [sVclistCell](#) [VclistCell](#)
Declaration of the VclistCell class as the VclistCell structure.
- typedef struct [sVclist](#) [Vclist](#)
Declaration of the Vclist class as the Vclist structure.

Enumerations

- enum [eVclist_DomainMode](#) { [CLIST_AUTO_DOMAIN](#) , [CLIST_MANUAL_DOMAIN](#) }
Atom cell list domain setup mode.

Functions

- VEXTERNC unsigned long int [Vclist_memChk](#) ([Vclist](#) *thee)
Get number of bytes in this object and its members.
- VEXTERNC double [Vclist_maxRadius](#) ([Vclist](#) *thee)
Get the max probe radius value (in A) the cell list was constructed with.

- VEXTERNC `Vclist * Vclist_ctor (Valist *alist, double max_radius, int npts[VAPBS_DIM], Vclist_DomainMode mode, double lower_corner[VAPBS_DIM], double upper_corner[VAPBS_DIM])`
Construct the cell list object.
- VEXTERNC `Vrc_Codes Vclist_ctor2 (Vclist *thee, Valist *alist, double max_radius, int npts[VAPBS_DIM], Vclist_DomainMode mode, double lower_corner[VAPBS_DIM], double upper_corner[VAPBS_DIM])`
FORTTRAN stub to construct the cell list object.
- VEXTERNC `void Vclist_dtor (Vclist **thee)`
Destroy object.
- VEXTERNC `void Vclist_dtor2 (Vclist *thee)`
FORTTRAN stub to destroy object.
- VEXTERNC `VclistCell * Vclist_getCell (Vclist *thee, double position[VAPBS_DIM])`
Return cell corresponding to specified position or return VNULL.
- VEXTERNC `VclistCell * VclistCell_ctor (int natoms)`
Allocate and construct a cell list cell object.
- VEXTERNC `Vrc_Codes VclistCell_ctor2 (VclistCell *thee, int natoms)`
Construct a cell list object.
- VEXTERNC `void VclistCell_dtor (VclistCell **thee)`
Destroy object.
- VEXTERNC `void VclistCell_dtor2 (VclistCell *thee)`
FORTTRAN stub to destroy object.

9.68.1 Detailed Description

Contains declarations for class Vclist.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```
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* APBS -- Adaptive Poisson-Boltzmann Solver
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* Pacific Northwest National Laboratory
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*
*

```

Definition in file [vclist.h](#).

9.69 vclist.h

[Go to the documentation of this file.](#)

```

00001
00062 #ifndef _VCLIST_H_
00063 #define _VCLIST_H_
00064
00065 #include "apbscfg.h"
00066
00067 #include "malloc/malloc.h"
00068 #if defined(HAVE_MC_H)
00069 #include "mc/mc.h"
00070 #endif
00071
00072 #include "generic/vhal.h"
00073 #include "generic/valist.h"
00074 #include "generic/vatom.h"
00075 #include "generic/vunit.h"
00076
00082 enum eVclist_DomainMode {
00083     CLIST_AUTO_DOMAIN,
00085     CLIST_MANUAL_DOMAIN
00087 };
00088
00094 typedef enum eVclist_DomainMode Vclist_DomainMode;
00095
00101 struct sVclistCell {
00102     Vatom **atoms;
00103     int natoms;
00104 };
00105
00110 typedef struct sVclistCell VclistCell;
00111
00117 struct sVclist {
00118
00119     Vmem *vmem;
00120     Valist *alist;
00121     Vclist_DomainMode mode;
00122     int npts[VAPBS_DIM];
00123     int n;
00124     double max_radius;
00125     VclistCell *cells;
00126     double lower_corner[VAPBS_DIM];
00127     double upper_corner[VAPBS_DIM];
00128     double spacs[VAPBS_DIM];
00130 };
00131

```



```

00136 typedef struct sVclist Vclist;
00137
00138 #if !defined(VINLINE_VCLIST)
00139
00145     VEXTERNC unsigned long int Vclist_memChk(
00146         Vclist *thee
00147     );
00148
00156     VEXTERNC double Vclist_maxRadius(
00157         Vclist *thee
00158     );
00159
00160 #else /* if defined(VINLINE_VCLIST) */
00161
00162 #   define Vclist_memChk(thee) (Vmem_bytes((thee)->vmem))
00163 #   define Vclist_maxRadius(thee) ((thee)->max_radius)
00164
00165 #endif /* if !defined(VINLINE_VCLIST) */
00166
00167 /* ////////////////////////////////////// */
00168 // Class Vclist: Non-Inlineable methods (vclist.c)
00169
00170
00175 VEXTERNC Vclist* Vclist_ctor(
00176     Valist *alist, /**< Molecule for cell list queries */
00177     double max_radius,
00178     int npts[VAPBS_DIM],
00180     Vclist_DomainMode mode,
00181     double lower_corner[VAPBS_DIM],
00184     double upper_corner[VAPBS_DIM]
00187 );
00188
00193 VEXTERNC Vrc_Codes Vclist_ctor2(
00194     Vclist *thee,
00195     Valist *alist,
00196     double max_radius,
00197     int npts[VAPBS_DIM],
00199     Vclist_DomainMode mode,
00200     double lower_corner[VAPBS_DIM],
00203     double upper_corner[VAPBS_DIM]
00206 );
00207
00212 VEXTERNC void Vclist_dtor(
00213     Vclist **thee
00214 );
00215
00220 VEXTERNC void Vclist_dtor2(
00221     Vclist *thee
00222 );
00223
00231 VEXTERNC VclistCell* Vclist_getCell(
00232     Vclist *thee,
00233     double position[VAPBS_DIM]
00234 );
00235
00242 VEXTERNC VclistCell* VclistCell_ctor(
00243     int natoms
00244 );
00245
00252 VEXTERNC Vrc_Codes VclistCell_ctor2(
00253     VclistCell *thee,
00254     int natoms
00255 );
00256
00261 VEXTERNC void VclistCell_dtor(
00262     VclistCell **thee
00263 );
00264
00269 VEXTERNC void VclistCell_dtor2(
00270     VclistCell *thee
00271 );
00272
00273 #endif /* ifndef _VCLIST_H_ */

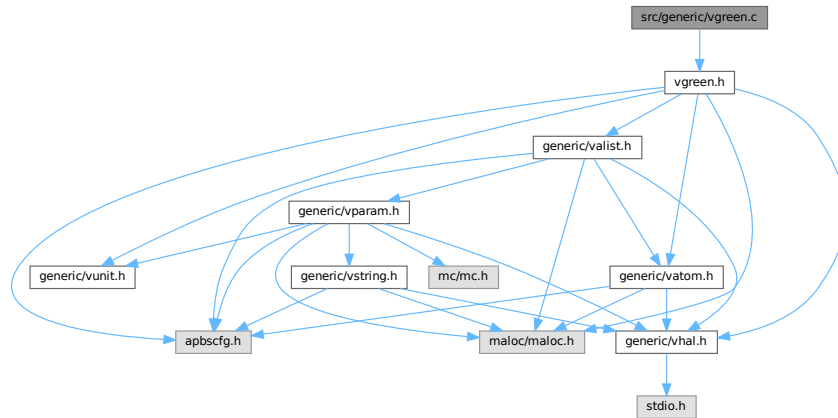
```

9.70 src/generic/vgreen.c File Reference

Class Vgreen methods.

```
#include "vgreen.h"
```

Include dependency graph for vgreen.c:



Functions

- VPRIVATE int [treesetup](#) ([Vgreen](#) *thee)
- VPRIVATE int [treecleanup](#) ([Vgreen](#) *thee)
- VPRIVATE int [treecalc](#) ([Vgreen](#) *thee, double *xtar, double *ytar, double *ztar, double *qtar, int numtars, double *tpengtar, double *x, double *y, double *z, double *q, int numpars, double *fx, double *fy, double *fz, int iflag, int farrdim, int arrdim)
- VPUBLIC [Valist](#) * [Vgreen_getValist](#) ([Vgreen](#) *thee)

Get the atom list associated with this Green's function object.
- VPUBLIC unsigned long int [Vgreen_memChk](#) ([Vgreen](#) *thee)

Return the memory used by this structure (and its contents) in bytes.
- VPUBLIC [Vgreen](#) * [Vgreen_ctor](#) ([Valist](#) *alist)

Construct the Green's function oracle.
- VPUBLIC int [Vgreen_ctor2](#) ([Vgreen](#) *thee, [Valist](#) *alist)

FORTTRAN stub to construct the Green's function oracle.
- VPUBLIC void [Vgreen_dtor](#) ([Vgreen](#) **thee)

Destruct the Green's function oracle.
- VPUBLIC void [Vgreen_dtor2](#) ([Vgreen](#) *thee)

FORTTRAN stub to destruct the Green's function oracle.
- VPUBLIC int [Vgreen_helmholtz](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *val, double kappa)

Get the Green's function for Helmholtz's equation integrated over the atomic point charges.
- VPUBLIC int [Vgreen_helmholtzD](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *gradx, double *grady, double *gradz, double kappa)

Get the gradient of Green's function for Helmholtz's equation integrated over the atomic point charges.
- VPUBLIC int [Vgreen_coulomb_direct](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *val)

Get the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation.
- VPUBLIC int [Vgreen_coulomb](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *val)

Get the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation or H. E. Johnston, R. Krasny FMM library (if available)

- `VPUBLIC int Vgreen_coulombD_direct (Vgreen *thee, int npos, double *x, double *y, double *z, double *pot, double *gradx, double *grady, double *gradz)`

Get gradient of the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation.

- `VPUBLIC int Vgreen_coulombD (Vgreen *thee, int npos, double *x, double *y, double *z, double *pot, double *gradx, double *grady, double *gradz)`

Get gradient of the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using either direct summation or H. E. Johnston/R. Krasny FMM library (if available)

9.70.1 Detailed Description

Class Vgreen methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
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* Pacific Northwest National Laboratory
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*
*
```

Definition in file [vgreen.c](#).

9.70.2 Function Documentation

9.70.2.1 treecalcul()

```
VPRIVATE int treecalcul (
    Vgreen * thee,
    double * xtar,
    double * ytar,
    double * ztar,
    double * qtar,
    int numtars,
    double * tpengtar,
    double * x,
    double * y,
    double * z,
    double * q,
    int numpars,
    double * fx,
    double * fy,
    double * fz,
    int iflag,
    int farrrdim,
    int arrdim )
```

Definition at line 525 of file [vgreen.c](#).

9.70.2.2 treecleanup()

```
VPRIVATE int treecleanup (
    Vgreen * thee )
```

Definition at line 505 of file [vgreen.c](#).

9.70.2.3 treesetup()

```
VPRIVATE int treesetup (
    Vgreen * thee )
```

Definition at line 425 of file [vgreen.c](#).

9.71 vgreen.c

[Go to the documentation of this file.](#)

00001

```

00057 #include "vgreen.h"
00058
00059 /* Define wrappers for F77 treecode routines */
00060 #ifdef HAVE_TREE
00061 # define F77TREEPEFORCE VF77_MANGLE(treepeforce, TREEPEFORCE)
00062 # define F77DIRECT_ENG_FORCE VF77_MANGLE(direct_eng_force, DIRECT_ENG_FORCE)
00063 # define F77CLEANUP VF77_MANGLE(mycleanup, MYCLEANUP)
00064 # define F77TREE_COMPP VF77_MANGLE(mytree_compp, MYTREE_COMP)
00065 # define F77TREE_COMPP VF77_MANGLE(mytree_compp, MYTREE_COMPP)
00066 # define F77CREATE_TREE VF77_MANGLE(mycreate_tree, MYCREATE_TREE)
00067 # define F77INITLEVELS VF77_MANGLE(myinitlevels, MYINITLEVELS)
00068 # define F77SETUP VF77_MANGLE(mysetup, MYSETUP)
00069 #endif /* ifdef HAVE_TREE */
00070
00071 /* Some constants associated with the tree code */
00072 #ifdef HAVE_TREE
00073 # define FMM_DIST_TOL VSMALL
00074 # define FMM_IFLAG 2
00075 # define FMM_ORDER 4
00076 # define FMM_THETA 0.5
00077 # define FMM_MAXPARNODE 150
00078 # define FMM_SHRINK 1
00079 # define FMM_MINLEVEL 50000
00080 # define FMM_MAXLEVEL 0
00081 #endif /* ifdef HAVE_TREE */
00082
00083 /*
00084  * @brief Setup treecode internal structures
00085  * @ingroup Vgreen
00086  * @author Nathan Baker
00087  * @param thee Vgreen object
00088  * @return 1 if successful, 0 otherwise
00089  */
00090 VPRIVATE int treesetup(Vgreen *thee);
00091
00092 /*
00093  * @brief Clean up treecode internal structures
00094  * @ingroup Vgreen
00095  * @author Nathan Baker
00096  * @param thee Vgreen object
00097  * @return 1 if successful, 0 otherwise
00098  */
00099 VPRIVATE int treecleanup(Vgreen *thee);
00100
00101 /*
00102  * @brief Calculate forces or potential
00103  * @ingroup Vgreen
00104  * @author Nathan Baker
00105  * @param thee Vgreen object
00106  * @return 1 if successful, 0 otherwise
00107  */
00108 VPRIVATE int treecalc(Vgreen *thee, double *xtar, double *ytar, double *ztar,
00109                      double *qtar, int numtars, double *tpengtar, double *x, double *y,
00110                      double *z, double *q, int numpars, double *fx, double *fy, double *fz,
00111                      int iflag, int farrdim, int arrdim);
00112
00113 #if !defined(VINLINE_VGREEN)
00114
00115 VPUBLIC Valist* Vgreen_getValist(Vgreen *thee) {
00116     VASSERT(thee != VNULL);
00117     return thee->alist;
00118 }
00119
00120 VPUBLIC unsigned long int Vgreen_memChk(Vgreen *thee) {
00121     if (thee == VNULL) return 0;
00122     return Vmem_bytes(thee->vmem);
00123 }
00124
00125 #endif /* if !defined(VINLINE_VGREEN) */
00126
00127 VPUBLIC Vgreen* Vgreen_ctor(Valist *alist) {
00128     /* Set up the structure */
00129     Vgreen *thee = VNULL;
00130     thee = (Vgreen *)Vmem_malloc(VNULL, 1, sizeof(Vgreen));
00131     VASSERT(thee != VNULL);
00132     VASSERT(Vgreen_ctor2(thee, alist));
00133 }

```

```

00164     return thee;
00165 }
00166
00167 VPUBLIC int Vgreen_ctor2(Vgreen *thee, Valist *alist) {
00168     VASSERT( thee != VNULL );
00169
00170     /* Memory management object */
00171     thee->vmem = Vmem_ctor("APBS:VGREEN");
00172
00173     /* Set up the atom list and grid manager */
00174     if (alist == VNULL) {
00175         Vnm_print(2, "Vgreen_ctor2: got null pointer to Valist object!\n");
00176     }
00177
00178     thee->alist = alist;
00179
00180     /* Setup FMM tree (if applicable) */
00181 #ifdef HAVE_TREE
00182     if (!treesetup(thee)) {
00183         Vnm_print(2, "Vgreen_ctor2: Error setting up FMM tree!\n");
00184         return 0;
00185     }
00186 #endif /* ifdef HAVE_TREE */
00187
00188     return 1;
00189 }
00190
00191
00192 VPUBLIC void Vgreen_dtor(Vgreen **thee) {
00193     if ((*thee) != VNULL) {
00194         Vgreen_dtor2(*thee);
00195         Vmem_free(VNULL, 1, sizeof(Vgreen), (void **)thee);
00196         (*thee) = VNULL;
00197     }
00198 }
00199
00200 VPUBLIC void Vgreen_dtor2(Vgreen *thee) {
00201
00202 #ifdef HAVE_TREE
00203     treecleanup(thee);
00204 #endif
00205     Vmem_dtor(&(thee->vmem));
00206 }
00207
00208
00209 VPUBLIC int Vgreen_helmholtz(Vgreen *thee, int npos, double *x, double *y,
00210     double *z, double *val, double kappa) {
00211
00212     Vnm_print(2, "Error -- Vgreen_helmholtz not implemented yet!\n");
00213     return 0;
00214 }
00215
00216 VPUBLIC int Vgreen_helmholtzD(Vgreen *thee, int npos, double *x, double *y,
00217     double *z, double *gradx, double *grady, double *gradz, double kappa) {
00218
00219     Vnm_print(2, "Error -- Vgreen_helmholtzD not implemented yet!\n");
00220     return 0;
00221 }
00222
00223
00224 VPUBLIC int Vgreen_coulomb_direct(Vgreen *thee, int npos, double *x,
00225     double *y, double *z, double *val) {
00226
00227     Vatom *atom;
00228     double *apos, charge, dist, dx, dy, dz, scale;
00229     double *q, qtemp, fx, fy, fz;
00230     int iatom, ipos;
00231
00232     if (thee == VNULL) {
00233         Vnm_print(2, "Vgreen_coulomb: Got NULL thee!\n");
00234         return 0;
00235     }
00236
00237     for (ipos=0; ipos<npos; ipos++) val[ipos] = 0.0;
00238
00239     for (iatom=0; iatom<Valist_getNumberAtoms(thee->alist); iatom++) {
00240         atom = Valist_getAtom(thee->alist, iatom);
00241         apos = Vatom_getPosition(atom);
00242         charge = Vatom_getCharge(atom);
00243         for (ipos=0; ipos<npos; ipos++) {
00244             dx = apos[0] - x[ipos];

```

```

00245         dy = apos[1] - y[ipos];
00246         dz = apos[2] - z[ipos];
00247         dist = VSQRT(VSQR(dx) + VSQR(dy) + VSQR(dz));
00248         if (dist > VSMALL) val[ipos] += (charge/dist);
00249     }
00250 }
00251
00252 scale = Vunit_ec/(4*Vunit_pi*Vunit_eps0*1.0e-10);
00253 for (ipos=0; ipos<npos; ipos++) val[ipos] = val[ipos]*scale;
00254
00255 return 1;
00256 }
00257
00258 VPUBLIC int Vgreen_coulomb(Vgreen *thee, int npos, double *x, double *y,
00259     double *z, double *val) {
00260     Vatom *atom;
00261     double *apos, charge, dist, dx, dy, dz, scale;
00262     double *q, qtemp, fx, fy, fz;
00263     int iatom, ipos;
00264
00265     if (thee == VNULL) {
00266         Vnm_print(2, "Vgreen_coulomb: Got NULL thee!\n");
00267         return 0;
00268     }
00269
00270     for (ipos=0; ipos<npos; ipos++) val[ipos] = 0.0;
00271
00272 #ifndef HAVE_TREE
00273
00274     /* Allocate charge array (if necessary) */
00275     if (Valist_getNumberAtoms(thee->alist) > 1) {
00276         if (npos > 1) {
00277             q = VNULL;
00278             q = Vmem_malloc(thee->vmem, npos, sizeof(double));
00279             if (q == VNULL) {
00280                 Vnm_print(2, "Vgreen_coulomb: Error allocating charge array!\n");
00281                 return 0;
00282             }
00283         } else {
00284             q = &qtemp;
00285         }
00286         for (ipos=0; ipos<npos; ipos++) q[ipos] = 1.0;
00287
00288         /* Calculate */
00289         treecalc(thee, x, y, z, q, npos, val, thee->xp, thee->yp, thee->zp,
00290             thee->qp, thee->np, &fx, &fy, &fz, 1, 1, thee->np);
00291     } else return Vgreen_coulomb_direct(thee, npos, x, y, z, val);
00292
00293     /* De-allocate charge array (if necessary) */
00294     if (npos > 1) Vmem_free(thee->vmem, npos, sizeof(double), (void **)&q);
00295
00296     scale = Vunit_ec/(4*Vunit_pi*Vunit_eps0*1.0e-10);
00297     for (ipos=0; ipos<npos; ipos++) val[ipos] = val[ipos]*scale;
00298
00299     return 1;
00300 }
00301
00302 #else /* ifdef HAVE_TREE */
00303
00304     return Vgreen_coulomb_direct(thee, npos, x, y, z, val);
00305 #endif
00306 }
00307
00308 }
00309
00310 VPUBLIC int Vgreen_coulombD_direct(Vgreen *thee, int npos,
00311     double *x, double *y, double *z, double *pot, double *gradx,
00312     double *grady, double *gradz) {
00313     Vatom *atom;
00314     double *apos, charge, dist, dist2, idist3, dy, dz, dx, scale;
00315     double *q, qtemp;
00316     int iatom, ipos;
00317
00318     if (thee == VNULL) {
00319         Vnm_print(2, "Vgreen_coulombD: Got VNULL thee!\n");
00320         return 0;
00321     }
00322
00323     for (ipos=0; ipos<npos; ipos++) {
00324         pot[ipos] = 0.0;

```

```

00326     gradx[ipos] = 0.0;
00327     grady[ipos] = 0.0;
00328     gradz[ipos] = 0.0;
00329 }
00330
00331 for (iatom=0; iatom<Valist_getNumberAtoms(thee->alist); iatom++) {
00332     atom = Valist_getAtom(thee->alist, iatom);
00333     apos = Vatom_getPosition(atom);
00334     charge = Vatom_getCharge(atom);
00335     for (ipos=0; ipos<npos; ipos++) {
00336         dx = apos[0] - x[ipos];
00337         dy = apos[1] - y[ipos];
00338         dz = apos[2] - z[ipos];
00339         dist2 = VSQR(dx) + VSQR(dy) + VSQR(dz);
00340         dist = VSQRT(dist2);
00341         if (dist > VSMALL) {
00342             idist3 = 1.0/(dist*dist2);
00343             gradx[ipos] -= (charge*dx*idist3);
00344             grady[ipos] -= (charge*dy*idist3);
00345             gradz[ipos] -= (charge*dz*idist3);
00346             pot[ipos] += (charge/dist);
00347         }
00348     }
00349 }
00350
00351 scale = Vunit_ec/(4*VPI*Vunit_eps0*(1.0e-10));
00352 for (ipos=0; ipos<npos; ipos++) {
00353     gradx[ipos] = gradx[ipos]*scale;
00354     grady[ipos] = grady[ipos]*scale;
00355     gradz[ipos] = gradz[ipos]*scale;
00356     pot[ipos] = pot[ipos]*scale;
00357 }
00358
00359 return 1;
00360 }
00361
00362 VPUBLIC int Vgreen_coulombD(Vgreen *thee, int npos, double *x, double *y,
00363     double *z, double *pot, double *gradx, double *grady, double *gradz) {
00364
00365     Vatom *atom;
00366     double *apos, charge, dist, dist2, idist3, dy, dz, dx, scale;
00367     double *q, qtemp;
00368     int iatom, ipos;
00369
00370     if (thee == VNULL) {
00371         Vnm_print(2, "Vgreen_coulombD: Got VNULL thee!\n");
00372         return 0;
00373     }
00374
00375     for (ipos=0; ipos<npos; ipos++) {
00376         pot[ipos] = 0.0;
00377         gradx[ipos] = 0.0;
00378         grady[ipos] = 0.0;
00379         gradz[ipos] = 0.0;
00380     }
00381
00382 #ifdef HAVE_TREE
00383
00384     if (Valist_getNumberAtoms(thee->alist) > 1) {
00385         if (npos > 1) {
00386             q = VNULL;
00387             q = Vmem_malloc(thee->vmem, npos, sizeof(double));
00388             if (q == VNULL) {
00389                 Vnm_print(2, "Vgreen_coulomb: Error allocating charge array!\n");
00390                 return 0;
00391             }
00392         } else {
00393             q = &(qtemp);
00394         }
00395         for (ipos=0; ipos<npos; ipos++) q[ipos] = 1.0;
00396
00397         /* Calculate */
00398         treecalc(thee, x, y, z, q, npos, pot, thee->xp, thee->yp, thee->zp,
00399             thee->qp, thee->np, gradx, grady, gradz, 2, npos, thee->np);
00400
00401         /* De-allocate charge array (if necessary) */
00402         if (npos > 1) Vmem_free(thee->vmem, npos, sizeof(double), (void **) &q);
00403     } else return Vgreen_coulombD_direct(thee, npos, x, y, z, pot,
00404         gradx, grady, gradz);
00405
00406     scale = Vunit_ec/(4*VPI*Vunit_eps0*(1.0e-10));

```



```

00407     for (ipos=0; ipos<npos; ipos++) {
00408         gradx[ipos] = gradx[ipos]*scale;
00409         grady[ipos] = grady[ipos]*scale;
00410         gradz[ipos] = gradz[ipos]*scale;
00411         pot[ipos] = pot[ipos]*scale;
00412     }
00413
00414     return 1;
00415
00416 #else /* ifdef HAVE_TREE */
00417
00418     return Vgreen_coulombD_direct(thee, npos, x, y, z, pot,
00419         gradx, grady, gradz);
00420
00421 #endif
00422 }
00423
00424
00425 VPRIVATE int treesetup(Vgreen *thee) {
00426
00427 #ifdef HAVE_TREE
00428
00429     double dist_tol = FMM_DIST_TOL;
00430     int iflag = FMM_IFLAG;
00431     double order = FMM_ORDER;
00432     int theta = FMM_THETA;
00433     int shrink = FMM_SHRINK;
00434     int maxparnode = FMM_MAXPARNODE;
00435     int minlevel = FMM_MINLEVEL;
00436     int maxlevel = FMM_MAXLEVEL;
00437     int level = 0;
00438     int one = 1;
00439     Vatom *atom;
00440     double xyzminmax[6], *pos;
00441     int i;
00442
00443     /* Set up particle arrays with atomic coordinates and charges */
00444     Vnm_print(0, "treesetup: Initializing FMM particle arrays...\n");
00445     thee->np = Valist_getNumberAtoms(thee->alist);
00446     thee->xp = VNULL;
00447     thee->xp = (double *)Vmem_malloc(thee->vmem, thee->np, sizeof(double));
00448     if (thee->xp == VNULL) {
00449         Vnm_print(2, "Vgreen_ctor2: Failed to allocate %d*sizeof(double)!\n",
00450             thee->np);
00451         return 0;
00452     }
00453     thee->yp = VNULL;
00454     thee->yp = (double *)Vmem_malloc(thee->vmem, thee->np, sizeof(double));
00455     if (thee->yp == VNULL) {
00456         Vnm_print(2, "Vgreen_ctor2: Failed to allocate %d*sizeof(double)!\n",
00457             thee->np);
00458         return 0;
00459     }
00460     thee->zp = VNULL;
00461     thee->zp = (double *)Vmem_malloc(thee->vmem, thee->np, sizeof(double));
00462     if (thee->zp == VNULL) {
00463         Vnm_print(2, "Vgreen_ctor2: Failed to allocate %d*sizeof(double)!\n",
00464             thee->np);
00465         return 0;
00466     }
00467     thee->qp = VNULL;
00468     thee->qp = (double *)Vmem_malloc(thee->vmem, thee->np, sizeof(double));
00469     if (thee->qp == VNULL) {
00470         Vnm_print(2, "Vgreen_ctor2: Failed to allocate %d*sizeof(double)!\n",
00471             thee->np);
00472         return 0;
00473     }
00474     for (i=0; i<thee->np; i++) {
00475         atom = Valist_getAtom(thee->alist, i);
00476         pos = Vatom_getPosition(atom);
00477         thee->xp[i] = pos[0];
00478         thee->yp[i] = pos[1];
00479         thee->zp[i] = pos[2];
00480         thee->qp[i] = Vatom_getCharge(atom);
00481     }
00482
00483     Vnm_print(0, "treesetup: Setting things up...\n");
00484     F77SETUP(thee->xp, thee->yp, thee->zp, &(thee->np), &order, &theta, &iflag,
00485         &dist_tol, xyzminmax, &(thee->np));
00486
00487

```

```

00488     Vnm_print(0, "treesetup: Initializing levels...\n");
00489     F77INITLEVELS(&minlevel, &maxlevel);
00490
00491     Vnm_print(0, "treesetup: Creating tree...\n");
00492     F77CREATE_TREE(&one, &(thee->np), thee->xp, thee->yp, thee->zp, thee->qp,
00493         &shrink, &maxparnode, xyzminmax, &level, &(thee->np));
00494
00495     return 1;
00496
00497 #else /* ifdef HAVE_TREE */
00498
00499     Vnm_print(2, "treesetup: Error! APBS not linked with treecode!\n");
00500     return 0;
00501
00502 #endif /* ifdef HAVE_TREE */
00503 }
00504
00505 VPRIVATE int treecleanup(Vgreen *thee) {
00506
00507 #ifdef HAVE_TREE
00508
00509     Vmem_free(thee->vmem, thee->np, sizeof(double), (void *)&(thee->xp));
00510     Vmem_free(thee->vmem, thee->np, sizeof(double), (void *)&(thee->yp));
00511     Vmem_free(thee->vmem, thee->np, sizeof(double), (void *)&(thee->zp));
00512     Vmem_free(thee->vmem, thee->np, sizeof(double), (void *)&(thee->qp));
00513     F77CLEANUP();
00514
00515     return 1;
00516
00517 #else /* ifdef HAVE_TREE */
00518
00519     Vnm_print(2, "treecleanup: Error! APBS not linked with treecode!\n");
00520     return 0;
00521
00522 #endif /* ifdef HAVE_TREE */
00523 }
00524
00525 VPRIVATE int treecalc(Vgreen *thee, double *xtar, double *ytar, double *ztar,
00526     double *qtar, int numtars, double *tpengtar, double *x, double *y,
00527     double *z, double *q, int numpars, double *fx, double *fy, double *fz,
00528     int iflag, int farrdim, int arrdim) {
00529
00530 #ifdef HAVE_TREE
00531     int i, level, err, maxlevel, minlevel, one;
00532     double xyzminmax[6];
00533
00534     if (iflag != 1) {
00535         F77TREE_COMPFP(xtar, ytar, ztar, qtar, &numtars, tpengtar, x, y, z, q,
00536             fx, fy, fz, &numpars, &farrdim, &arrdim);
00537     } else {
00538         F77TREE_COMPP(xtar, ytar, ztar, qtar, &numtars, tpengtar, &farrdim, x,
00539             y, z, q, &numpars, &arrdim);
00540     }
00541
00542     return 1;
00543
00544 #else /* ifdef HAVE_TREE */
00545
00546     Vnm_print(2, "treecalc: Error! APBS not linked with treecode!\n");
00547     return 0;
00548
00549 #endif /* ifdef HAVE_TREE */
00550
00551 #endif /* ifdef HAVE_TREE */
00552 }

```

9.72 src/generic/vgreen.h File Reference

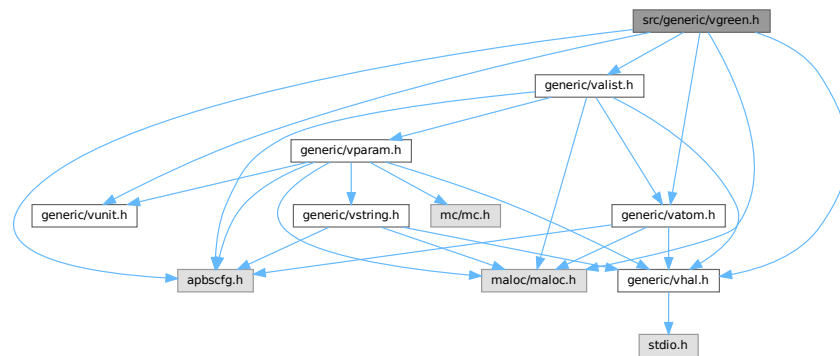
Contains declarations for class Vgreen.

```

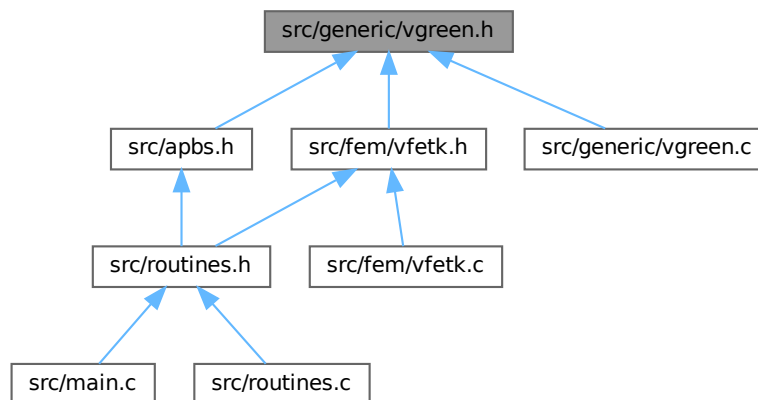
#include "apbscfg.h"
#include "malloc/malloc.h"
#include "generic/vhal.h"
#include "generic/vunit.h"
#include "generic/vatom.h"
#include "generic/valist.h"

```

Include dependency graph for vgreen.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVgreen](#)
Contains public data members for Vgreen class/module.

Typedefs

- typedef struct [sVgreen](#) [Vgreen](#)
Declaration of the Vgreen class as the Vgreen structure.

Functions

- VEXTERNC [Valist](#) * [Vgreen_getValist](#) ([Vgreen](#) *thee)
Get the atom list associated with this Green's function object.

- VEXTERNC unsigned long int [Vgreen_memChk](#) ([Vgreen](#) *thee)
Return the memory used by this structure (and its contents) in bytes.
- VEXTERNC [Vgreen](#) * [Vgreen_ctor](#) ([Valist](#) *alist)
Construct the Green's function oracle.
- VEXTERNC int [Vgreen_ctor2](#) ([Vgreen](#) *thee, [Valist](#) *alist)
FORTTRAN stub to construct the Green's function oracle.
- VEXTERNC void [Vgreen_dtor](#) ([Vgreen](#) **thee)
Destruct the Green's function oracle.
- VEXTERNC void [Vgreen_dtor2](#) ([Vgreen](#) *thee)
FORTTRAN stub to destruct the Green's function oracle.
- VEXTERNC int [Vgreen_helmholtz](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *val, double kappa)
Get the Green's function for Helmholtz's equation integrated over the atomic point charges.
- VEXTERNC int [Vgreen_helmholtzD](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *gradx, double *grady, double *gradz, double kappa)
Get the gradient of Green's function for Helmholtz's equation integrated over the atomic point charges.
- VEXTERNC int [Vgreen_coulomb_direct](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *val)
Get the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation.
- VEXTERNC int [Vgreen_coulomb](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *val)
Get the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation or H. E. Johnston, R. Krasny FMM library (if available)
- VEXTERNC int [Vgreen_coulombD_direct](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *pot, double *gradx, double *grady, double *gradz)
Get gradient of the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation.
- VEXTERNC int [Vgreen_coulombD](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *pot, double *gradx, double *grady, double *gradz)
Get gradient of the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using either direct summation or H. E. Johnston/R. Krasny FMM library (if available)

9.72.1 Detailed Description

Contains declarations for class [Vgreen](#).

Version

\$Id\$

Author

Nathan A. Baker

Definition in file [vgreen.h](#).

9.73 vgreen.h

[Go to the documentation of this file.](#)

```
00001
00065 #ifndef _VGREEN_H_
00066 #define _VGREEN_H_
00067
00068 #include "apbscfg.h"
00069
```

```

00070 #include "malloc/malloc.h"
00071
00072 #include "generic/vhal.h"
00073 #include "generic/vunit.h"
00074 #include "generic/vatom.h"
00075 #include "generic/valist.h"
00076
00082 struct sVgreen {
00083
00084     Valist *alist;
00085     Vmem *vmem;
00086     double *xp;
00088     double *yp;
00090     double *zp;
00092     double *qp;
00094     int np;
00095 };
00096
00101 typedef struct sVgreen Vgreen;
00102
00103 /* ////////////////////////////////////////
00104 // Class Vgreen: Inlineable methods (vgreen.c)
00106
00107 #if !defined(VINLINE_VGREEN)
00108
00116     VEXTERNC Valist* Vgreen_getValist(Vgreen *thee);
00117
00125     VEXTERNC unsigned long int Vgreen_memChk(Vgreen *thee);
00126
00127 #else /* if defined(VINLINE_VGREEN) */
00128 #   define Vgreen_getValist(thee) ((thee)->alist)
00129 #   define Vgreen_memChk(thee) (Vmem_bytes((thee)->vmem))
00130 #endif /* if !defined(VINLINE_VGREEN) */
00131
00132 /* ////////////////////////////////////////
00133 // Class Vgreen: Non-Inlineable methods (vgreen.c)
00135
00142 VEXTERNC Vgreen* Vgreen_ctor(Valist *alist);
00143
00151 VEXTERNC int Vgreen_ctor2(Vgreen *thee, Valist *alist);
00152
00158 VEXTERNC void Vgreen_dtor(Vgreen **thee);
00159
00165 VEXTERNC void Vgreen_dtor2(Vgreen *thee);
00166
00191 VEXTERNC int Vgreen_helmholtz(Vgreen *thee, int npos, double *x, double *y,
00192     double *z, double *val, double kappa);
00193
00221 VEXTERNC int Vgreen_helmholtzD(Vgreen *thee, int npos, double *x, double *y,
00222     double *z, double *gradx, double *grady, double *gradz, double kappa);
00223
00244 VEXTERNC int Vgreen_coulomb_direct(Vgreen *thee, int npos, double *x,
00245     double *y, double *z, double *val);
00246
00267 VEXTERNC int Vgreen_coulomb(Vgreen *thee, int npos, double *x, double *y,
00268     double *z, double *val);
00269
00293 VEXTERNC int Vgreen_coulombD_direct(Vgreen *thee, int npos, double *x,
00294     double *y, double *z, double *pot, double *gradx, double *grady, double
00295     *gradz);
00296
00321 VEXTERNC int Vgreen_coulombD(Vgreen *thee, int npos, double *x, double *y,
00322     double *z, double *pot, double *gradx, double *grady, double *gradz);
00323
00324 #endif /* ifndef _VGREEN_H_ */

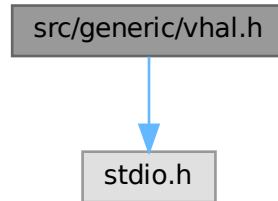
```

9.74 src/generic/vhal.h File Reference

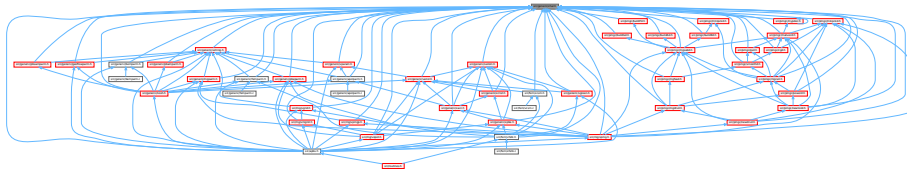
Contains generic macro definitions for APBS.

```
#include "stdio.h"
```

Include dependency graph for vhal.h:



This graph shows which files directly or indirectly include this file:



Macros

- `#define APBS_TIMER_WALL_CLOCK` 26
APBS total execution timer ID.
- `#define APBS_TIMER_SETUP` 27
APBS setup timer ID.
- `#define APBS_TIMER_SOLVER` 28
APBS solver timer ID.
- `#define APBS_TIMER_ENERGY` 29
APBS energy timer ID.
- `#define APBS_TIMER_FORCE` 30
APBS force timer ID.
- `#define APBS_TIMER_TEMP1` 31
APBS temp timer #1 ID.
- `#define APBS_TIMER_TEMP2` 32
APBS temp timer #2 ID.
- `#define MAXMOL` 5
The maximum number of molecules that can be involved in a single PBE calculation.
- `#define MAXION` 10
The maximum number of ion species that can be involved in a single PBE calculation.
- `#define MAXFOCUS` 5
The maximum number of times an MG calculation can be focused.
- `#define VMGNLEV` 4

- Minimum number of levels in a multigrid calculations.*

 - #define `VREDFRAC` 0.25
- Maximum reduction of grid spacing during a focusing calculation.*

 - #define `VAPBS_NVS` 4
- Number of vertices per simplex (hard-coded to 3D)*

 - #define `VAPBS_DIM` 3
- Our dimension.*

 - #define `VAPBS_RIGHT` 0
- Face definition for a volume.*

 - #define `VAPBS_FRONT` 1
- Face definition for a volume.*

 - #define `VAPBS_UP` 2
- Face definition for a volume.*

 - #define `VAPBS_LEFT` 3
- Face definition for a volume.*

 - #define `VAPBS_BACK` 4
- Face definition for a volume.*

 - #define `VAPBS_DOWN` 5
- Face definition for a volume.*

 - #define `VPMGSMALL` 1e-12
- A small number used in Vpmg to decide if points are on/off grid-lines or non-zero (etc.)*

 - #define `SINH_MIN` -85.0
- Used to set the min values acceptable for sinh chopping.*

 - #define `SINH_MAX` 85.0
- Used to set the max values acceptable for sinh chopping.*

 - #define `MAX_HASH_DIM` 75
- #define `VF77_MANGLE`(name, NAME) name

Name-mangling macro for using FORTRAN functions in C code.
- #define `VFLOOR`(value) floor(value)

Wrapped floor to fix floating point issues in the Intel compiler.
- #define `VEMBED`(rctag)

Allows embedding of RCS ID tags in object files.
- #define `PRINT_FUNC` __PRETTY_FUNCTION__
- #define `OS_SEP_STR` "/"
- #define `OS_SEP_CHAR` '/'
- #define `ANNOUNCE_FUNCTION`
- #define `WARN_UNTESTED`
- #define `WARN_PARTTESTED`
- #define `VCHANNELEDMESSAGE0`(channel, msg)
- #define `VCHANNELEDMESSAGE1`(channel, msg, arg0)
- #define `VCHANNELEDMESSAGE2`(channel, msg, arg0, arg1)
- #define `VCHANNELEDMESSAGE3`(channel, msg, arg0, arg1, arg2)
- #define `VMESSAGE0`(msg) VCHANNELEDMESSAGE0(0, msg)
- #define `VMESSAGE1`(msg, arg0) VCHANNELEDMESSAGE1(0, msg, arg0)
- #define `VMESSAGE2`(msg, arg0, arg1) VCHANNELEDMESSAGE2(0, msg, arg0, arg1)
- #define `VMESSAGE3`(msg, arg0, arg1, arg2) VCHANNELEDMESSAGE3(0, msg, arg0, arg1, arg2)
- #define `VERRMSG0`(msg) VCHANNELEDMESSAGE0(2, msg)
- #define `VERRMSG1`(msg, arg0) VCHANNELEDMESSAGE1(2, msg, arg0)

- #define [VERRMSG2](#)(msg, arg0, arg1) VCHANNELEDMESSAGE2(2, msg, arg0, arg1)
- #define [VERRMSG3](#)(msg, arg0, arg1, arg2) VCHANNELEDMESSAGE3(2, msg, arg0, arg1, arg2)
- #define [VASSERT_MSG0](#)(cnd, msg)
- #define [VASSERT_MSG1](#)(cnd, msg, arg)
- #define [VASSERT_MSG2](#)(cnd, msg, arg0, arg1)
- #define [VWARN_MSG0](#)(cnd, msg)
- #define [VWARN_MSG1](#)(cnd, msg, arg0)
- #define [VWARN_MSG2](#)(cnd, msg, arg0, arg1)
- #define [VABORT_MSG0](#)(msg)
- #define [VABORT_MSG1](#)(msg, arg)
- #define [VABORT_MSG2](#)(msg, arg0, arg1)
- #define [PRINT_INT](#)(expr)
- #define [PRINT_DBL](#)(expr)
- #define [VMALLOC](#)(vmem, n, type) ((type*)Vmem_malloc(vmem, n, sizeof(type)))
- #define [VFREE](#)(vmem, n, type, ptr) (Vmem_free(vmem, n, sizeof(type), (void **)&(ptr)))
- #define [VFILL](#)(vec, n, val)
- #define [VCOPY](#)(srcvec, dstvec, i, n)
- #define [VAT](#)(array, i) ((array)[(i) - 1])
- #define [RAT](#)(array, i) ((array) + i - 1)

Typedefs

- typedef enum [eVrc_Codes](#) [Vrc_Codes](#)
- typedef enum [eVsol_Meth](#) [Vsol_Meth](#)
- typedef enum [eVsurf_Meth](#) [Vsurf_Meth](#)
Declaration of the Vsurf_Meth type as the Vsurf_Meth enum.
- typedef enum [eVhal_PBEType](#) [Vhal_PBEType](#)
Declaration of the Vhal_PBEType type as the Vhal_PBEType enum.
- typedef enum [eVhal_IPKEYType](#) [Vhal_IPKEYType](#)
Declaration of the Vhal_IPKEYType type as the Vhal_IPKEYType enum.
- typedef enum [eVhal_NONLINType](#) [Vhal_NONLINType](#)
Declaration of the Vhal_NONLINType type as the Vhal_NONLINType enum.
- typedef enum [eVoutput_Format](#) [Voutput_Format](#)
Declaration of the Voutput_Format type as the VOutput_Format enum.
- typedef enum [eVbcfl](#) [Vbcfl](#)
Declare Vbcfl type.
- typedef enum [eVchrg_Meth](#) [Vchrg_Meth](#)
Declaration of the Vchrg_Meth type as the Vchrg_Meth enum.
- typedef enum [eVchrg_Src](#) [Vchrg_Src](#)
Declaration of the Vchrg_Src type as the Vchrg_Meth enum.
- typedef enum [eVdata_Type](#) [Vdata_Type](#)
Declaration of the Vdata_Type type as the Vdata_Type enum.
- typedef enum [eVdata_Format](#) [Vdata_Format](#)
Declaration of the Vdata_Format type as the Vdata_Format enum.

Enumerations

- enum `eVrc_Codes` { `VRC_WARNING` = -1 , `VRC_FAILURE` = 0 , `VRC_SUCCESS` = 1 }
Return code enumerations.
- enum `eVsol_Meth` {
`VSOL_CGMG` , `VSOL_Newton` , `VSOL_MG` , `VSOL_CG` ,
`VSOL_SOR` , `VSOL_RBGS` , `VSOL_WJ` , `VSOL_Richardson` ,
`VSOL_CGMGAqua` , `VSOL_NewtonAqua` }
Solution Method enumerations.
- enum `eVsurf_Meth` {
`VSM_MOL` = 0 , `VSM_MOLSMOOTH` = 1 , `VSM_SPLINE` = 2 , `VSM_SPLINE3` = 3 ,
`VSM_SPLINE4` = 4 }
Types of molecular surface definitions.
- enum `eVhal_PBEType` {
`PBE_LPBE` , `PBE_NPBE` , `PBE_LRPBE` , `PBE_NRPBE` ,
`PBE_SMPBE` }
Version of PBE to solve.
- enum `eVhal_IPKEYType` { `IPKEY_SMPBE` = -2 , `IPKEY_LPBE` , `IPKEY_NPBE` }
Type of ipkey to use for MG methods.
- enum `eVhal_NONLINType` {
`NONLIN_LPBE` = 0 , `NONLIN_NPBE` , `NONLIN_SMPBE` , `NONLIN_LPBEAQUA` ,
`NONLIN_NPBEAQUA` }
Type of nonlinear to use for MG methods.
- enum `eVoutput_Format` { `OUTPUT_NULL` , `OUTPUT_FLAT` }
Output file format.
- enum `eVbcfl` {
`BCFL_ZERO` = 0 , `BCFL_SDH` = 1 , `BCFL_MDH` = 2 , `BCFL_UNUSED` = 3 ,
`BCFL_FOCUS` = 4 , `BCFL_MEM` = 5 , `BCFL_MAP` = 6 }
Types of boundary conditions.
- enum `eVchrg_Meth` { `VCM_TRIL` = 0 , `VCM_BSPL2` = 1 , `VCM_BSPL4` = 2 }
Types of charge discretization methods.
- enum `eVchrg_Src` { `VCM_CHARGE` = 0 , `VCM_PERMANENT` = 1 , `VCM_INDUCED` = 2 , `VCM_NLINDUCED` = 3 }
Charge source.
- enum `eVdata_Type` {
`VDI_CHARGE` , `VDI_POT` , `VDI_ATOMPOT` , `VDI_SMOL` ,
`VDI_SSPL` , `VDI_VDW` , `VDI_IVDW` , `VDI_LAP` ,
`VDI_EDENS` , `VDI_NDENS` , `VDI_QDENS` , `VDI_DIELX` ,
`VDI_DIELY` , `VDI_DIELZ` , `VDI_KAPPA` }
Types of (scalar) data that can be written out of APBS.
- enum `eVdata_Format` {
`VDF_DX` = 0 , `VDF_UHBD` = 1 , `VDF_AVS` = 2 , `VDF_MCSF` = 3 ,
`VDF_GZ` = 4 , `VDF_FLAT` = 5 , `VDF_DXBIN` = 6 }
Format of data for APBS I/O.

Functions

- `char * wrap_text` (char *str, int right_margin, int left_padding)

9.74.1 Detailed Description

Contains generic macro definitions for APBS.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```
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* APBS -- Adaptive Poisson-Boltzmann Solver
*
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*
*
```

Definition in file [vhal.h](#).

9.74.2 Macro Definition Documentation

9.74.2.1 ANNOUNCE_FUNCTION

```
#define ANNOUNCE_FUNCTION
```

Definition at line 600 of file [vhal.h](#).

9.74.2.2 MAX_HASH_DIM

```
#define MAX_HASH_DIM 75
```

Definition at line 458 of file [vhal.h](#).

9.74.2.3 OS_SEP_CHAR

```
#define OS_SEP_CHAR '/'
```

Definition at line 573 of file [vhal.h](#).

9.74.2.4 OS_SEP_STR

```
#define OS_SEP_STR "/"
```

Definition at line 572 of file [vhal.h](#).

9.74.2.5 PRINT_DBL

```
#define PRINT_DBL(  
    expr )
```

Definition at line 945 of file [vhal.h](#).

9.74.2.6 PRINT_FUNC

```
#define PRINT_FUNC __PRETTY_FUNCTION__
```

OS specific flags and etcetera

Definition at line 571 of file [vhal.h](#).

9.74.2.7 PRINT_INT

```
#define PRINT_INT(  
    expr )
```

Definition at line 944 of file [vhal.h](#).

9.74.2.8 RAT

```
#define RAT(  
    array,  
    i ) ((array) + i - 1)
```

Definition at line 969 of file [vhal.h](#).

9.74.2.9 VABORT_MSG0

```
#define VABORT_MSG0(  
    msg )
```

Value:

```
do {  
    Vnm_print(2, "[%s()]: ABORTING:\n" \br/>              "    %s\n\n", \br/>              __FUNCTION__, msg); \br/>    abort();  
} while (0)
```

Definition at line 899 of file [vhal.h](#).

9.74.2.10 VABORT_MSG1

```
#define VABORT_MSG1(  
    msg,  
    arg )
```

Value:

```
do {  
    char buff[1000];  
    snprintf( buff, 1000, msg, arg );  
    Vnm_print(2, "[%s()]: ABORTING:\n"  
        "    %s\n\n",  
        __FUNCTION__, buff);  
    abort();  
} while(0)
```

Definition at line 907 of file [vhal.h](#).

9.74.2.11 VABORT_MSG2

```
#define VABORT_MSG2(  
    msg,  
    arg0,  
    arg1 )
```

Value:

```
do {  
    char buff[1000];  
    snprintf( buff, 1000, msg, arg0, arg1);  
    Vnm_print(2, "[%s()]: ABORTING:\n"  
        "    %s\n\n",  
        __FUNCTION__, buff);  
    abort();  
} while(0)
```

Definition at line 917 of file [vhal.h](#).

9.74.2.12 VASSERT_MSG0

```
#define VASSERT_MSG0(  
    cnd,  
    msg )
```

Value:

```
do {  
    if( (cnd) == 0 ) {  
        Vnm_print(2, "[%s()]: ERROR:\n"  
            "    Assertion Failed (%s): %s\n\n",  
            __FUNCTION__, #cnd, msg);  
        abort();  
    }  
} while(0)
```

Definition at line 731 of file [vhal.h](#).

9.74.2.13 VASSERT_MSG1

```
#define VASSERT_MSG1(  
    cnd,  
    msg,  
    arg )
```

Value:

```
do {
```

```

        if( (cnd) == 0 ) {
            char buff[1000];
            snprintf( buff, 1000, msg, arg );
            Vnm_print(2, "[%s()]: ERROR:\n"
                    "        Assertion Failed (%s): %s\n\n",
                    __FUNCTION__, #cnd, buff);
            abort();
        }
    } while(0)

```

Definition at line 741 of file [vhal.h](#).

9.74.2.14 VASSERT_MSG2

```

#define VASSERT_MSG2(
    cnd,
    msg,
    arg0,
    arg1 )

```

Value:

```

do {
    if( (cnd) == 0 ) {
        char buff[1000];
        snprintf( buff, 1000, msg, arg0, arg1 );
        Vnm_print(2, "[%s()]: ERROR:\n"
                "        Assertion Failed (%s): %s\n\n",
                __FUNCTION__, #cnd, buff);
        abort();
    }
} while(0)

```

Definition at line 753 of file [vhal.h](#).

9.74.2.15 VAT

```

#define VAT(
    array,
    i ) ((array)[(i) - 1])

```

Definition at line 968 of file [vhal.h](#).

9.74.2.16 VCHANNELEDMESSAGE0

```

#define VCHANNELEDMESSAGE0(
    channel,
    msg )

```

Value:

```

do {
    Vnm_print(channel, "%s: %s\n", __FUNCTION__, msg);
} while(0)

```

Definition at line 653 of file [vhal.h](#).

9.74.2.17 VCHANNELEDMESSAGE1

```

#define VCHANNELEDMESSAGE1(
    channel,
    msg,
    arg0 )

```

Value:

```

do {
    char buff[1000];
    snprintf( buff, 1000, msg, arg0 );
}

```

```
Vnm_print(channel, "%s: %s\n", __FUNCTION__, buff); \
} while(0)
```

Definition at line 658 of file [vhal.h](#).

9.74.2.18 VCHANNELEDMESSAGE2

```
#define VCHANNELEDMESSAGE2(  
    channel,  
    msg,  
    arg0,  
    arg1 )
```

Value:

```
do {  
    char buff[1000];  
    snprintf( buff, 1000, msg, arg0, arg1 );  
    Vnm_print(channel, "%s: %s\n", __FUNCTION__, buff); \
} while(0)
```

Definition at line 665 of file [vhal.h](#).

9.74.2.19 VCHANNELEDMESSAGE3

```
#define VCHANNELEDMESSAGE3(  
    channel,  
    msg,  
    arg0,  
    arg1,  
    arg2 )
```

Value:

```
do {  
    char buff[1000];  
    snprintf(buff, 1000, msg, arg0, arg1, arg2);  
    Vnm_print(channel, "%s: %s\n", __FUNCTION__, buff); \
} while(0)
```

Definition at line 672 of file [vhal.h](#).

9.74.2.20 VCOPY

```
#define VCOPY(  
    srcvec,  
    dstvec,  
    i,  
    n )
```

Value:

```
do {  
    for (i = 0; i < n; i++)  
        dstvec[i] = srcvec[i]; \
} while(0)
```

Definition at line 959 of file [vhal.h](#).

9.74.2.21 VERRMSG0

```
#define VERRMSG0(  
    msg ) VCHANNELEDMESSAGE0(2, msg)
```

Definition at line 684 of file [vhal.h](#).

9.74.2.22 VERRMSG1

```
#define VERRMSG1(  
    msg,  
    arg0 ) VCHANNELEDMESSAGE1(2, msg, arg0)
```

Definition at line 685 of file [vhal.h](#).

9.74.2.23 VERRMSG2

```
#define VERRMSG2(  
    msg,  
    arg0,  
    arg1 ) VCHANNELEDMESSAGE2(2, msg, arg0, arg1)
```

Definition at line 686 of file [vhal.h](#).

9.74.2.24 VERRMSG3

```
#define VERRMSG3(  
    msg,  
    arg0,  
    arg1,  
    arg2 ) VCHANNELEDMESSAGE3(2, msg, arg0, arg1, arg2)
```

Definition at line 687 of file [vhal.h](#).

9.74.2.25 VFILL

```
#define VFILL(  
    vec,  
    n,  
    val )
```

Value:

```
do {  
    int fill_idx;  
    for (fill_idx = 0; fill_idx < n; fill_idx++)  
        vec[fill_idx] = val;  
} while(0)
```

Definition at line 952 of file [vhal.h](#).

9.74.2.26 VFREE

```
#define VFREE(  
    vmem,  
    n,  
    type,  
    ptr ) (Vmem_free(vmem, n, sizeof(type), (void **)&(ptr)))
```

Definition at line 950 of file [vhal.h](#).

9.74.2.27 VMALLOC

```
#define VMALLOC(  
    vmem,
```

```

    n,
    type ) ((type*)Vmem_malloc(vmem, n, sizeof(type)))

```

Definition at line 948 of file [vhal.h](#).

9.74.2.28 VMESSAGE0

```

#define VMESSAGE0(
    msg ) VCHANNELEDMESSAGE0(0, msg)

```

Definition at line 679 of file [vhal.h](#).

9.74.2.29 VMESSAGE1

```

#define VMESSAGE1(
    msg,
    arg0 ) VCHANNELEDMESSAGE1(0, msg, arg0)

```

Definition at line 680 of file [vhal.h](#).

9.74.2.30 VMESSAGE2

```

#define VMESSAGE2(
    msg,
    arg0,
    arg1 ) VCHANNELEDMESSAGE2(0, msg, arg0, arg1)

```

Definition at line 681 of file [vhal.h](#).

9.74.2.31 VMESSAGE3

```

#define VMESSAGE3(
    msg,
    arg0,
    arg1,
    arg2 ) VCHANNELEDMESSAGE3(0, msg, arg0, arg1, arg2)

```

Definition at line 682 of file [vhal.h](#).

9.74.2.32 VWARN_MSG0

```

#define VWARN_MSG0(
    cnd,
    msg )

```

Value:

```

do {
    if( (cnd) == 0 ) {
        Vnm_print(
            2,
            "[%s()]: WARNING:\n"
            "    %s\n",
            __FUNCTION__,
            msg
        );
    }
} while(0)

```

Definition at line 825 of file [vhal.h](#).

9.74.2.33 VWARN_MSG1

```
#define VWARN_MSG1(
    cnd,
    msg,
    arg0 )
```

Value:

```
do {
    if( (cnd) == 0 ) {
        char buff[1000];
        snprintf(buff, 1000, msg, arg0);
        Vnm_print(
            2,
            "[%s()]: WARNING:\n"
            "    %s\n\n",
            __FUNCTION__,
            buff
        );
    }
} while (0)
```

Definition at line 838 of file [vhal.h](#).**9.74.2.34 VWARN_MSG2**

```
#define VWARN_MSG2(
    cnd,
    msg,
    arg0,
    arg1 )
```

Value:

```
do {
    if( (cnd) == 0 ) {
        char buff[1000];
        snprintf(buff, 1000, msg, arg0, arg1);
        Vnm_print(
            2,
            "[%s()]: WARNING:\n"
            "    %s\n\n",
            __FUNCTION__,
            buff
        );
    }
} while (0)
```

Definition at line 853 of file [vhal.h](#).**9.74.2.35 WARN_PARTTESTED**

```
#define WARN_PARTTESTED
```

Definition at line 602 of file [vhal.h](#).**9.74.2.36 WARN_UNTESTED**

```
#define WARN_UNTESTED
```

Definition at line 601 of file [vhal.h](#).**9.74.3 Typedef Documentation**

9.74.3.1 Vrc_Codes

typedef enum eVrc_Codes Vrc_Codes
Definition at line 73 of file vhal.h.

9.74.3.2 Vsol_Meth

typedef enum eVsol_Meth Vsol_Meth
Definition at line 95 of file vhal.h.

9.75 vhal.h

[Go to the documentation of this file.](#)

```

00001
00055 #ifndef _VAPBSHAL_H_
00056 #define _VAPBSHAL_H_
00057
00058 #include "stdio.h"
00059
00066 enum eVrc_Codes {
00067     VRC_WARNING=-1,
00069     VRC_FAILURE=0,
00070     VRC_SUCCESS=1
00072 };
00073 typedef enum eVrc_Codes Vrc_Codes;
00074
00081 enum eVsol_Meth {
00082
00083     VSOL_CGMG,          /* 0: conjugate gradient multigrid */
00084     VSOL_Newton,        /* 1: newton */
00085     VSOL_MG,            /* 2: multigrid */
00086     VSOL_CG,            /* 3: conjugate gradient */
00087     VSOL_SOR,           /* 4: successive overrelaxation */
00088     VSOL_RBGS,          /* 5: red-black gauss-seidel */
00089     VSOL_WJ,            /* 6: weighted jacobi */
00090     VSOL_Richardson,    /* 7: richardson */
00091     VSOL_CGMGAqua,      /* 8: conjugate gradient multigrid aqua */
00092     VSOL_NewtonAqua     /* 9: newton aqua */
00093
00094 };
00095 typedef enum eVsol_Meth Vsol_Meth;
00096
00102 enum eVsurf_Meth {
00103     VSM_MOL=0,
00107     VSM_MOLSMOOTH=1,
00109     VSM_SPLINE=2,
00119     VSM_SPLINE3=3,
00123     VSM_SPLINE4=4
00127 };
00128
00133 typedef enum eVsurf_Meth Vsurf_Meth;
00134
00139 enum eVhal_PBEType {
00140     PBE_LPBE,
00141     PBE_NPBE,
00142     PBE_LRPBE,
00143     PBE_NRPBE,
00144     PBE_SMPBE
00145 };
00146
00151 typedef enum eVhal_PBEType Vhal_PBEType;
00152
00157 enum eVhal_IPKEYType {
00158     IPKEY_SMPBE = -2,
00159     IPKEY_LPBE,
00160     IPKEY_NPBE
00161 };
00162
00167 typedef enum eVhal_IPKEYType Vhal_IPKEYType;
00168
00173 enum eVhal_NONLINType {
00174     NONLIN_LPBE = 0,

```

```

00175     NONLIN_NPBE,
00176     NONLIN_SMPBE,
00177     NONLIN_LPBEAQUA,
00178     NONLIN_NPBEAQUA
00179 };
00180
00185 typedef enum eVhal_NONLINType Vhal_NONLINType;
00186
00191 enum eVoutput_Format {
00192     OUTPUT_NULL,
00193     OUTPUT_FLAT,
00194 };
00195
00200 typedef enum eVoutput_Format Voutput_Format;
00201
00207 enum eVbcfl {
00208     BCFL_ZERO=0,
00209     BCFL_SDH=1,
00211     BCFL_MDH=2,
00213     BCFL_UNUSED=3,
00214     BCFL_FOCUS=4,
00215     BCFL_MEM=5,
00216     BCFL_MAP=6
00217 };
00218
00223 typedef enum eVbcfl Vbcfl;
00224
00230 enum eVchrg_Meth {
00231     VCM_TRIL=0,
00234     VCM_BSPL2=1,
00237     VCM_BSPL4=2
00238 };
00239
00244 typedef enum eVchrg_Meth Vchrg_Meth;
00245
00251 enum eVchrg_Src {
00252     VCM_CHARGE=0,
00253     VCM_PERMANENT=1,
00254     VCM_INDUCED=2,
00255     VCM_NLINDUCED=3
00256 };
00257
00262 typedef enum eVchrg_Src Vchrg_Src;
00263
00269 enum eVdata_Type {
00270     VDT_CHARGE,
00271     VDT_POT,
00272     VDT_ATOMPOT,
00273     VDT_SMOL,
00275     VDT_SSPL,
00277     VDT_VDW,
00279     VDT_IVDW,
00281     VDT_LAP,
00282     VDT_EDENS,
00284     VDT_NDENS,
00286     VDT_QDENS,
00288     VDT_DIELX,
00290     VDT_DIELY,
00292     VDT_DIELZ,
00294     VDT_KAPPA
00296 };
00297
00302 typedef enum eVdata_Type Vdata_Type;
00303
00309 enum eVdata_Format {
00310     VDF_DX=0,
00311     VDF_UHBD=1,
00312     VDF_AVS=2,
00313     VDF_MCSF=3,
00314     VDF_GZ=4,
00315     VDF_FLAT=5,
00316     VDF_DXBIN=6
00317 };
00318
00323 typedef enum eVdata_Format Vdata_Format;
00324
00329 #define APBS_TIMER_WALL_CLOCK 26
00330
00335 #define APBS_TIMER_SETUP 27
00336
00341 #define APBS_TIMER_SOLVER 28

```

```
00342
00347 #define APBS_TIMER_ENERGY 29
00348
00353 #define APBS_TIMER_FORCE 30
00354
00359 #define APBS_TIMER_TEMP1 31
00360
00365 #define APBS_TIMER_TEMP2 32
00366
00371 #define MAXMOL 5
00372
00377 #define MAXION 10
00378
00382 #define MAXFOCUS 5
00383
00387 #define VMGNLEV 4
00388
00392 #define VREDFRAC 0.25
00393
00397 #define VAPBS_NVS 4
00398
00402 #define VAPBS_DIM 3
00403
00408 #define VAPBS_RIGHT 0
00409
00414 #define VAPBS_FRONT 1
00415
00420 #define VAPBS_UP 2
00421
00426 #define VAPBS_LEFT 3
00427
00432 #define VAPBS_BACK 4
00433
00438 #define VAPBS_DOWN 5
00439
00444 #define VPMGSMALL 1e-12
00445
00450 #define SINH_MIN -85.0
00451
00456 #define SINH_MAX 85.0
00457
00458 #define MAX_HASH_DIM 75
00459
00460 #if defined(VDEBUG)
00461 #   if !defined(APBS_NOINLINE)
00462 #       define APBS_NOINLINE 1
00463 #   endif
00464 #endif
00465
00466 #if !defined(APBS_NOINLINE)
00467
00471 #   define VINLINE_VACC
00472
00476 #   define VINLINE_VATOM
00477
00481 #   define VINLINE_VCSM
00482
00486 #   define VINLINE_VPBE
00487
00491 #   define VINLINE_VPEE
00492
00496 #   define VINLINE_VGREEN
00497
00501 #   define VINLINE_VFETK
00502
00506 #   define VINLINE_VPMG
00507
00512 #endif
00513
00514 /* Fortran name mangling */
00515 #if defined(VF77_UPPERCASE)
00516 #   if defined(VF77_NOUNDERSCORE)
00517 #       define VF77_MANGLE(name,NAME) NAME
00518 #   elif defined(VF77_ONEUNDERSCORE)
00519 #       define VF77_MANGLE(name,NAME) NAME##_
00520 #   else
00521 #       define VF77_MANGLE(name,NAME) name
00522 #   endif
00523 #else
00524 #   if defined(VF77_NOUNDERSCORE)
00525 #       define VF77_MANGLE(name,NAME) name
```

```

00526 #   elif defined(VF77_ONEUNDERSCORE)
00527 #       define VF77_MANGLE(name,NAME) name ## _
00528 #   else
00532 #       define VF77_MANGLE(name,NAME) name
00533 #   endif
00534 #endif
00535
00536 /* Floating Point Error */
00537 #if defined(FLOAT_EPSILON)
00538 #   define VFLOOR(value) \
00539       ((floor(value) != floor(value + FLOAT_EPSILON)) ? \
00540        floor(value + FLOAT_EPSILON) : floor(value))
00541 #else
00547 #   define VFLOOR(value) floor(value)
00548 #endif
00549
00550 /* String embedding for ident */
00551 #if defined(HAVE_EMBED)
00556 #   define VEMBED(rctag) \
00557       VPRIVATE const char* rctag; \
00558       static void* use_rcsid=(0 ? &use_rcsid : (void*)&rcsid);
00559 #else
00564 #   define VEMBED(rctag)
00565 #endif /* if defined(HAVE_EMBED) */
00566
00567
00568
00570 #if !defined(__WIN32) || defined(__MINGW32__)
00571 #define PRINT_FUNC __PRETTY_FUNCTION__
00572 #define OS_SEP_STR "/"
00573 #define OS_SEP_CHAR '/'
00574 #else
00575 #define OS_SEP_STR "\\\"
00576 #define OS_SEP_CHAR '\\\"
00577 #define PRINT_FUNC __FUNCSIG__
00578 #define snprintf sprintf_s
00579 #endif
00580
00581 #ifdef VERBOSE_DEBUG
00582 #define ANNOUNCE_FUNCTION
00583     do {
00584         Vnm_print(2, "%s() [%s:%d]\n",
00585                 PRINT_FUNC, __FILE__, __LINE__ ); \
00586     } while(0)
00587
00588 #define WARN_UNTESTED
00589     do {
00590         Vnm_print(2, "%s() [%s:%d]: Untested Translation!\n", \
00591                 __FUNCTION__, __FILE__, __LINE__); \
00592     } while(0)
00593
00594 #define WARN_PARTTESTED
00595     do{
00596         Vnm_print(2, "%s() [%s:%d]: Partially Tested Translation.\n", \
00597                 __FUNCTION__, __FILE__, __LINE__); \
00598     } while(0)
00599 #else
00600 #define ANNOUNCE_FUNCTION
00601 #define WARN_UNTESTED
00602 #define WARN_PARTTESTED
00603 #endif
00604
00605
00606
00607 /* Utility messages.  Print out messages with location information */
00608 #ifdef DEBUG
00609 #define VCHANNELEDMESSAGE0(channel, msg)
00610     do {
00611         Vnm_print(channel, "%s:%d [%s()]: MESSAGE:\n"
00612                 "    %s\n\n",
00613                 __FILE__, __LINE__, __FUNCTION__, msg); \
00614     } while(0)
00615
00616 #define VCHANNELEDMESSAGE1(channel, msg, arg)
00617     do {
00618         char buff[1000];
00619         snprintf( buff, 1000, msg, arg );
00620         Vnm_print(channel, "%s:%d [%s()]: MESSAGE:\n"
00621                 "    %s\n\n",
00622                 __FILE__, __LINE__, __FUNCTION__, buff); \
00623     } while(0)

```

```

00624
00625 #define VCHANNELEDMESSAGE2(channel, msg, arg0, arg1)          \
00626     do {                                                        \
00627         char buff[1000];                                        \
00628         snprintf( buff, 1000, msg, arg0, arg1 );               \
00629         Vnm_print(channel, "%s:%d [%s()]: MESSAGE:\n"         \
00630             "    %s\n\n",                                     \
00631             __FILE__, __LINE__, __FUNCTION__, buff); \
00632     } while(0)
00633
00634 #define VCHANNELEDMESSAGE3(channel, msg, arg0, arg1, arg2)      \
00635     do {                                                        \
00636         char buff[1000];                                        \
00637         snprintf(buff, 1000, msg, arg0, arg1, arg2);           \
00638         Vnm_print(channel, "%s:%d [%s()]: MESSAGE:\n"         \
00639             "    %s\n\n",                                     \
00640             __FILE__, __LINE__, __FUNCTION__, buff); \
00641     } while(0)
00642
00643 #define VMESAGE0(msg) VCHANNELEDMESSAGE0(2, msg)
00644 #define VMESAGE1(msg, arg0) VCHANNELEDMESSAGE1(2, msg, arg0)
00645 #define VMESAGE2(msg, arg0, arg1) VCHANNELEDMESSAGE2(2, msg, arg0, arg1)
00646 #define VMESAGE3(msg, arg0, arg1, arg2) VCHANNELEDMESSAGE3(2, msg, arg0, arg1, arg2)
00647
00648 #define VERRMSG0(msg) VMESAGE0(msg)
00649 #define VERRMSG1(msg, arg0) VMESAGE1(msg, arg0)
00650 #define VERRMSG2(msg, arg0, arg1) VMESAGE2(msg, arg0, arg1)
00651 #define VERRMSG3(msg, arg0, arg1, arg2) VMESAGE3(msg, arg0, arg1, arg2)
00652 #else
00653 #define VCHANNELEDMESSAGE0(channel, msg)                        \
00654     do {                                                        \
00655         Vnm_print(channel, "%s: %s\n", __FUNCTION__, msg); \
00656     } while(0)
00657
00658 #define VCHANNELEDMESSAGE1(channel, msg, arg0)                \
00659     do {                                                        \
00660         char buff[1000];                                        \
00661         snprintf( buff, 1000, msg, arg0 );                     \
00662         Vnm_print(channel, "%s: %s\n", __FUNCTION__, buff); \
00663     } while(0)
00664
00665 #define VCHANNELEDMESSAGE2(channel, msg, arg0, arg1)          \
00666     do {                                                        \
00667         char buff[1000];                                        \
00668         snprintf( buff, 1000, msg, arg0, arg1 );               \
00669         Vnm_print(channel, "%s: %s\n", __FUNCTION__, buff); \
00670     } while(0)
00671
00672 #define VCHANNELEDMESSAGE3(channel, msg, arg0, arg1, arg2)      \
00673     do {                                                        \
00674         char buff[1000];                                        \
00675         snprintf(buff, 1000, msg, arg0, arg1, arg2);           \
00676         Vnm_print(channel, "%s: %s\n", __FUNCTION__, buff); \
00677     } while(0)
00678
00679 #define VMESAGE0(msg) VCHANNELEDMESSAGE0(0, msg)
00680 #define VMESAGE1(msg, arg0) VCHANNELEDMESSAGE1(0, msg, arg0)
00681 #define VMESAGE2(msg, arg0, arg1) VCHANNELEDMESSAGE2(0, msg, arg0, arg1)
00682 #define VMESAGE3(msg, arg0, arg1, arg2) VCHANNELEDMESSAGE3(0, msg, arg0, arg1, arg2)
00683
00684 #define VERRMSG0(msg) VCHANNELEDMESSAGE0(2, msg)
00685 #define VERRMSG1(msg, arg0) VCHANNELEDMESSAGE1(2, msg, arg0)
00686 #define VERRMSG2(msg, arg0, arg1) VCHANNELEDMESSAGE2(2, msg, arg0, arg1)
00687 #define VERRMSG3(msg, arg0, arg1, arg2) VCHANNELEDMESSAGE3(2, msg, arg0, arg1, arg2)
00688 #endif
00689
00690
00691
00692 /* Utility assertions. If they fail, they print out messages with possible
00693  * arguments and then abort
00694  * The do{...} while(0) simply enforces that a semicolon appears at the end
00695  */
00696 #ifdef DEBUG
00697 #define VASSERT_MSG0(cnd, msg)
00698     do {
00699         if( (cnd) == 0 ) {
00700             Vnm_print(2, "%s:%d [%s()]: ERROR:\n"
00701                 "    Assertion Failed (%s): %s\n\n",
00702                 __FILE__, __LINE__, __FUNCTION__, #cnd, msg);
00703             abort();
00704         }

```

```

00705     } while(0)
00706
00707 #define VASSERT_MSG1(cnd, msg, arg)
00708     do {
00709         if( (cnd) == 0 ) {
00710             char buff[1000];
00711             snprintf( buff, 1000, msg, arg );
00712             Vnm_print(2, "%s:%d [%s()]: ERROR:\n"
00713                 "      Assertion Failed (%s): %s\n\n",
00714                 __FILE__, __LINE__, __FUNCTION__, #cnd, buff);
00715             abort();
00716         }
00717     } while(0)
00718
00719 #define VASSERT_MSG2(cnd, msg, arg0, arg1)
00720     do {
00721         if( (cnd) == 0 ) {
00722             char buff[1000];
00723             snprintf( buff, 1000, msg, arg0, arg1 );
00724             Vnm_print(2, "%s:%d [%s()]: ERROR:\n"
00725                 "      Assertion Failed (%s): %s\n\n",
00726                 __FILE__, __LINE__, __FUNCTION__, #cnd, buff);
00727             abort();
00728         }
00729     } while(0)
00730 #else
00731 #define VASSERT_MSG0(cnd, msg)
00732     do {
00733         if( (cnd) == 0 ) {
00734             Vnm_print(2, "[%s()]: ERROR:\n"
00735                 "      Assertion Failed (%s): %s\n\n",
00736                 __FUNCTION__, #cnd, msg);
00737             abort();
00738         }
00739     } while(0)
00740
00741 #define VASSERT_MSG1(cnd, msg, arg)
00742     do {
00743         if( (cnd) == 0 ) {
00744             char buff[1000];
00745             snprintf( buff, 1000, msg, arg );
00746             Vnm_print(2, "[%s()]: ERROR:\n"
00747                 "      Assertion Failed (%s): %s\n\n",
00748                 __FUNCTION__, #cnd, buff);
00749             abort();
00750         }
00751     } while(0)
00752
00753 #define VASSERT_MSG2(cnd, msg, arg0, arg1)
00754     do {
00755         if( (cnd) == 0 ) {
00756             char buff[1000];
00757             snprintf( buff, 1000, msg, arg0, arg1 );
00758             Vnm_print(2, "[%s()]: ERROR:\n"
00759                 "      Assertion Failed (%s): %s\n\n",
00760                 __FUNCTION__, #cnd, buff);
00761             abort();
00762         }
00763     } while(0)
00764 #endif
00765
00766
00767
00768 /* Utility warning. Tests a condition and if it fails prints out a message
00769  * with optional arguments
00770  * The do{...} while(0) simply enforces that a semicolon at the end
00771  */
00772 #ifdef DEBUG
00773 #define VWARN_MSG0(cnd, msg)
00774     do {
00775         if( (cnd) == 0 ) {
00776             Vnm_print(
00777                 2,
00778                 "%s:%d [%s()]: WARNING:\n"
00779                 "      Condition Failed (%s): %s\n\n",
00780                 __FILE__,
00781                 __LINE__,
00782                 __FUNCTION__,
00783                 #cnd,
00784                 msg
00785             );

```

```

00786     }
00787     } while(0)
00788
00789 #define VWARN_MSG1(cnd, msg, arg0)
00790     do {
00791         if( (cnd) == 0 ) {
00792             char buff[1000];
00793             snprintf(buff, 1000, msg, arg0);
00794             Vnm_print(
00795                 2,
00796                 "%s:%d [%s()]: WARNING:\n"
00797                 "    Condition Failed (%s):\n    %s\n\n",
00798                 __FILE__,
00799                 __LINE__,
00800                 __FUNCTION__,
00801                 #cnd,
00802                 buff
00803             );
00804         }
00805     } while(0)
00806
00807 #define VWARN_MSG2(cnd, msg, arg0, arg1)
00808     do {
00809         if( (cnd) == 0 ) {
00810             char buff[1000];
00811             snprintf(buff, 1000, msg, arg0, arg1);
00812             Vnm_print(
00813                 2,
00814                 "%s:%d [%s()]: WARNING:\n"
00815                 "    Condition Failed (%s):\n    %s\n\n",
00816                 __FILE__,
00817                 __LINE__,
00818                 __FUNCTION__,
00819                 #cnd,
00820                 buff
00821             );
00822         }
00823     } while(0)
00824 #else
00825 #define VWARN_MSG0(cnd, msg)
00826     do {
00827         if( (cnd) == 0 ) {
00828             Vnm_print(
00829                 2,
00830                 "[%s()]: WARNING:\n"
00831                 "    %s\n\n",
00832                 __FUNCTION__,
00833                 msg
00834             );
00835         }
00836     } while(0)
00837
00838 #define VWARN_MSG1(cnd, msg, arg0)
00839     do {
00840         if( (cnd) == 0 ) {
00841             char buff[1000];
00842             snprintf(buff, 1000, msg, arg0);
00843             Vnm_print(
00844                 2,
00845                 "[%s()]: WARNING:\n"
00846                 "    %s\n\n",
00847                 __FUNCTION__,
00848                 buff
00849             );
00850         }
00851     } while(0)
00852
00853 #define VWARN_MSG2(cnd, msg, arg0, arg1)
00854     do {
00855         if( (cnd) == 0 ) {
00856             char buff[1000];
00857             snprintf(buff, 1000, msg, arg0, arg1);
00858             Vnm_print(
00859                 2,
00860                 "[%s()]: WARNING:\n"
00861                 "    %s\n\n",
00862                 __FUNCTION__,
00863                 buff
00864             );
00865         }
00866     } while(0)

```



```

00867 #endif
00868
00869 /* Utility Abort. Prints a message with optional arugments and aborts */
00870 #ifdef DEBUG
00871 #define VABORT_MSG0(msg) \
00872     do { \
00873         Vnm_print(2, "%s:%d [%s()]: ABORTING:\n" \
00874             "    %s\n\n", \
00875             __FILE__, __LINE__, __FUNCTION__, msg); \
00876         abort(); \
00877     } while(0)
00878
00879 #define VABORT_MSG1(msg, arg) \
00880     do { \
00881         char buff[1000]; \
00882         snprintf( buff, 1000, msg, arg ); \
00883         Vnm_print(2, "%s:%d [%s()]: ABORTING:\n" \
00884             "    %s\n\n", \
00885             __FILE__, __LINE__, __FUNCTION__, buff); \
00886         abort(); \
00887     } while(0)
00888
00889 #define VABORT_MSG2(msg, arg0, arg1) \
00890     do { \
00891         char buff[1000]; \
00892         snprintf( buff, 1000, msg, arg0, arg1); \
00893         Vnm_print(2, "%s:%d [%s()]: ABORTING:\n" \
00894             "    %s\n\n", \
00895             __FILE__, __LINE__, __FUNCTION__, buff); \
00896         abort(); \
00897     } while(0)
00898 #else
00899 #define VABORT_MSG0(msg) \
00900     do { \
00901         Vnm_print(2, "[%s()]: ABORTING:\n" \
00902             "    %s\n\n", \
00903             __FUNCTION__, msg); \
00904         abort(); \
00905     } while(0)
00906
00907 #define VABORT_MSG1(msg, arg) \
00908     do { \
00909         char buff[1000]; \
00910         snprintf( buff, 1000, msg, arg ); \
00911         Vnm_print(2, "[%s()]: ABORTING:\n" \
00912             "    %s\n\n", \
00913             __FUNCTION__, buff); \
00914         abort(); \
00915     } while(0)
00916
00917 #define VABORT_MSG2(msg, arg0, arg1) \
00918     do { \
00919         char buff[1000]; \
00920         snprintf( buff, 1000, msg, arg0, arg1); \
00921         Vnm_print(2, "[%s()]: ABORTING:\n" \
00922             "    %s\n\n", \
00923             __FUNCTION__, buff); \
00924         abort(); \
00925     } while(0)
00926 #endif
00927
00928
00929
00930 /* Utility expression printers. Print the expression and its value */
00931 #ifdef DEBUG
00932 #define PRINT_INT(expr) \
00933     do { \
00934         Vnm_print(2, "%s:%d [%s()]: %s == %d\n", \
00935             __FILE__, __LINE__, __FUNCTION__, #expr, expr); \
00936     } while(0)
00937
00938 #define PRINT_DBL(expr) \
00939     do { \
00940         Vnm_print(2, "%s:%d [%s()]: %s == %f\n", \
00941             __FILE__, __LINE__, __FUNCTION__, #expr, expr); \
00942     } while(0)
00943 #else
00944 #define PRINT_INT(expr)
00945 #define PRINT_DBL(expr)
00946 #endif
00947

```

```

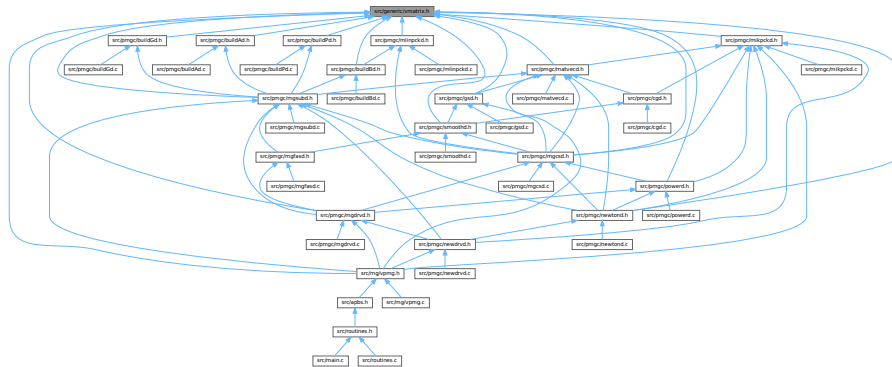
00948 #define VMALLOC(vmem, n, type) ((type*)Vmem_malloc(vmem, n, sizeof(type)))
00949
00950 #define VFREE(vmem, n, type, ptr) (Vmem_free(vmem, n, sizeof(type), (void **)&(ptr)))
00951
00952 #define VFILL(vec, n, val) \
00953     do { \
00954         int fill_idx; \
00955         for (fill_idx = 0; fill_idx < n; fill_idx++) \
00956             vec[fill_idx] = val; \
00957     } while(0)
00958
00959 #define VCOPY(srcvec, dstvec, i, n) \
00960     do { \
00961         for (i = 0; i < n; i++) \
00962             dstvec[i] = srcvec[i]; \
00963     } while(0)
00964
00965
00966 char* wrap_text( char* str, int right_margin, int left_padding );
00967
00968 #define VAT(array, i) ((array)[(i) - 1])
00969 #define RAT(array, i) ((array) + i - 1)
00970
00971 #endif /* #ifndef _VAPBSHAL_H_ */

```

9.76 src/generic/vmatrix.h File Reference

Contains inclusions for matrix data wrappers.

This graph shows which files directly or indirectly include this file:



Macros

- #define [MAT2](#)(mat, dx, dy)
- #define [RAT2](#)(mat, x, y) &[VAT2](#)(mat, x, y)
- #define [VAT2](#)(mat, x, y) mat[(y - 1) * dx_##mat + (x - 1)]
- #define [MAT3](#)(mat, dx, dy, dz)
- #define [RAT3](#)(mat, x, y, z) &[VAT3](#)(mat, x, y, z)
- #define [VAT3](#)(mat, x, y, z)

9.76.1 Detailed Description

Contains inclusions for matrix data wrappers.

Version

Author

Tucker A. Beck

Attention

```

*
* APBS -- Adaptive Poisson-Boltzmann Solver
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* Pacific Northwest National Laboratory
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* Additional contributing authors listed in the code documentation.
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*
*

```

Definition in file [vmatrix.h](#).

9.76.2 Macro Definition Documentation**9.76.2.1 MAT2**

```

#define MAT2(
    mat,
    dx,
    dy )

```

Value:

```
int dx_##mat = dx;    \
int dy_##mat = dy
```

Definition at line 64 of file [vmatrix.h](#).

9.76.2.2 MAT3

```
#define MAT3(
    mat,
    dx,
    dy,
    dz )
```

Value:

```
int dx_##mat = dx;    \
int dy_##mat = dy;    \
int dz_##mat = dz
```

Definition at line 76 of file [vmatrix.h](#).

9.76.2.3 RAT2

```
#define RAT2(
    mat,
    x,
    y ) &VAT2(mat, x, y)
```

Definition at line 68 of file [vmatrix.h](#).

9.76.2.4 RAT3

```
#define RAT3(
    mat,
    x,
    y,
    z ) &VAT3(mat, x, y, z)
```

Definition at line 81 of file [vmatrix.h](#).

9.76.2.5 VAT2

```
#define VAT2(
    mat,
    x,
    y ) mat[(y - 1) * dx_##mat + (x - 1)]
```

Definition at line 71 of file [vmatrix.h](#).

9.76.2.6 VAT3

```
#define VAT3(
    mat,
    x,
    y,
    z )
```

Value:

```
mat[(z - 1) * dy_##mat * dx_##mat + \
    (y - 1) * dx_##mat + \
```

```
(x - 1)]
```

Definition at line 84 of file [vmatrix.h](#).

9.77 vmatrix.h

[Go to the documentation of this file.](#)

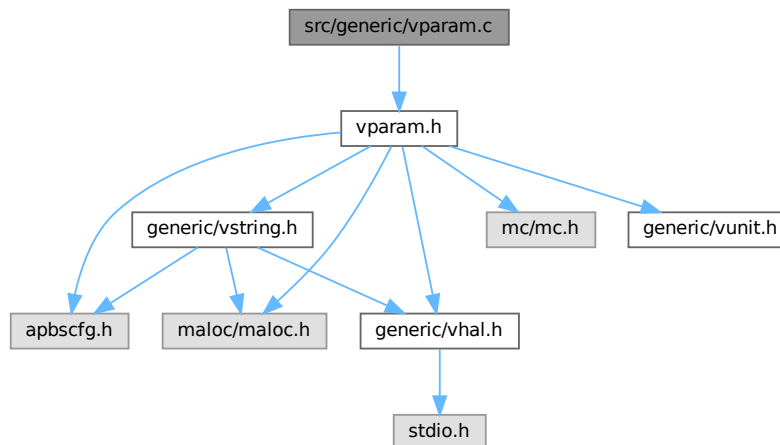
```
00001
00061 #ifndef _VMATRIX_H_
00062 #define _VMATRIX_H_
00063
00064 #define MAT2(mat, dx, dy) \
00065     int dx_##mat = dx; \
00066     int dy_##mat = dy
00067
00068 #define RAT2(mat, x, y) \
00069     &VAT2(mat, x, y)
00070
00071 #define VAT2(mat, x, y) \
00072     mat[(y - 1) * dx_##mat + (x - 1)]
00073
00074
00075
00076 #define MAT3(mat, dx, dy, dz) \
00077     int dx_##mat = dx; \
00078     int dy_##mat = dy; \
00079     int dz_##mat = dz
00080
00081 #define RAT3(mat, x, y, z) \
00082     &VAT3(mat, x, y, z)
00083
00084 #define VAT3(mat, x, y, z) \
00085     mat[(z - 1) * dy_##mat * dx_##mat + \
00086         (y - 1) * dx_##mat + \
00087         (x - 1)]
00088
00089 #endif /* _VMATRIX_H_ */
```

9.78 src/generic/vparam.c File Reference

Class [Vparam](#) methods.

```
#include "vparam.h"
```

Include dependency graph for vparam.c:



Functions

- VPRIVATE int [readFlatFileLine](#) (Vio *sock, [Vparam_AtomData](#) *atom)
Read a single line of the flat file database.
- VPRIVATE int [readXMLFileAtom](#) (Vio *sock, [Vparam_AtomData](#) *atom)
Read atom information from an XML file.
- VPUBLIC unsigned long int [Vparam_memChk](#) ([Vparam](#) *thee)
Get number of bytes in this object and its members.
- VPUBLIC [Vparam_AtomData](#) * [Vparam_AtomData_ctor](#) ()
Construct the object.
- VPUBLIC int [Vparam_AtomData_ctor2](#) ([Vparam_AtomData](#) *thee)
FORTTRAN stub to construct the object.
- VPUBLIC void [Vparam_AtomData_dtor](#) ([Vparam_AtomData](#) **thee)
Destroy object.
- VPUBLIC void [Vparam_AtomData_dtor2](#) ([Vparam_AtomData](#) *thee)
FORTTRAN stub to destroy object.
- VPUBLIC [Vparam_ResData](#) * [Vparam_ResData_ctor](#) (Vmem *mem)
Construct the object.
- VPUBLIC int [Vparam_ResData_ctor2](#) ([Vparam_ResData](#) *thee, Vmem *mem)
FORTTRAN stub to construct the object.
- VPUBLIC void [Vparam_ResData_dtor](#) ([Vparam_ResData](#) **thee)
Destroy object.
- VPUBLIC void [Vparam_ResData_dtor2](#) ([Vparam_ResData](#) *thee)
FORTTRAN stub to destroy object.
- VPUBLIC [Vparam](#) * [Vparam_ctor](#) ()
Construct the object.
- VPUBLIC int [Vparam_ctor2](#) ([Vparam](#) *thee)
FORTTRAN stub to construct the object.
- VPUBLIC void [Vparam_dtor](#) ([Vparam](#) **thee)
Destroy object.
- VPUBLIC void [Vparam_dtor2](#) ([Vparam](#) *thee)
FORTTRAN stub to destroy object.
- VPUBLIC [Vparam_ResData](#) * [Vparam_getResData](#) ([Vparam](#) *thee, char resName[VMAX_ARGLEN])
Get residue data.
- VPUBLIC [Vparam_AtomData](#) * [Vparam_getAtomData](#) ([Vparam](#) *thee, char resName[VMAX_ARGLEN], char atomName[VMAX_ARGLEN])
Get atom data.
- VPUBLIC int [Vparam_readXMLFile](#) ([Vparam](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname)
Read an XML format parameter database.
- VPUBLIC int [Vparam_readFlatFile](#) ([Vparam](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname)
Read a flat-file format parameter database.
- VEXTERNC void [Vparam_AtomData_copyTo](#) ([Vparam_AtomData](#) *thee, [Vparam_AtomData](#) *dest)
Copy current atom object to destination.
- VEXTERNC void [Vparam_ResData_copyTo](#) ([Vparam_ResData](#) *thee, [Vparam_ResData](#) *dest)
Copy current residue object to destination.
- VEXTERNC void [Vparam_AtomData_copyFrom](#) ([Vparam_AtomData](#) *thee, [Vparam_AtomData](#) *src)
Copy current atom object from another.

Variables

- VPRIVATE char * [MCwhiteChars](#) = " =,;\t\n\r"
Whitespace characters for socket reads.
- VPRIVATE char * [MCcommChars](#) = "#%"
Comment characters for socket reads.
- VPRIVATE char * [MCxmlwhiteChars](#) = " =,;\t\n\r<>"
Whitespace characters for XML socket reads.

9.78.1 Detailed Description

Class [Vparam](#) methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
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```

```

* INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN
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* THE POSSIBILITY OF SUCH DAMAGE.
*
*

```

Definition in file [vparam.c](#).

9.79 vparam.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "vparam.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061
00065 VPRIVATE char *MCwhiteChars = " =,;\t\n\r";
00066
00071 VPRIVATE char *MCcommChars = "##";
00072
00077 VPRIVATE char *MCxmlwhiteChars = " =,;\t\n\r<>";
00078
00087 VPRIVATE int readFlatFileLine(Vio *sock, Vparam_AtomData *atom);
00088
00097 VPRIVATE int readXMLFileAtom(Vio *sock, Vparam_AtomData *atom);
00098
00099
00100 #if !defined(VINLINE_VPARAM)
00101
00102 VPUBLIC unsigned long int Vparam_memChk(Vparam *thee) {
00103     if (thee == VNULL) return 0;
00104     return Vmem_bytes(thee->vmem);
00105 }
00106
00107 #endif /* if !defined(VINLINE_VPARAM) */
00108
00109 VPUBLIC Vparam_AtomData* Vparam_AtomData_ctor() {
00110
00111     Vparam_AtomData *thee = VNULL;
00112
00113     /* Set up the structure */
00114     thee = (Vparam_AtomData*)Vmem_malloc(VNULL, 1, sizeof(Vparam_AtomData) );
00115     VASSERT(thee != VNULL);
00116     VASSERT(Vparam_AtomData_ctor2(thee));
00117
00118     return thee;
00119 }
00120
00121 VPUBLIC int Vparam_AtomData_ctor2(Vparam_AtomData *thee) { return 1; }
00122
00123 VPUBLIC void Vparam_AtomData_dtor(Vparam_AtomData **thee) {
00124
00125     if ((*thee) != VNULL) {
00126         Vparam_AtomData_dtor2(*thee);
00127         Vmem_free(VNULL, 1, sizeof(Vparam_AtomData), (void **)thee);
00128         (*thee) = VNULL;
00129     }
00130
00131 }
00132
00133 VPUBLIC void Vparam_AtomData_dtor2(Vparam_AtomData *thee) { ; }
00134
00135 VPUBLIC Vparam_ResData* Vparam_ResData_ctor(Vmem *mem) {
00136
00137     Vparam_ResData *thee = VNULL;
00138
00139     /* Set up the structure */
00140     thee = (Vparam_ResData*)Vmem_malloc(mem, 1, sizeof(Vparam_ResData) );
00141     VASSERT(thee != VNULL);
00142     VASSERT(Vparam_ResData_ctor2(thee, mem));
00143
00144     return thee;
00145 }
00146

```



```

00147 VPUBLIC int Vparam_ResData_ctor2(Vparam_ResData *thee, Vmem *mem) {
00148
00149     if (thee == VNULL) {
00150         Vnm_print(2, "Vparam_ResData_ctor2: Got VNULL thee!\n");
00151         return 0;
00152     }
00153     thee->vmem = mem;
00154     thee->nAtomData = 0;
00155     thee->atomData = VNULL;
00156
00157     return 1;
00158 }
00159
00160 VPUBLIC void Vparam_ResData_dtor(Vparam_ResData **thee) {
00161
00162     if ((*thee) != VNULL) {
00163         Vparam_ResData_dtor2(*thee);
00164         Vmem_free((*thee)->vmem, 1, sizeof(Vparam_ResData), (void **)thee);
00165         (*thee) = VNULL;
00166     }
00167
00168 }
00169
00170 VPUBLIC void Vparam_ResData_dtor2(Vparam_ResData *thee) {
00171
00172     if (thee == VNULL) return;
00173     if (thee->nAtomData > 0) {
00174         Vmem_free(thee->vmem, thee->nAtomData, sizeof(Vparam_AtomData),
00175             (void **)&(thee->atomData));
00176     }
00177     thee->nAtomData = 0;
00178     thee->atomData = VNULL;
00179 }
00180
00181 VPUBLIC Vparam* Vparam_ctor() {
00182
00183     Vparam *thee = VNULL;
00184
00185     /* Set up the structure */
00186     thee = (Vparam*)Vmem_malloc(VNULL, 1, sizeof(Vparam) );
00187     VASSERT(thee != VNULL);
00188     VASSERT(Vparam_ctor2(thee));
00189
00190     return thee;
00191 }
00192
00193 VPUBLIC int Vparam_ctor2(Vparam *thee) {
00194
00195     if (thee == VNULL) {
00196         Vnm_print(2, "Vparam_ctor2: got VNULL thee!\n");
00197         return 0;
00198     }
00199
00200     thee->vmem = VNULL;
00201     thee->vmem = Vmem_ctor("APBS:VPARAM");
00202     if (thee->vmem == VNULL) {
00203         Vnm_print(2, "Vparam_ctor2: failed to init Vmem!\n");
00204         return 0;
00205     }
00206
00207     thee->nResData = 0;
00208     thee->resData = VNULL;
00209
00210     return 1;
00211 }
00212
00213 VPUBLIC void Vparam_dtor(Vparam **thee) {
00214
00215     if ((*thee) != VNULL) {
00216         Vparam_dtor2(*thee);
00217         Vmem_free(VNULL, 1, sizeof(Vparam), (void **)thee);
00218         (*thee) = VNULL;
00219     }
00220
00221 }
00222
00223 VPUBLIC void Vparam_dtor2(Vparam *thee) {
00224
00225     int i;
00226
00227     if (thee == VNULL) return;

```

```

00228
00229     /* Destroy the residue data */
00230     for (i=0; i<thee->nResData; i++) Vparam_ResData_dtor2(&(thee->resData[i]));
00231     if (thee->nResData > 0) Vmem_free(thee->vmem, thee->nResData,
00232         sizeof(Vparam_ResData), (void **)&(thee->resData));
00233     thee->nResData = 0;
00234     thee->resData = VNULL;
00235
00236     if (thee->vmem != VNULL) Vmem_dtor(&(thee->vmem));
00237     thee->vmem = VNULL;
00238
00239 }
00240
00241 VPUBLIC Vparam_ResData* Vparam_getResData(Vparam *thee,
00242     char resName[VMAX_ARGLEN]) {
00243     int i;
00244     Vparam_ResData *res = VNULL;
00245
00246     VASSERT(thee != VNULL);
00247
00248     if ((thee->nResData == 0) || (thee->resData == VNULL)) {
00249         res = VNULL;
00250         return res;
00251     }
00252
00253     /* Look for the matching residue */
00254     for (i=0; i<thee->nResData; i++) {
00255         res = &(thee->resData[i]);
00256         if (Vstring_strcasecmp(resName, res->name) == 0) return res;
00257     }
00258
00259     /* Didn't find a matching residue */
00260     res = VNULL;
00261     Vnm_print(2, "Vparam_getResData: unable to find res=%s\n", resName);
00262     return res;
00263 }
00264
00265
00266 VPUBLIC Vparam_AtomData* Vparam_getAtomData(Vparam *thee,
00267     char resName[VMAX_ARGLEN], char atomName[VMAX_ARGLEN]) {
00268     int i;
00269     Vparam_ResData *res = VNULL;
00270     Vparam_AtomData *atom = VNULL;
00271
00272     VASSERT(thee != VNULL);
00273
00274     if ((thee->nResData == 0) || (thee->resData == VNULL)) {
00275         atom = VNULL;
00276         return atom;
00277     }
00278
00279     /* Look for the matching residue */
00280     res = Vparam_getResData(thee, resName);
00281     if (res == VNULL) {
00282         atom = VNULL;
00283         Vnm_print(2, "Vparam_getAtomData: Unable to find residue %s!\n", resName);
00284         return atom;
00285     }
00286     for (i=0; i<res->nAtomData; i++) {
00287         atom = &(res->atomData[i]);
00288         if (atom == VNULL) {
00289             Vnm_print(2, "Vparam_getAtomData: got NULL atom!\n");
00290             return VNULL;
00291         }
00292         if (Vstring_strcasecmp(atomName, atom->atomName) == 0) {
00293             return atom;
00294         }
00295     }
00296
00297     /* Didn't find a matching atom/residue */
00298     atom = VNULL;
00299     Vnm_print(2, "Vparam_getAtomData: unable to find atom '%s', res '%s'\n",
00300         atomName, resName);
00301     return atom;
00302 }
00303
00304
00305 VPUBLIC int Vparam_readXMLFile(Vparam *thee, const char *iodev,
00306     const char *iofmt, const char *thost, const char *fname) {
00307
00308

```

```

00309     int i, ires, natoms, nalloc, ralloc;
00310     Vparam_AtomData *atoms = VNULL;
00311     Vparam_AtomData *tatoms = VNULL;
00312     Vparam_AtomData *atom = VNULL;
00313     Vparam_ResData *res = VNULL;
00314     Vparam_ResData *residues = VNULL;
00315     Vparam_ResData *tresidues = VNULL;
00316     Vio *sock = VNULL;
00317     char currResName[VMAX_ARGLEN];
00318     char tok[VMAX_ARGLEN];
00319     char endtag[VMAX_ARGLEN];
00320
00321     VASSERT(thee != VNULL);
00322
00323     /* Setup communication */
00324     sock = Vio_ctor(iodev, iofmt, thost, fname, "r");
00325     if (sock == VNULL) {
00326         Vnm_print(2, "Vparam_readXMLFile: Problem opening virtual socket %s\n",
00327             fname);
00328         return 0;
00329     }
00330     if (Vio_accept(sock, 0) < 0) {
00331         Vnm_print(2, "Vparam_readXMLFile: Problem accepting virtual socket %s\n",
00332             fname);
00333         return 0;
00334     }
00335     Vio_setWhiteChars(sock, MCxmlwhiteChars);
00336     Vio_setCommChars(sock, MCcommChars);
00337
00338     /* Clear existing parameters */
00339     if (thee->nResData > 0) {
00340         Vnm_print(2, "WARNING -- CLEARING PARAMETER DATABASE!\n");
00341         for (i=0; i<thee->nResData; i++) {
00342             Vparam_ResData_dtor2(&(thee->resData[i]));
00343         }
00344         Vmem_free(thee->vmem, thee->nResData,
00345             sizeof(Vparam_ResData), (void *)&(thee->resData));
00346     }
00347
00348     strcpy(endtag, "/");
00349
00350     /* Set up temporary residue list */
00351
00352     ralloc = 50;
00353     residues = (Vparam_ResData*)Vmem_malloc(thee->vmem, ralloc, sizeof(Vparam_ResData));
00354
00355     /* Read until we run out of entries, allocating space as needed */
00356     while (1) {
00357
00358         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00359
00360         /* The first token should be the start tag */
00361
00362         if (Vstring_strcasecmp(endtag, "/") == 0) strcat(endtag, tok);
00363
00364         if (Vstring_strcasecmp(tok, "residue") == 0) {
00365             if (thee->nResData >= ralloc) {
00366                 tresidues = (Vparam_ResData*)Vmem_malloc(thee->vmem, 2*ralloc, sizeof(Vparam_ResData));
00367                 VASSERT(tresidues != VNULL);
00368                 for (i=0; i<thee->nResData; i++) {
00369                     Vparam_ResData_copyTo(&(residues[i]), &(tresidues[i]));
00370                 }
00371                 Vmem_free(thee->vmem, ralloc, sizeof(Vparam_ResData),
00372                     (void *)&(residues));
00373                 residues = tresidues;
00374                 tresidues = VNULL;
00375                 ralloc = 2*ralloc;
00376             }
00377
00378             /* Initial space for this residue's atoms */
00379             nalloc = 20;
00380             natoms = 0;
00381             atoms = (Vparam_AtomData*)Vmem_malloc(thee->vmem, nalloc, sizeof(Vparam_AtomData));
00382
00383         } else if (Vstring_strcasecmp(tok, "name") == 0) {
00384             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1); /* value */
00385             strcpy(currResName, tok);
00386             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1); /* </name> */
00387         } else if (Vstring_strcasecmp(tok, "atom") == 0) {
00388             if (natoms >= nalloc) {
00389                 tatoms = (Vparam_AtomData*)Vmem_malloc(thee->vmem, 2*nalloc, sizeof(Vparam_AtomData));

```

```

00390         VASSERT(tatoms != VNULL);
00391         for (i=0; i<natoms; i++) {
00392             Vparam_AtomData_copyTo(&(atoms[i]), &(tatoms[i]));
00393         }
00394         Vmem_free(thee->vmem, nalloc, sizeof(Vparam_AtomData),
00395             (void **)&(atoms));
00396         atoms = tatoms;
00397         tatoms = VNULL;
00398         nalloc = 2*nalloc;
00399     }
00400     atom = &(atoms[natoms]);
00401     if (!readXMLFileAtom(sock, atom)) break;
00402     natoms++;
00403 }
00404 } else if (Vstring_strcasecmp(tok, "/residue") == 0) {
00405     res = &(residues[thee->nResData]);
00406     Vparam_ResData_ctor2(res, thee->vmem);
00407     res->atomData = (Vparam_AtomData*)Vmem_malloc(thee->vmem, natoms,
00408         sizeof(Vparam_AtomData));
00409     res->nAtomData = natoms;
00410     strcpy(res->name, currResName);
00411     for (i=0; i<natoms; i++) {
00412         strcpy(atoms[i].resName, currResName);
00413         Vparam_AtomData_copyTo(&(atoms[i]), &(res->atomData[i]));
00414     }
00415     Vmem_free(thee->vmem, nalloc, sizeof(Vparam_AtomData), (void **)&(atoms));
00416     (thee->nResData)++;
00417 }
00418 } else if (Vstring_strcasecmp(tok, endtag) == 0) break;
00419 }
00420 }
00421
00422 /* Initialize and copy the residues into the Vparam object */
00423
00424 thee->resData = (Vparam_ResData*)Vmem_malloc(thee->vmem, thee->nResData,
00425     sizeof(Vparam_ResData));
00426 for (ires=0; ires<thee->nResData; ires++) {
00427     Vparam_ResData_copyTo(&(residues[ires]), &(thee->resData[ires]));
00428 }
00429
00430 /* Destroy temporary atom space */
00431 Vmem_free(thee->vmem, ralloc, sizeof(Vparam_ResData), (void **)&(residues));
00432
00433 /* Shut down communication */
00434 Vio_acceptFree(sock);
00435 Vio_dtor(&sock);
00436
00437 return 1;
00438
00439 ERROR1:
00440     Vnm_print(2, "Vparam_readXMLFile: Got unexpected EOF reading parameter file!\n");
00441     return 0;
00442 }
00443 }
00444
00445 VPUBLIC int Vparam_readFlatFile(Vparam *thee, const char *iodev,
00446     const char *iofmt, const char *thost, const char *fname) {
00447     int i, iatom, jatom, ires, natoms, nalloc;
00448     Vparam_AtomData *atoms = VNULL;
00449     Vparam_AtomData *tatoms = VNULL;
00450     Vparam_AtomData *atom = VNULL;
00451     Vparam_ResData *res = VNULL;
00452     Vio *sock = VNULL;
00453     char currResName[VMAX_ARGLEN];
00454
00455     VASSERT(thee != VNULL);
00456
00457     /* Setup communication */
00458     sock = Vio_ctor(iodev, iofmt, thost, fname, "r");
00459     if (sock == VNULL) {
00460         Vnm_print(2, "Vparam_readFlatFile: Problem opening virtual socket %s\n",
00461             fname);
00462         return 0;
00463     }
00464     if (Vio_accept(sock, 0) < 0) {
00465         Vnm_print(2, "Vparam_readFlatFile: Problem accepting virtual socket %s\n",
00466             fname);
00467         return 0;
00468     }
00469     Vio_setWhiteChars(sock, MCwhiteChars);

```

```

00471     Vio_setCommChars(sock, MCcommChars);
00472
00473     /* Clear existing parameters */
00474     if (thee->nResData > 0) {
00475         Vnm_print(2, "WARNING -- CLEARING PARAMETER DATABASE!\n");
00476         for (i=0; i<thee->nResData; i++) {
00477             Vparam_ResData_dtor2(&(thee->resData[i]));
00478         }
00479         Vmem_free(thee->vmem, thee->nResData,
00480             sizeof(Vparam_ResData), (void **)&(thee->resData));
00481     }
00482
00483     /* Initial space for atoms */
00484     nalloc = 200;
00485     natoms = 0;
00486     atoms = (Vparam_AtomData*)Vmem_malloc(thee->vmem, nalloc, sizeof(Vparam_AtomData));
00487
00488     /* Read until we run out of entries, allocating space as needed */
00489     while (1) {
00490         if (natoms >= nalloc) {
00491             tatoms = (Vparam_AtomData*)Vmem_malloc(thee->vmem, 2*nalloc, sizeof(Vparam_AtomData));
00492             VASSERT(tatoms != VNULL);
00493             for (i=0; i<natoms; i++) {
00494                 Vparam_AtomData_copyTo(&(atoms[i]), &(tatoms[i]));
00495             }
00496             Vmem_free(thee->vmem, nalloc, sizeof(Vparam_AtomData),
00497                 (void **)&(atoms));
00498             atoms = tatoms;
00499             tatoms = VNULL;
00500             nalloc = 2*nalloc;
00501         }
00502         atom = &(atoms[natoms]);
00503         if (!readFlatFileLine(sock, atom)) break;
00504         natoms++;
00505     }
00506     if (natoms == 0) return 0;
00507
00508     /* Count the number of residues */
00509     thee->nResData = 1;
00510     strcpy(currResName, atoms[0].resName);
00511     for (i=1; i<natoms; i++) {
00512         if (Vstring_strcasecmp(atoms[i].resName, currResName) != 0) {
00513             strcpy(currResName, atoms[i].resName);
00514             (thee->nResData)++;
00515         }
00516     }
00517
00518     /* Create the residues */
00519     thee->resData = (Vparam_ResData*)Vmem_malloc(thee->vmem, thee->nResData,
00520         sizeof(Vparam_ResData));
00521     VASSERT(thee->resData != VNULL);
00522     for (i=0; i<(thee->nResData); i++) {
00523         res = &(thee->resData[i]);
00524         Vparam_ResData_ctor2(res, thee->vmem);
00525     }
00526
00527     /* Count the number of atoms per residue */
00528     ires = 0;
00529     res = &(thee->resData[ires]);
00530     res->nAtomData = 1;
00531     strcpy(res->name, atoms[0].resName);
00532     for (i=1; i<natoms; i++) {
00533         if (Vstring_strcasecmp(atoms[i].resName, res->name) != 0) {
00534             (ires)++;
00535             res = &(thee->resData[ires]);
00536             res->nAtomData = 1;
00537             strcpy(res->name, atoms[i].resName);
00538         } else (res->nAtomData)++;
00539     }
00540
00541     /* Allocate per-residue space for atoms */
00542     for (ires=0; ires<thee->nResData; ires++) {
00543         res = &(thee->resData[ires]);
00544         res->atomData = (Vparam_AtomData*)Vmem_malloc(thee->vmem, res->nAtomData,
00545             sizeof(Vparam_AtomData));
00546     }
00547
00548     /* Copy atoms into residues */
00549     iatom = 0;
00550     Vparam_AtomData_copyTo(&(atoms[0]), &(res->atomData[iatom]));
00551     for (ires=0; ires<thee->nResData; ires++) {

```

```

00552         res = &(thee->resData[ires]);
00553         for (jatom=0; jatom<res->nAtomData; jatom++) {
00554             Vparam_AtomData_copyTo(&(atoms[iatom]), &(res->atomData[jatom]));
00555             iatom++;
00556         }
00557     }
00558
00559     /* Shut down communication */
00560     Vio_acceptFree(sock);
00561     Vio_dtor(&sock);
00562
00563     /* Destroy temporary atom space */
00564     Vmem_free(thee->vmem, nalloc, sizeof(Vparam_AtomData), (void **)&(atoms));
00565
00566     return 1;
00567 }
00568
00569 }
00570
00571 VEXTERN void Vparam_AtomData_copyTo(Vparam_AtomData *thee,
00572     Vparam_AtomData *dest) {
00573     VASSERT(thee != VNULL);
00574     VASSERT(dest != VNULL);
00575
00576     strcpy(dest->atomName, thee->atomName);
00577     strcpy(dest->resName, thee->resName);
00578     dest->charge = thee->charge;
00579     dest->radius = thee->radius;
00580     dest->epsilon = thee->epsilon;
00581 }
00582
00583 }
00584
00585 VEXTERN void Vparam_ResData_copyTo(Vparam_ResData *thee,
00586     Vparam_ResData *dest) {
00587     int i;
00588
00589     VASSERT(thee != VNULL);
00590     VASSERT(dest != VNULL);
00591
00592     strcpy(dest->name, thee->name);
00593     dest->vmem = thee->vmem;
00594     dest->nAtomData = thee->nAtomData;
00595
00596     dest->atomData = (Vparam_AtomData*)Vmem_malloc(thee->vmem, dest->nAtomData,
00597         sizeof(Vparam_AtomData));
00598
00599     for (i=0; i<dest->nAtomData; i++) {
00600         Vparam_AtomData_copyTo(&(thee->atomData[i]), &(dest->atomData[i]));
00601     }
00602     Vmem_free(thee->vmem, thee->nAtomData, sizeof(Vparam_AtomData),
00603         (void **)&(thee->atomData));
00604 }
00605
00606 }
00607 VEXTERN void Vparam_AtomData_copyFrom(Vparam_AtomData *thee,
00608     Vparam_AtomData *src) { Vparam_AtomData_copyTo(src, thee); }
00609
00610 VPRIVATE int readXMLFileAtom(Vio *sock, Vparam_AtomData *atom) {
00611     double dtmp;
00612     char tok[VMAX_BUFSIZE];
00613     int chgflag, radflag, nameflag;
00614
00615     VASSERT(atom != VNULL);
00616
00617     if (Vio_scanf(sock, "%s", tok) != 1) return 0;
00618
00619     chgflag = 0;
00620     radflag = 0;
00621     nameflag = 0;
00622
00623     while (1)
00624     {
00625         if (Vstring_strcasecmp(tok, "name") == 0) {
00626             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00627             if (strlen(tok) > VMAX_ARGLEN) {
00628                 Vnm_print(2, "Vparam_readXMLFileAtom: string (%s) too long \
00629 (%d)!\n", tok, strlen(tok));
00630                 return 0;
00631             }
00632         }

```

```

00633         nameflag = 1;
00634         strcpy(atom->atomName, tok);
00635     } else if (Vstring_strcasecmp(tok, "charge") == 0) {
00636         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00637         if (sscanf(tok, "%lf", &dtmp) != 1) {
00638             Vnm_print(2, "Vparam_readXMLFileAtom: Unexpected token (%s) while \
00639 parsing charge!\n", tok);
00640             return 0;
00641         }
00642         chgflag = 1;
00643         atom->charge = dtmp;
00644     } else if (Vstring_strcasecmp(tok, "radius") == 0) {
00645         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00646         if (sscanf(tok, "%lf", &dtmp) != 1) {
00647             Vnm_print(2, "Vparam_readXMLFileAtom: Unexpected token (%s) while \
00648 parsing radius!\n", tok);
00649             return 0;
00650         }
00651         radflag = 1;
00652         atom->radius = dtmp;
00653     } else if (Vstring_strcasecmp(tok, "epsilon") == 0) {
00654         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00655         if (sscanf(tok, "%lf", &dtmp) != 1) {
00656             Vnm_print(2, "Vparam_readXMLFileAtom: Unexpected token (%s) while \
00657 parsing epsilon!\n", tok);
00658             return 0;
00659         }
00660         atom->epsilon = dtmp;
00661     } else if ((Vstring_strcasecmp(tok, "/atom") == 0) ||
00662                (Vstring_strcasecmp(tok, "atom") == 0)){
00663         if (chgflag && radflag && nameflag) return 1;
00664         else if (!chgflag) {
00665             Vnm_print(2, "Vparam_readXMLFileAtom: Reached end of atom without \
00666 setting the charge!\n");
00667             return 0;
00668         } else if (!radflag) {
00669             Vnm_print(2, "Vparam_readXMLFileAtom: Reached end of atom without \
00670 setting the radius!\n");
00671             return 0;
00672         } else if (!nameflag) {
00673             Vnm_print(2, "Vparam_readXMLFileAtom: Reached end of atom without \
00674 setting the name!\n");
00675             return 0;
00676         }
00677     }
00678     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00679 }
00680
00681 /* If we get here something wrong has happened */
00682 VJMPERR1(1);
00683
00684
00685 VERROR1:
00686     Vnm_print(2, "Vparam_readXMLFileAtom: Got unexpected EOF reading parameter file!\n");
00687     return 0;
00688 }
00689
00690
00691 VPRIVATE int readFlatFileLine(Vio *sock, Vparam_AtomData *atom) {
00692
00693     double dtmp;
00694     char tok[VMAX_BUFSIZE];
00695
00696     VASSERT(atom != VNULL);
00697
00698     if (Vio_scanf(sock, "%s", tok) != 1) return 0;
00699     if (strlen(tok) > VMAX_ARGLEN) {
00700         Vnm_print(2, "Vparam_readFlatFile: string (%s) too long (%d)!\n",
00701                 tok, strlen(tok));
00702         return 0;
00703     }
00704     strcpy(atom->resName, tok);
00705     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00706     if (strlen(tok) > VMAX_ARGLEN) {
00707         Vnm_print(2, "Vparam_readFlatFile: string (%s) too long (%d)!\n",
00708                 tok, strlen(tok));
00709         return 0;
00710     }
00711     strcpy(atom->atomName, tok);
00712     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00713     if (sscanf(tok, "%lf", &dtmp) != 1) {

```

```

00714         Vnm_print(2, "Vparam_readFlatFile: Unexpected token (%s) while \
00715 parsing charge!\n", tok);
00716         return 0;
00717     }
00718     atom->charge = dtmp;
00719     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00720     if (sscanf(tok, "%lf", &dtmp) != 1) {
00721         Vnm_print(2, "Vparam_readFlatFile: Unexpected token (%s) while \
00722 parsing radius!\n", tok);
00723         return 0;
00724     }
00725     atom->radius = dtmp;
00726     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00727     if (sscanf(tok, "%lf", &dtmp) != 1) {
00728         Vnm_print(2, "Vparam_readFlatFile: Unexpected token (%s) while \
00729 parsing radius!\n", tok);
00730         return 0;
00731     }
00732     atom->epsilon = dtmp;
00733     return 1;
00734 }
00735
00736 ERROR1:
00737     Vnm_print(2, "Vparam_readFlatFile: Got unexpected EOF reading parameter file!\n");
00738     return 0;
00739 }

```

9.80 src/generic/vparam.h File Reference

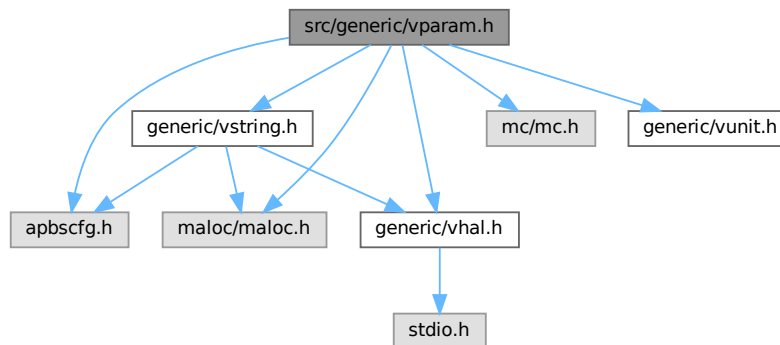
Contains declarations for class [Vparam](#).

```

#include "apbscfg.h"
#include "maloc/maloc.h"
#include "mc/mc.h"
#include "generic/vhal.h"
#include "generic/vunit.h"
#include "generic/vstring.h"

```

Include dependency graph for vparam.h:



[illegible]

- struct **sVparam_AtomData**
AtomData sub-class; stores atom data.
- struct **Vparam_ResData**
ResData sub-class; stores residue data.
- struct **Vparam**
Reads and assigns charge/radii parameters.

- typedef struct [sVparam_AtomData](#) [Vparam_AtomData](#)
Declaration of the [Vparam_AtomData](#) class as the [sVparam_AtomData](#) structure.
- typedef struct [Vparam_ResData](#) [Vparam_ResData](#)
Declaration of the [Vparam_ResData](#) class as the [Vparam_ResData](#) structure.
- typedef struct [Vparam](#) [Vparam](#)
Declaration of the [Vparam](#) class as the [Vparam](#) structure.

- VEXTERNC unsigned long int `Vparam_memChk (Vparam *thee)`
Get number of bytes in this object and its members.
- VEXTERNC `Vparam_AtomData * Vparam_AtomData_ctor ()`
Construct the object.
- VEXTERNC int `Vparam_AtomData_ctor2 (Vparam_AtomData *thee)`
FORTRAN stub to construct the object.
- VEXTERNC void `Vparam_AtomData_dtor (Vparam_AtomData **thee)`
Destroy object.
- VEXTERNC void `Vparam_AtomData_dtor2 (Vparam_AtomData *thee)`
FORTRAN stub to destroy object.
- VEXTERNC void `Vparam_AtomData_copyTo (Vparam_AtomData *thee, Vparam_AtomData *dest)`
Copy current atom object to destination.
- VEXTERNC void `Vparam_ResData_copyTo (Vparam_ResData *thee, Vparam_ResData *dest)`

- Copy current residue object to destination.*

 - VEXTERNC void `Vparam_AtomData_copyFrom` (`Vparam_AtomData *thee`, `Vparam_AtomData *src`)
- Copy current atom object from another.*

 - VEXTERNC `Vparam_ResData * Vparam_ResData_ctor` (`Vmem *mem`)
- Construct the object.*

 - VEXTERNC int `Vparam_ResData_ctor2` (`Vparam_ResData *thee`, `Vmem *mem`)
- FORTTRAN stub to construct the object.*

 - VEXTERNC void `Vparam_ResData_dtor` (`Vparam_ResData **thee`)
- Destroy object.*

 - VEXTERNC void `Vparam_ResData_dtor2` (`Vparam_ResData *thee`)
- FORTTRAN stub to destroy object.*

 - VEXTERNC `Vparam * Vparam_ctor` ()
- Construct the object.*

 - VEXTERNC int `Vparam_ctor2` (`Vparam *thee`)
- FORTTRAN stub to construct the object.*

 - VEXTERNC void `Vparam_dtor` (`Vparam **thee`)
- Destroy object.*

 - VEXTERNC void `Vparam_dtor2` (`Vparam *thee`)
- FORTTRAN stub to destroy object.*

 - VEXTERNC `Vparam_ResData * Vparam_getResData` (`Vparam *thee`, `char resName[VMAX_ARGLEN]`)
- Get residue data.*

 - VEXTERNC `Vparam_AtomData * Vparam_getAtomData` (`Vparam *thee`, `char resName[VMAX_ARGLEN]`, `char atomName[VMAX_ARGLEN]`)
- Get atom data.*

 - VEXTERNC int `Vparam_readFlatFile` (`Vparam *thee`, `const char *iodev`, `const char *iofmt`, `const char *thost`, `const char *fname`)
- Read a flat-file format parameter database.*

 - VEXTERNC int `Vparam_readXMLFile` (`Vparam *thee`, `const char *iodev`, `const char *iofmt`, `const char *thost`, `const char *fname`)
- Read an XML format parameter database.*

9.80.1 Detailed Description

Contains declarations for class `Vparam`.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```

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*
*

```

Definition in file [vparam.h](#).

9.81 vparam.h

[Go to the documentation of this file.](#)

```

00001
00062 #ifndef _VPARAM_H_
00063 #define _VPARAM_H_
00064
00065 #include "apbscfg.h"
00066
00067 #include "malloc/malloc.h"
00068 #if defined(HAVE_MC_H)
00069 #include "mc/mc.h"
00070 #endif
00071
00072 #include "generic/vhal.h"
00073 #include "generic/vunit.h"
00074 #include "generic/vstring.h"
00075

```

```

00092 struct sVparam_AtomData {
00093     char  atomName[VMAX_ARGLEN];
00094     char  resName[VMAX_ARGLEN];
00095     double charge;
00096     double radius;
00097     double epsilon;
00099 };
00100
00106 typedef struct sVparam_AtomData Vparam_AtomData;
00107
00114 struct Vparam_ResData {
00115     Vmem *vmem;
00116     char  name[VMAX_ARGLEN];
00117     int   nAtomData;
00119     Vparam_AtomData *atomData;
00120 };
00121
00127 typedef struct Vparam_ResData Vparam_ResData;
00128
00135 struct Vparam {
00136
00137     Vmem *vmem;
00138     int   nResData;
00140     Vparam_ResData *resData;
00141 };
00142
00147 typedef struct Vparam Vparam;
00148
00149 /* ////////////////////////////////////////
00150 // Class Vparam: Inlineable methods (vparam.c)
00152 #if !defined(VINLINE_VPARAM)
00154
00161     VEXTERNC unsigned long int Vparam_memChk(Vparam *thee);
00162
00163 #else /* if defined(VINLINE_VPARAM) */
00164 #   define Vparam_memChk(thee) (Vmem_bytes((thee)->vmem))
00166 #endif /* if !defined(VINLINE_VPARAM) */
00168
00169 /* ////////////////////////////////////////
00170 // Class Vparam: Non-Inlineable methods (vparam.c)
00172
00177 VEXTERNC Vparam_AtomData* Vparam_AtomData_ctor();
00178
00184 VEXTERNC int Vparam_AtomData_ctor2(Vparam_AtomData *thee);
00185
00190 VEXTERNC void Vparam_AtomData_dtor(Vparam_AtomData **thee);
00191
00196 VEXTERNC void Vparam_AtomData_dtor2(Vparam_AtomData *thee);
00197
00205 VEXTERNC void Vparam_AtomData_copyTo(Vparam_AtomData *thee,
00206     Vparam_AtomData *dest);
00207
00215 VEXTERNC void Vparam_ResData_copyTo(Vparam_ResData *thee,
00216     Vparam_ResData *dest);
00217
00225 VEXTERNC void Vparam_AtomData_copyFrom(Vparam_AtomData *thee,
00226     Vparam_AtomData *src);
00227
00233 VEXTERNC Vparam_ResData* Vparam_ResData_ctor(Vmem *mem);
00234
00241 VEXTERNC int Vparam_ResData_ctor2(Vparam_ResData *thee, Vmem *mem);
00242
00247 VEXTERNC void Vparam_ResData_dtor(Vparam_ResData **thee);
00248
00253 VEXTERNC void Vparam_ResData_dtor2(Vparam_ResData *thee);
00254
00259 VEXTERNC Vparam* Vparam_ctor();
00260
00266 VEXTERNC int Vparam_ctor2(Vparam *thee);
00267
00272 VEXTERNC void Vparam_dtor(Vparam **thee);
00273
00278 VEXTERNC void Vparam_dtor2(Vparam *thee);
00279
00290 VEXTERNC Vparam_ResData* Vparam_getResData(Vparam *thee,
00291     char resName[VMAX_ARGLEN]);
00292
00304 VEXTERNC Vparam_AtomData* Vparam_getAtomData(Vparam *thee,

```

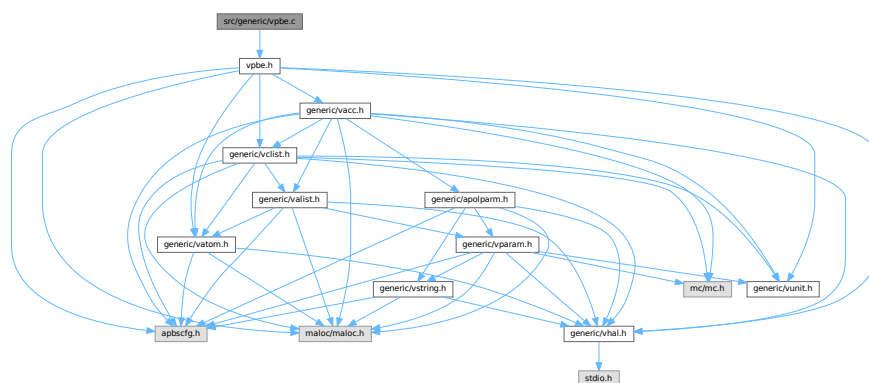
```
00305 char resName[VMAX_ARGLEN], char atomName[VMAX_ARGLEN]);
00306
00336 VEXTERNC int Vparam_readFlatFile(Vparam *thee, const char *iodev,
00336     const char *iofmt, const char *thost, const char *fname);
00337
00348 VEXTERNC int Vparam_readXMLFile(Vparam *thee, const char *iodev,
00348     const char *iofmt, const char *thost, const char *fname);
00350
00351 #endif /* ifndef VPARAM_H */
```

9.82 src/generic/vpbe.c File Reference

Class Vpbe methods.

```
#include "vpbe.h"
```

Include dependency graph for vpbe.c:



Macros

- #define MAX SPLINE WINDOW 0.5

Functions

- VPUBLIC Valist * Vpbe_getValist (Vpbe *three)
Get atom list.
- VPUBLIC Vacc * Vpbe_getVacc (Vpbe *three)
Get accessibility oracle.
- VPUBLIC double Vpbe_getBulkIonicStrength (Vpbe *three)
Get bulk ionic strength.
- VPUBLIC double Vpbe_getTemperature (Vpbe *three)
Get temperature.
- VPUBLIC double Vpbe_getSoluteDiel (Vpbe *three)
Get solute dielectric constant.
- VPUBLIC double * Vpbe_getSoluteCenter (Vpbe *three)
Get coordinates of solute center.
- VPUBLIC double Vpbe_getSolventDiel (Vpbe *three)
Get solvent dielectric constant.
- VPUBLIC double Vpbe_getSolventRadius (Vpbe *three)
Get solvent molecule radius.

- VPUBLIC double [Vpbe_getMaxIonRadius](#) (Vpbe *thee)
Get maximum radius of ion species.
- VPUBLIC double [Vpbe_getXkappa](#) (Vpbe *thee)
Get Debye-Huckel parameter.
- VPUBLIC double [Vpbe_getDeblen](#) (Vpbe *thee)
Get Debye-Huckel screening length.
- VPUBLIC double [Vpbe_getZkappa2](#) (Vpbe *thee)
Get modified squared Debye-Huckel parameter.
- VPUBLIC double [Vpbe_getZmagic](#) (Vpbe *thee)
Get charge scaling factor.
- VPUBLIC double [Vpbe_getSoluteRadius](#) (Vpbe *thee)
Get sphere radius which bounds biomolecule.
- VPUBLIC double [Vpbe_getSoluteXlen](#) (Vpbe *thee)
Get length of solute in x dimension.
- VPUBLIC double [Vpbe_getSoluteYlen](#) (Vpbe *thee)
Get length of solute in y dimension.
- VPUBLIC double [Vpbe_getSoluteZlen](#) (Vpbe *thee)
Get length of solute in z dimension.
- VPUBLIC double [Vpbe_getSoluteCharge](#) (Vpbe *thee)
Get total solute charge.
- VPUBLIC double [Vpbe_getzmem](#) (Vpbe *thee)
Get z position of the membrane bottom.
- VPUBLIC double [Vpbe_getLmem](#) (Vpbe *thee)
Get length of the membrane (A)
author Michael Grabe.
- VPUBLIC double [Vpbe_getmembraneDiel](#) (Vpbe *thee)
Get membrane dielectric constant.
- VPUBLIC double [Vpbe_getmemv](#) (Vpbe *thee)
Get membrane potential (kT)
- VPUBLIC Vpbe * [Vpbe_ctor](#) (Valist *alist, int ionNum, double *ionConc, double *ionRadii, double *ionQ, double T, double soluteDiel, double solventDiel, double solventRadius, int focusFlag, double sdens, double z_mem, double L, double membraneDiel, double V)
Construct Vpbe object.
- VPUBLIC int [Vpbe_ctor2](#) (Vpbe *thee, Valist *alist, int ionNum, double *ionConc, double *ionRadii, double *ionQ, double T, double soluteDiel, double solventDiel, double solventRadius, int focusFlag, double sdens, double z_↔mem, double L, double membraneDiel, double V)
FORTTRAN stub to construct Vpbe objct.
- VPUBLIC void [Vpbe_dtor](#) (Vpbe **thee)
Object destructor.
- VPUBLIC void [Vpbe_dtor2](#) (Vpbe *thee)
FORTTRAN stub object destructor.
- VPUBLIC double [Vpbe_getCoulombEnergy1](#) (Vpbe *thee)
Calculate coulombic energy of set of charges.
- VPUBLIC unsigned long int [Vpbe_memChk](#) (Vpbe *thee)
Return the memory used by this structure (and its contents) in bytes.
- VPUBLIC int [Vpbe_getIons](#) (Vpbe *thee, int *nion, double ionConc[[MAXION](#)], double ionRadii[[MAXION](#)], double ionQ[[MAXION](#)])
Get information about the counterion species present.

9.82.1 Detailed Description

Class Vpbe methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
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*
*
```

Definition in file [vpbe.c](#).

9.82.2 Macro Definition Documentation

9.82.2.1 MAX_SPLINE_WINDOW

#define MAX_SPLINE_WINDOW 0.5

Definition at line 62 of file [vpbe.c](#).

9.83 vpbe.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "vpbe.h"
00058
00059 /* ////////////////////////////////////////
00060 // Class Vpbe: Private method declaration
00062 #define MAX_SPLINE_WINDOW 0.5
00063
00064 /* ////////////////////////////////////////
00065 // Class Vpbe: Inlineable methods
00067 #if !defined(VINLINE_VPBE)
00068
00069 VPUBLIC Valist* Vpbe_getValist(Vpbe *thee) {
00070
00071     VASSERT(thee != VNULL);
00072     return thee->alist;
00073 }
00074 }
00075
00076 VPUBLIC Vacc* Vpbe_getVacc(Vpbe *thee) {
00077
00078     VASSERT(thee != VNULL);
00079     VASSERT(thee->paramFlag);
00080     return thee->acc;
00081 }
00082 }
00083
00084 VPUBLIC double Vpbe_getBulkIonicStrength(Vpbe *thee) {
00085
00086     VASSERT(thee != VNULL);
00087     VASSERT(thee->paramFlag);
00088     return thee->bulkIonicStrength;
00089 }
00090
00091 VPUBLIC double Vpbe_getTemperature(Vpbe *thee) {
00092
00093     VASSERT(thee != VNULL);
00094     VASSERT(thee->paramFlag);
00095     return thee->T;
00096 }
00097 }
00098
00099 VPUBLIC double Vpbe_getSoluteDiel(Vpbe *thee) {
00100
00101     VASSERT(thee != VNULL);
00102     VASSERT(thee->paramFlag);
00103     return thee->soluteDiel;
00104 }
00105 }
00106
00107 VPUBLIC double* Vpbe_getSoluteCenter(Vpbe *thee) {
00108
00109     VASSERT(thee != VNULL);
00110     return thee->soluteCenter;
00111 }
00112
00113 VPUBLIC double Vpbe_getSolventDiel(Vpbe *thee) {
00114
00115     VASSERT(thee != VNULL);
00116     VASSERT(thee->paramFlag);
00117     return thee->solventDiel;
00118 }
00119
00120 VPUBLIC double Vpbe_getSolventRadius(Vpbe *thee) {
00121
00122     VASSERT(thee != VNULL);
00123     VASSERT(thee->paramFlag);
00124     return thee->solventRadius;
00125 }
00126

```



```

00127 VPUBLIC double Vpbe_getMaxIonRadius(Vpbe *thee) {
00128
00129     VASSERT(thee != VNULL);
00130     VASSERT(thee->paramFlag);
00131     return thee->maxIonRadius;
00132 }
00133
00134 VPUBLIC double Vpbe_getXkappa(Vpbe *thee) {
00135
00136     VASSERT(thee != VNULL);
00137     VASSERT(thee->paramFlag);
00138     return thee->xkappa;
00139 }
00140
00141 VPUBLIC double Vpbe_getDeblen(Vpbe *thee) {
00142
00143     VASSERT(thee != VNULL);
00144     VASSERT(thee->paramFlag);
00145     return thee->deblen;
00146 }
00147
00148 VPUBLIC double Vpbe_getZkappa2(Vpbe *thee) {
00149
00150     VASSERT(thee != VNULL);
00151     VASSERT(thee->paramFlag);
00152     return thee->zkappa2;
00153 }
00154
00155 VPUBLIC double Vpbe_getZmagic(Vpbe *thee) {
00156
00157     VASSERT(thee != VNULL);
00158     VASSERT(thee->paramFlag);
00159     return thee->zmagic;
00160 }
00161
00162 VPUBLIC double Vpbe_getSoluteRadius(Vpbe *thee) {
00163
00164     VASSERT(thee != VNULL);
00165     return thee->soluteRadius;
00166 }
00167
00168 VPUBLIC double Vpbe_getSoluteXlen(Vpbe *thee) {
00169
00170     VASSERT(thee != VNULL);
00171     return thee->soluteXlen;
00172 }
00173
00174 VPUBLIC double Vpbe_getSoluteYlen(Vpbe *thee) {
00175
00176     VASSERT(thee != VNULL);
00177     return thee->soluteYlen;
00178 }
00179
00180 VPUBLIC double Vpbe_getSoluteZlen(Vpbe *thee) {
00181
00182     VASSERT(thee != VNULL);
00183     return thee->soluteZlen;
00184 }
00185
00186 VPUBLIC double Vpbe_getSoluteCharge(Vpbe *thee) {
00187
00188     VASSERT(thee != VNULL);
00189     return thee->soluteCharge;
00190 }
00191
00192 /* ////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////
00193 // Routine: Vpbe_getzmem
00194 // Purpose: This routine returns values stored in the structure thee.
00195 // Author: Michael Grabe
00197 VPUBLIC double Vpbe_getzmem(Vpbe *thee) {
00198
00199     VASSERT(thee != VNULL);
00200     VASSERT(thee->param2Flag);
00201     return thee->z_mem;
00202 }
00203
00204 /* ////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////
00205 // Routine: Vpbe_getLmem
00206 // Purpose: This routine returns values stored in the structure thee.
00207 // Author: Michael Grabe
00209 VPUBLIC double Vpbe_getLmem(Vpbe *thee) {

```

```

00210
00211     VASSERT(thee != VNULL);
00212     VASSERT(thee->param2Flag);
00213     return thee->L;
00214 }
00215
00216 /* ////////////////////////////////////////
00217 // Routine: Vpbe_getmembraneDiel
00218 // Purpose: This routine returns values stored in the structure thee.
00219 // Author: Michael Grabe
00221 VPUBLIC double Vpbe_getmembraneDiel(Vpbe *thee) {
00222
00223     VASSERT(thee != VNULL);
00224     VASSERT(thee->param2Flag);
00225     return thee->membraneDiel;
00226 }
00227
00228 /* ////////////////////////////////////////
00229 // Routine: Vpbe_getmemv
00230 // Purpose: This routine returns values stored in the structure thee.
00231 // Author: Michael Grabe
00233 VPUBLIC double Vpbe_getmemv(Vpbe *thee) {
00234
00235     VASSERT(thee != VNULL);
00236     VASSERT(thee->param2Flag);
00237     return thee->V;
00238 }
00239
00240 #endif /* if !defined(VINLINE_VPBE) */
00241
00242 /* ////////////////////////////////////////
00243 // Class Vpbe: Non-inlineable methods
00245
00246 VPUBLIC Vpbe* Vpbe_ctor(Valist *alist, int ionNum, double *ionConc,
00247                        double *ionRadii, double *ionQ, double T,
00248                        double soluteDiel, double solventDiel,
00249                        double solventRadius, int focusFlag, double sdens,
00250                        double z_mem, double L, double membraneDiel, double V ) {
00251
00252     /* Set up the structure */
00253     Vpbe *thee = VNULL;
00254     thee = (Vpbe*)Vmem_malloc(VNULL, 1, sizeof(Vpbe) );
00255     VASSERT( thee != VNULL);
00256     VASSERT( Vpbe_ctor2(thee, alist, ionNum, ionConc, ionRadii, ionQ,
00257                        T, soluteDiel, solventDiel, solventRadius, focusFlag, sdens,
00258                        z_mem, L, membraneDiel, V) );
00259
00260     return thee;
00261 }
00262
00263
00264 VPUBLIC int Vpbe_ctor2(Vpbe *thee, Valist *alist, int ionNum,
00265                      double *ionConc, double *ionRadii,
00266                      double *ionQ, double T, double soluteDiel,
00267                      double solventDiel, double solventRadius, int focusFlag,
00268                      double sdens, double z_mem, double L, double membraneDiel,
00269                      double V) {
00270
00271     int i, iatom, inhash[3];
00272     double atomRadius;
00273     Vatom *atom;
00274     double center[3] = {0.0, 0.0, 0.0};
00275     double lower_corner[3] = {0.0, 0.0, 0.0};
00276     double upper_corner[3] = {0.0, 0.0, 0.0};
00277     double disp[3], dist, radius, charge, xmin, xmax, ymin, ymax, zmin, zmax;
00278     double x, y, z, netCharge;
00279     double nhash[3];
00280     const double N_A = 6.022045000e+23;
00281     const double e_c = 4.803242384e-10;
00282     const double k_B = 1.380662000e-16;
00283     const double pi = 4. * VATAN(1.);
00284
00285     /* Set up memory management object */
00286     thee->vmem = Vmem_ctor("APBS:VPBE");
00287
00288     VASSERT(thee != VNULL);
00289     if (alist == VNULL) {
00290         Vnm_print(2, "Vpbe_ctor2: Got null pointer to Valist object!\n");
00291         return 0;
00292     }
00293

```

```

00294      /* **** STUFF THAT GETS DONE FOR EVERYONE **** */
00295      /* Set pointers */
00296      thee->alist = alist;
00297      thee->paramFlag = 0;
00298
00299      /* Determine solute center */
00300      center[0] = thee->alist->center[0];
00301      center[1] = thee->alist->center[1];
00302      center[2] = thee->alist->center[2];
00303      thee->soluteCenter[0] = center[0];
00304      thee->soluteCenter[1] = center[1];
00305      thee->soluteCenter[2] = center[2];
00306
00307      /* Determine solute length and charge*/
00308      radius = 0;
00309      atom = Valist_getAtom(thee->alist, 0);
00310      xmin = Vatom_getPosition(atom)[0];
00311      xmax = Vatom_getPosition(atom)[0];
00312      ymin = Vatom_getPosition(atom)[1];
00313      ymax = Vatom_getPosition(atom)[1];
00314      zmin = Vatom_getPosition(atom)[2];
00315      zmax = Vatom_getPosition(atom)[2];
00316      charge = 0;
00317      for (iatom=0; iatom<Valist_getNumberAtoms(thee->alist); iatom++) {
00318          atom = Valist_getAtom(thee->alist, iatom);
00319          atomRadius = Vatom_getRadius(atom);
00320          x = Vatom_getPosition(atom)[0];
00321          y = Vatom_getPosition(atom)[1];
00322          z = Vatom_getPosition(atom)[2];
00323          if ((x+atomRadius) > xmax) xmax = x + atomRadius;
00324          if ((x-atomRadius) < xmin) xmin = x - atomRadius;
00325          if ((y+atomRadius) > ymax) ymax = y + atomRadius;
00326          if ((y-atomRadius) < ymin) ymin = y - atomRadius;
00327          if ((z+atomRadius) > zmax) zmax = z + atomRadius;
00328          if ((z-atomRadius) < zmin) zmin = z - atomRadius;
00329          disp[0] = (x - center[0]);
00330          disp[1] = (y - center[1]);
00331          disp[2] = (z - center[2]);
00332          dist = (disp[0]*disp[0]) + (disp[1]*disp[1]) + (disp[2]*disp[2]);
00333          dist = VSQRT(dist) + atomRadius;
00334          if (dist > radius) radius = dist;
00335          charge += Vatom_getCharge(Valist_getAtom(thee->alist, iatom));
00336      }
00337      thee->soluteRadius = radius;
00338      Vnm_print(0, "Vpbe_ctor2: solute radius = %g\n", radius);
00339      thee->soluteXlen = xmax - xmin;
00340      thee->soluteYlen = ymax - ymin;
00341      thee->soluteZlen = zmax - zmin;
00342      Vnm_print(0, "Vpbe_ctor2: solute dimensions = %g x %g x %g\n",
00343              thee->soluteXlen, thee->soluteYlen, thee->soluteZlen);
00344      thee->soluteCharge = charge;
00345      Vnm_print(0, "Vpbe_ctor2: solute charge = %g\n", charge);
00346
00347      /* Set parameters */
00348      thee->numIon = ionNum;
00349      if (thee->numIon >= MAXION) {
00350          Vnm_print(2, "Vpbe_ctor2: Too many ion species (MAX = %d)!\n",
00351                  MAXION);
00352          return 0;
00353      }
00354      thee->bulkIonicStrength = 0.0;
00355      thee->maxIonRadius = 0.0;
00356      netCharge = 0.0;
00357      for (i=0; i<thee->numIon; i++) {
00358          thee->ionConc[i] = ionConc[i];
00359          thee->ionRadii[i] = ionRadii[i];
00360          if (ionRadii[i] > thee->maxIonRadius) thee->maxIonRadius = ionRadii[i];
00361          thee->ionQ[i] = ionQ[i];
00362          thee->bulkIonicStrength += (0.5*ionConc[i]*VSQR(ionQ[i]));
00363          netCharge += (ionConc[i]*ionQ[i]);
00364      }
00365      #ifndef VAPBSQUIET
00366          Vnm_print(1, " Vpbe_ctor: Using max ion radius (%g A) for exclusion \
00367 function\n", thee->maxIonRadius);
00368      #endif
00369      if (VABS(netCharge) > VSMALL) {
00370          Vnm_print(2, "Vpbe_ctor2: You have a counterion charge imbalance!\n");
00371          Vnm_print(2, "Vpbe_ctor2: Net charge conc. = %g M\n", netCharge);
00372          return 0;
00373      }
00374      thee->T = T;

```

```

00375     thee->soluteDiel = soluteDiel;
00376     thee->solventDiel = solventDiel;
00377     thee->solventRadius = solventRadius;
00378
00379     /* Compute parameters:
00380     *
00381     *  $\kappa^2 = (8 \pi N_A e_c^2) I_s / (1000 \epsilon_w k_B T)$ 
00382     *  $\kappa = 0.325567 * I_s^{1/2}$  angstroms-1
00383     *  $deblen = 1 / \kappa$ 
00384     *  $= 3.071564378 * I_s^{1/2}$  angstroms
00385     *  $\bar{\kappa}^2 = \epsilon_w * \kappa^2$ 
00386     *  $z_{magic} = (4 * \pi * e_c^2) / (k_B T)$  (we scale the diagonal later)
00387     *  $= 7046.528838$ 
00388     */
00389     if (thee->T == 0.0) {
00390         Vnm_print(2, "Vpbe_ctor2: You set the temperature to 0 K.\n");
00391         Vnm_print(2, "Vpbe_ctor2: That violates the 3rd Law of Thermo!");
00392         return 0;
00393     }
00394     if (thee->bulkIonicStrength == 0.) {
00395         thee->xkappa = 0.;
00396         thee->deblen = 0.;
00397         thee->zkappa2 = 0.;
00398     } else {
00399         thee->xkappa = VSQRT( thee->bulkIonicStrength * 1.0e-16 *
00400             ((8.0 * pi * N_A * e_c * e_c) /
00401              (1000.0 * thee->solventDiel * k_B * T))
00402         );
00403         thee->deblen = 1. / thee->xkappa;
00404         thee->zkappa2 = thee->solventDiel * VSQR(thee->xkappa);
00405     }
00406     Vnm_print(0, "Vpbe_ctor2: bulk ionic strength = %g\n",
00407         thee->bulkIonicStrength);
00408     Vnm_print(0, "Vpbe_ctor2: xkappa = %g\n", thee->xkappa);
00409     Vnm_print(0, "Vpbe_ctor2: Debye length = %g\n", thee->deblen);
00410     Vnm_print(0, "Vpbe_ctor2: zkappa2 = %g\n", thee->zkappa2);
00411     thee->zmagic = ((4.0 * pi * e_c * e_c) / (k_B * thee->T)) * 1.0e+8;
00412     Vnm_print(0, "Vpbe_ctor2: zmagic = %g\n", thee->zmagic);
00413
00414     /* Compute accessibility objects:
00415     * - Allow for extra room in the case of spline windowing
00416     * - Place some limits on the size of the hash table in the case of very
00417     *   large molecules
00418     */
00419     if (thee->maxIonRadius > thee->solventRadius)
00420         radius = thee->maxIonRadius + MAX_SPLINE_WINDOW;
00421     else radius = thee->solventRadius + MAX_SPLINE_WINDOW;
00422
00423     nhash[0] = (thee->soluteXlen)/0.5;
00424     nhash[1] = (thee->soluteYlen)/0.5;
00425     nhash[2] = (thee->soluteZlen)/0.5;
00426     for (i=0; i<3; i++) inhash[i] = (int) (nhash[i]);
00427
00428     for (i=0; i<3; i++){
00429         if (inhash[i] < 3) inhash[i] = 3;
00430         if (inhash[i] > MAX_HASH_DIM) inhash[i] = MAX_HASH_DIM;
00431     }
00432     Vnm_print(0, "Vpbe_ctor2: Constructing Vclist with %d x %d x %d table\n",
00433         inhash[0], inhash[1], inhash[2]);
00434
00435     thee->clist = Vclist_ctor(thee->alist, radius, inhash,
00436         CLIST_AUTO_DOMAIN, lower_corner, upper_corner);
00437
00438     VASSERT(thee->clist != VNULL);
00439     thee->acc = Vacc_ctor(thee->alist, thee->clist, sdens);
00440
00441     VASSERT(thee->acc != VNULL);
00442
00443     /* SMPBE Added */
00444     thee->smsize = 0.0;
00445     thee->smvolume = 0.0;
00446     thee->ipkey = 0;
00447
00448     thee->paramFlag = 1;
00449
00450     /*-----*/
00451     /* added by Michael Grabe */
00452     /*-----*/
00453
00454     thee->z_mem = z_mem;
00455     thee->L = L;

```

```

00456     thee->membraneDiel = membraneDiel;
00457     thee->V = V;
00458
00459     if (V != 0.0) thee->param2Flag = 1;
00460     else thee->param2Flag = 0;
00461
00462     /*-----*/
00463
00464     return 1;
00465 }
00466
00467 VPUBLIC void Vpbe_dtor(Vpbe **thee) {
00468     if ((*thee) != VNULL) {
00469         Vpbe_dtor2(*thee);
00470         Vmem_free(VNULL, 1, sizeof(Vpbe), (void **)thee);
00471         (*thee) = VNULL;
00472     }
00473 }
00474
00475 VPUBLIC void Vpbe_dtor2(Vpbe *thee) {
00476     Vclist_dtor(&(thee->clist));
00477     Vacc_dtor(&(thee->acc));
00478     Vmem_dtor(&(thee->vmem));
00479 }
00480
00481 VPUBLIC double Vpbe_getCoulombEnergy1(Vpbe *thee) {
00482
00483     int i, j, k, natoms;
00484
00485     double dist, *ipos, *jpos, icharge, jcharge;
00486     double energy = 0.0;
00487     double eps, T;
00488     Vatom *iatom, *jatom;
00489     Valist *alist;
00490
00491     VASSERT(thee != VNULL);
00492     alist = Vpbe_getValist(thee);
00493     VASSERT(alist != VNULL);
00494     natoms = Valist_getNumberAtoms(alist);
00495
00496     /* Do the sum */
00497     for (i=0; i<natoms; i++) {
00498         iatom = Valist_getAtom(alist,i);
00499         icharge = Vatom_getCharge(iatom);
00500         ipos = Vatom_getPosition(iatom);
00501         for (j=i+1; j<natoms; j++) {
00502             jatom = Valist_getAtom(alist,j);
00503             jcharge = Vatom_getCharge(jatom);
00504             jpos = Vatom_getPosition(jatom);
00505             dist = 0;
00506             for (k=0; k<3; k++) dist += ((ipos[k]-jpos[k])*(ipos[k]-jpos[k]));
00507             dist = VSQRT(dist);
00508             energy = energy + icharge*jcharge/dist;
00509         }
00510     }
00511
00512     /* Convert the result to J */
00513     T = Vpbe_getTemperature(thee);
00514     eps = Vpbe_getSoluteDiel(thee);
00515     energy = energy*Vunit_ec*Vunit_ec/(4*Vunit_pi*Vunit_eps0*eps*(1.0e-10));
00516
00517     /* Scale by Boltzmann energy */
00518     energy = energy/(Vunit_kb*T);
00519
00520     return energy;
00521 }
00522
00523 VPUBLIC unsigned long int Vpbe_memChk(Vpbe *thee) {
00524
00525     unsigned long int memUse = 0;
00526
00527     if (thee == VNULL) return 0;
00528
00529     memUse = memUse + sizeof(Vpbe);
00530     memUse = memUse + (unsigned long int)Vacc_memChk(thee->acc);
00531
00532     return memUse;
00533 }
00534
00535 VPUBLIC int Vpbe_getIons(Vpbe *thee, int *nion, double ionConc[MAXION],
00536     double ionRadii[MAXION], double ionQ[MAXION]) {

```

```

00537
00538     int i;
00539
00540     VASSERT(thee != VNULL);
00541
00542     *nion = thee->numIon;
00543     for (i=0; i<(*nion); i++) {
00544         ionConc[i] = thee->ionConc[i];
00545         ionRadii[i] = thee->ionRadii[i];
00546         ionQ[i] = thee->ionQ[i];
00547     }
00548
00549     return *nion;
00550 }

```

9.84 src/generic/vpbe.h File Reference

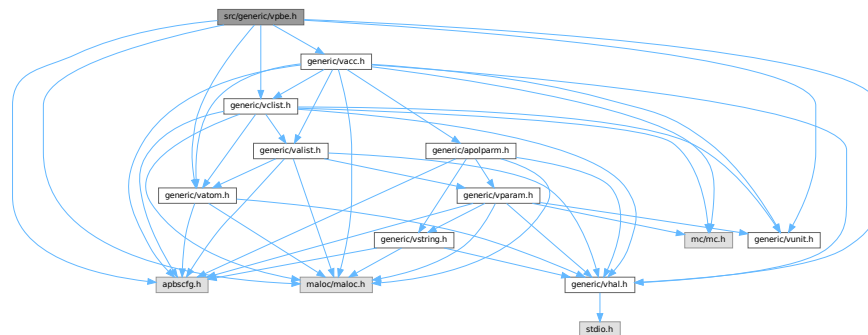
Contains declarations for class Vpbe.

```

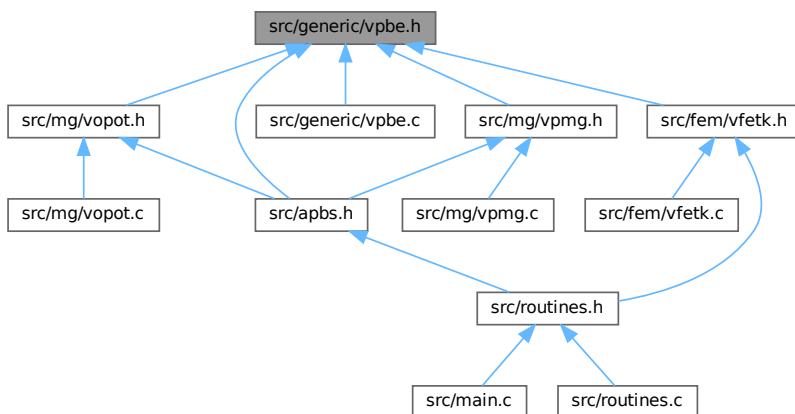
#include "apbscfg.h"
#include "maloc/maloc.h"
#include "generic/vhal.h"
#include "generic/vunit.h"
#include "generic/vatom.h"
#include "generic/vacc.h"
#include "generic/vclist.h"

```

Include dependency graph for vpbe.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVpbe](#)
Contains public data members for Vpbe class/module.

Typedefs

- typedef struct [sVpbe](#) [Vpbe](#)
Declaration of the Vpbe class as the Vpbe structure.

Functions

- VEXTERNC [Valist](#) * [Vpbe_getValist](#) ([Vpbe](#) *thee)
Get atom list.
- VEXTERNC [Vacc](#) * [Vpbe_getVacc](#) ([Vpbe](#) *thee)
Get accessibility oracle.
- VEXTERNC double [Vpbe_getBulkIonicStrength](#) ([Vpbe](#) *thee)
Get bulk ionic strength.
- VEXTERNC double [Vpbe_getMaxIonRadius](#) ([Vpbe](#) *thee)
Get maximum radius of ion species.
- VEXTERNC double [Vpbe_getTemperature](#) ([Vpbe](#) *thee)
Get temperature.
- VEXTERNC double [Vpbe_getSoluteDiel](#) ([Vpbe](#) *thee)
Get solute dielectric constant.
- VEXTERNC double [Vpbe_getGamma](#) ([Vpbe](#) *thee)
Get apolar coefficient.
- VEXTERNC double [Vpbe_getSoluteRadius](#) ([Vpbe](#) *thee)
Get sphere radius which bounds biomolecule.
- VEXTERNC double [Vpbe_getSoluteXlen](#) ([Vpbe](#) *thee)
Get length of solute in x dimension.

- VEXTERNC double [Vpbe_getSoluteYlen](#) ([Vpbe](#) *thee)
Get length of solute in y dimension.
- VEXTERNC double [Vpbe_getSoluteZlen](#) ([Vpbe](#) *thee)
Get length of solute in z dimension.
- VEXTERNC double * [Vpbe_getSoluteCenter](#) ([Vpbe](#) *thee)
Get coordinates of solute center.
- VEXTERNC double [Vpbe_getSoluteCharge](#) ([Vpbe](#) *thee)
Get total solute charge.
- VEXTERNC double [Vpbe_getSolventDiel](#) ([Vpbe](#) *thee)
Get solvent dielectric constant.
- VEXTERNC double [Vpbe_getSolventRadius](#) ([Vpbe](#) *thee)
Get solvent molecule radius.
- VEXTERNC double [Vpbe_getXkappa](#) ([Vpbe](#) *thee)
Get Debye-Huckel parameter.
- VEXTERNC double [Vpbe_getDeblen](#) ([Vpbe](#) *thee)
Get Debye-Huckel screening length.
- VEXTERNC double [Vpbe_getZkappa2](#) ([Vpbe](#) *thee)
Get modified squared Debye-Huckel parameter.
- VEXTERNC double [Vpbe_getZmagic](#) ([Vpbe](#) *thee)
Get charge scaling factor.
- VEXTERNC double [Vpbe_getzmem](#) ([Vpbe](#) *thee)
Get z position of the membrane bottom.
- VEXTERNC double [Vpbe_getLmem](#) ([Vpbe](#) *thee)
Get length of the membrane (A)
author Michael Grabe.
- VEXTERNC double [Vpbe_getmembraneDiel](#) ([Vpbe](#) *thee)
Get membrane dielectric constant.
- VEXTERNC double [Vpbe_getmemv](#) ([Vpbe](#) *thee)
Get membrane potential (kT)
- VEXTERNC [Vpbe](#) * [Vpbe_ctor](#) ([Valist](#) *alist, int ionNum, double *ionConc, double *ionRadii, double *ionQ, double T, double soluteDiel, double solventDiel, double solventRadius, int focusFlag, double sdens, double z_↵mem, double L, double membraneDiel, double V)
Construct Vpbe object.
- VEXTERNC int [Vpbe_ctor2](#) ([Vpbe](#) *thee, [Valist](#) *alist, int ionNum, double *ionConc, double *ionRadii, double *ionQ, double T, double soluteDiel, double solventDiel, double solventRadius, int focusFlag, double sdens, double z_mem, double L, double membraneDiel, double V)
FORTTRAN stub to construct Vpbe objct.
- VEXTERNC int [Vpbe_getlons](#) ([Vpbe](#) *thee, int *nion, double ionConc[[MAXION](#)], double ionRadii[[MAXION](#)], double ionQ[[MAXION](#)])
Get information about the counterion species present.
- VEXTERNC void [Vpbe_dtor](#) ([Vpbe](#) **thee)
Object destructor.
- VEXTERNC void [Vpbe_dtor2](#) ([Vpbe](#) *thee)
FORTTRAN stub object destructor.
- VEXTERNC double [Vpbe_getCoulombEnergy1](#) ([Vpbe](#) *thee)
Calculate coulombic energy of set of charges.
- VEXTERNC unsigned long int [Vpbe_memChk](#) ([Vpbe](#) *thee)
Return the memory used by this structure (and its contents) in bytes.

9.84.1 Detailed Description

Contains declarations for class Vpbe.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
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* Pacific Northwest National Laboratory
*
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*
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* THE POSSIBILITY OF SUCH DAMAGE.
*
*
```

Definition in file [vpbe.h](#).

9.85 vpbe.h

[Go to the documentation of this file.](#)

```

00001
00066 #ifndef _VPBE_H_
00067 #define _VPBE_H_
00068
00069 #include "apbscfg.h"
00070
00071 #include "malloc/malloc.h"
00072
00073 #include "generic/vhal.h"
00074 #include "generic/vunit.h"
00075 #include "generic/vatom.h"
00076 #include "generic/vacc.h"
00077 #include "generic/vclist.h"
00078
00084 struct sVpbe {
00085
00086     Vmem *vmem;
00088     Valist *alist;
00089     Vclist *clist;
00090     Vacc *acc;
00092     double T;
00093     double soluteDiel;
00094     double solventDiel;
00095     double solventRadius;
00099     double bulkIonicStrength;
00100     double maxIonRadius;
00103     int numIon;
00104     double ionConc[MAXION];
00105     double ionRadii[MAXION];
00106     double ionQ[MAXION];
00108     double xkappa;
00109     double deblen;
00110     double zkappa2;
00111     double zmagic;
00113     double soluteCenter[3];
00114     double soluteRadius;
00115     double soluteXlen;
00116     double soluteYlen;
00117     double soluteZlen;
00118     double soluteCharge;
00120     double smvolume;
00121     double smsize;
00122     int ipkey;
00125     int paramFlag;
00127     /*-----*/
00128     /* Added by Michael Grabe */
00129     /*-----*/
00130
00131     double z_mem;
00132     double L;
00133     double membraneDiel;
00134     double V;
00135     int param2Flag;
00136     /*-----*/
00137
00138 };
00139
00144 typedef struct sVpbe Vpbe;
00145
00146 /* ////////////////////////////////////// */
00147 // Class Vpbe: Inlineable methods (vpbe.c)
00149
00150 #if !defined(VINLINE_VPBE)
00151
00158 VEXTERNC Valist* Vpbe_getValist(Vpbe *thee);
00159
00166 VEXTERNC Vacc* Vpbe_getVacc(Vpbe *thee);
00167
00174 VEXTERNC double Vpbe_getBulkIonicStrength(Vpbe *thee);
00175
00182 VEXTERNC double Vpbe_getMaxIonRadius(Vpbe *thee);
00183
00190 VEXTERNC double Vpbe_getTemperature(Vpbe *thee);
00191
00198 VEXTERNC double Vpbe_getSoluteDiel(Vpbe *thee);
00199
00206 VEXTERNC double Vpbe_getGamma(Vpbe *thee);
00207
00214 VEXTERNC double Vpbe_getSoluteRadius(Vpbe *thee);
00215
00222 VEXTERNC double Vpbe_getSoluteXlen(Vpbe *thee);

```

```

00223
00230 VEXTERNC double  Vpbe_getSoluteYlen(Vpbe *thee);
00231
00238 VEXTERNC double  Vpbe_getSoluteZlen(Vpbe *thee);
00239
00246 VEXTERNC double* Vpbe_getSoluteCenter(Vpbe *thee);
00247
00254 VEXTERNC double  Vpbe_getSoluteCharge(Vpbe *thee);
00255
00262 VEXTERNC double  Vpbe_getSolventDiel(Vpbe *thee);
00263
00270 VEXTERNC double  Vpbe_getSolventRadius(Vpbe *thee);
00271
00278 VEXTERNC double  Vpbe_getXkappa(Vpbe *thee);
00279
00286 VEXTERNC double  Vpbe_getDeblen(Vpbe *thee);
00287
00294 VEXTERNC double  Vpbe_getZkappa2(Vpbe *thee);
00295
00302 VEXTERNC double  Vpbe_getZmagic(Vpbe *thee);
00303
00304 /*-----*/
00305 /* Added by Michael Grabe */
00306 /*-----*/
00307
00314 VEXTERNC double  Vpbe_getzmem(Vpbe *thee);
00315
00322 VEXTERNC double  Vpbe_getLmem(Vpbe *thee);
00323
00330 VEXTERNC double  Vpbe_getmembraneDiel(Vpbe *thee);
00331
00337 VEXTERNC double  Vpbe_getmemv(Vpbe *thee);
00338
00339 /*-----*/
00340
00341 #else /* if defined(VINLINE_VPBE) */
00342 #   define Vpbe_getValist(thee) ((thee)->alist)
00343 #   define Vpbe_getVacc(thee) ((thee)->acc)
00344 #   define Vpbe_getBulkIonicStrength(thee) ((thee)->bulkIonicStrength)
00345 #   define Vpbe_getTemperature(thee) ((thee)->T)
00346 #   define Vpbe_getSoluteDiel(thee) ((thee)->soluteDiel)
00347 #   define Vpbe_getSoluteCenter(thee) ((thee)->soluteCenter)
00348 #   define Vpbe_getSoluteRadius(thee) ((thee)->soluteRadius)
00349 #   define Vpbe_getSoluteXlen(thee) ((thee)->soluteXlen)
00350 #   define Vpbe_getSoluteYlen(thee) ((thee)->soluteYlen)
00351 #   define Vpbe_getSoluteZlen(thee) ((thee)->soluteZlen)
00352 #   define Vpbe_getSoluteCharge(thee) ((thee)->soluteCharge)
00353 #   define Vpbe_getSolventDiel(thee) ((thee)->solventDiel)
00354 #   define Vpbe_getSolventRadius(thee) ((thee)->solventRadius)
00355 #   define Vpbe_getMaxIonRadius(thee) ((thee)->maxIonRadius)
00356 #   define Vpbe_getXkappa(thee) ((thee)->xkappa)
00357 #   define Vpbe_getDeblen(thee) ((thee)->deblen)
00358 #   define Vpbe_getZkappa2(thee) ((thee)->zkappa2)
00359 #   define Vpbe_getZmagic(thee) ((thee)->zmagic)
00360
00361 /*-----*/
00362 /* Added by Michael Grabe */
00363 /*-----*/
00364
00365 #   define Vpbe_getzmem(thee) ((thee)->z_mem)
00366 #   define Vpbe_getLmem(thee) ((thee)->L)
00367 #   define Vpbe_getmembraneDiel(thee) ((thee)->membraneDiel)
00368 #   define Vpbe_getmemv(thee) ((thee)->V)
00369
00370 /*-----*/
00371
00372
00373 #endif /* if !defined(VINLINE_VPBE) */
00374
00375 /* ////////////////////////////////////// */
00376 // Class Vpbe: Non-Inlineable methods (vpbe.c)
00377
00399 VEXTERNC Vpbe*  Vpbe_ctor(
00400     Valist *alist, /**< Atom list */
00401     int ionNum,
00402     double *ionConc,
00403     double *ionRadii,
00404     double *ionQ,
00405     double T,
00406     double soluteDiel,
00407     double solventDiel,

```

```

00408             double solventRadius,
00409             int focusFlag,
00410             double sdens,
00411             double z_mem,
00412             double L,
00413             double membraneDiel,
00414             double V
00415         );
00416
00437 VEXTERNC int    Vpbe_ctor2(
00438                 Vpbe *thee,
00439                 Valist *alist,
00440                 int ionNum,
00441                 double *ionConc,
00442                 double *ionRadii,
00443                 double *ionQ,
00444                 double T,
00445                 double soluteDiel,
00446                 double solventDiel,
00447                 double solventRadius,
00448                 int focusFlag,
00449                 double sdens,
00450                 double z_mem,
00451                 double L,
00452                 double membraneDiel,
00453                 double V
00454             );
00455
00466 VEXTERNC int    Vpbe_getIons(Vpbe *thee, int *nion, double ionConc[MAXION],
00467                               double ionRadii[MAXION], double ionQ[MAXION]);
00468
00474 VEXTERNC void    Vpbe_dtor(Vpbe **thee);
00475
00481 VEXTERNC void    Vpbe_dtor2(Vpbe *thee);
00482
00497 VEXTERNC double  Vpbe_getCoulombEnergy1(Vpbe *thee);
00498
00506 VEXTERNC unsigned long int Vpbe_memChk(Vpbe *thee);
00507
00508 #endif /* ifndef _VPBE_H_ */

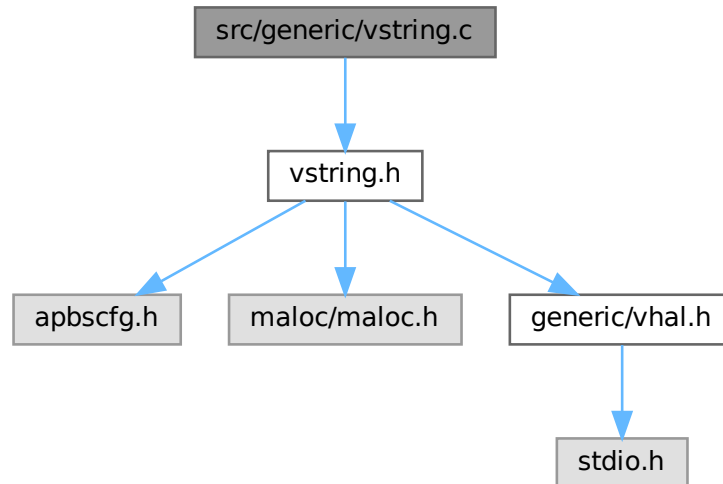
```

9.86 src/generic/vstring.c File Reference

Class Vstring methods.

```
#include "vstring.h"
```

Include dependency graph for vstring.c:



Functions

- VPUBLIC int [Vstring_strcasecmp](#) (const char *s1, const char *s2)
Case-insensitive string comparison (BSD standard)
- VPUBLIC int [Vstring_isdigit](#) (const char *tok)
A modified sscanf that examines the complete string.
- char * [Vstring_wrappedtext](#) (const char *str, int right_margin, int left_padding)

9.86.1 Detailed Description

Class Vstring methods.

Author

Nathan Baker

Version

Attention

```

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* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
*

```

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*
*

```

Definition in file [vstring.c](#).

9.87 vstring.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "vstring.h"
00058
00059 /* ////////////////////////////////////////
00060 // Routine: Vstring_strcasecmp
00061 //
00062 //      Copyright (c) 1988-1993 The Regents of the University of
00063 //                      California.
00064 //      Copyright (c) 1995-1996 Sun Microsystems, Inc.
00066 VPUBLIC int Vstring_strcasecmp(const char *s1, const char *s2) {
00067
00068 #if !defined(HAVE_STRCASECMP)
00069     unsigned char charmap[] = {
00070         0x00, 0x01, 0x02, 0x03, 0x04, 0x05, 0x06, 0x07,
00071         0x08, 0x09, 0x0a, 0x0b, 0x0c, 0x0d, 0x0e, 0x0f,
00072         0x10, 0x11, 0x12, 0x13, 0x14, 0x15, 0x16, 0x17,
00073         0x18, 0x19, 0x1a, 0x1b, 0x1c, 0x1d, 0x1e, 0x1f,
00074         0x20, 0x21, 0x22, 0x23, 0x24, 0x25, 0x26, 0x27,
00075         0x28, 0x29, 0x2a, 0x2b, 0x2c, 0x2d, 0x2e, 0x2f,
00076         0x30, 0x31, 0x32, 0x33, 0x34, 0x35, 0x36, 0x37,
00077         0x38, 0x39, 0x3a, 0x3b, 0x3c, 0x3d, 0x3e, 0x3f,
00078         0x40, 0x61, 0x62, 0x63, 0x64, 0x65, 0x66, 0x67,
00079         0x68, 0x69, 0x6a, 0x6b, 0x6c, 0x6d, 0x6e, 0x6f,
00080         0x70, 0x71, 0x72, 0x73, 0x74, 0x75, 0x76, 0x77,
00081         0x78, 0x79, 0x7a, 0x5b, 0x5c, 0x5d, 0x5e, 0x5f,
00082         0x60, 0x61, 0x62, 0x63, 0x64, 0x65, 0x66, 0x67,

```

```

00083     0x68, 0x69, 0x6a, 0x6b, 0x6c, 0x6d, 0x6e, 0x6f,
00084     0x70, 0x71, 0x72, 0x73, 0x74, 0x75, 0x76, 0x77,
00085     0x78, 0x79, 0x7a, 0x7b, 0x7c, 0x7d, 0x7e, 0x7f,
00086     0x80, 0x81, 0x82, 0x83, 0x84, 0x85, 0x86, 0x87,
00087     0x88, 0x89, 0x8a, 0x8b, 0x8c, 0x8d, 0x8e, 0x8f,
00088     0x90, 0x91, 0x92, 0x93, 0x94, 0x95, 0x96, 0x97,
00089     0x98, 0x99, 0x9a, 0x9b, 0x9c, 0x9d, 0x9e, 0x9f,
00090     0xa0, 0xa1, 0xa2, 0xa3, 0xa4, 0xa5, 0xa6, 0xa7,
00091     0xa8, 0xa9, 0xaa, 0xab, 0xac, 0xad, 0xae, 0xaf,
00092     0xb0, 0xb1, 0xb2, 0xb3, 0xb4, 0xb5, 0xb6, 0xb7,
00093     0xb8, 0xb9, 0xba, 0xbb, 0xbc, 0xbd, 0xbe, 0xbf,
00094     0xc0, 0xc1, 0xc2, 0xc3, 0xc4, 0xc5, 0xc6, 0xc7,
00095     0xc8, 0xc9, 0xca, 0xcb, 0xcc, 0xcd, 0xce, 0xcf,
00096     0xd0, 0xd1, 0xd2, 0xd3, 0xd4, 0xd5, 0xd6, 0xd7,
00097     0xd8, 0xd9, 0xda, 0xdb, 0xdc, 0xdd, 0xde, 0xdf,
00098     0xe0, 0xe1, 0xe2, 0xe3, 0xe4, 0xe5, 0xe6, 0xe7,
00099     0xe8, 0xe9, 0xea, 0xeb, 0xec, 0xed, 0xee, 0xef,
00100     0xf0, 0xf1, 0xf2, 0xf3, 0xf4, 0xf5, 0xf6, 0xf7,
00101     0xf8, 0xf9, 0xfa, 0xfb, 0xfc, 0xfd, 0xfe, 0xff,
00102 };
00103
00104 unsigned char u1, u2;
00105
00106 for ( ; ; s1++, s2++) {
00107     u1 = (unsigned char) *s1;
00108     u2 = (unsigned char) *s2;
00109     if ((u1 == '\0') || (charmap[u1] != charmap[u2])) {
00110         break;
00111     }
00112 }
00113 return charmap[u1] - charmap[u2];
00114
00115 #else
00116     return strcasecmp(s1, s2);
00117
00118 #endif
00119 }
00120
00121 }
00122
00123 /* ////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////// */
00124 // Routine: Vstring_isdigit
00125 //
00126 //     Improves upon sscanf to see if a token is an int or not
00127 //
00128 //     Returns isdigit: 1 if a digit, 0 otherwise
00129 //
00130 // PUBLIC int Vstring_isdigit(const char *tok) {
00131 //     int i, isdigit, ti;
00132 //     char checkchar[1];
00133 //     char name[VMAX_BUFSIZE];
00134 //     strcpy(name, tok);
00135 //     isdigit = 1;
00136 //     for(i=0; ; i++){
00137 //         checkchar[0] = name[i];
00138 //         if (name[i] == '\0'){
00139 //             break;
00140 //         }
00141 //         if (sscanf(checkchar, "%d", &ti) != 1){
00142 //             isdigit = 0;
00143 //             break;
00144 //         }
00145 //     }
00146 //     return isdigit;
00147 // }
00148
00149
00150 char* Vstring_wrappedtext(const char* str, int right_margin, int left_padding)
00151 {
00152     int span = right_margin - left_padding;
00153     int i = 0;
00154     int k = 0;
00155     int j = 0;
00156     int line_len = 0;
00157     int hyphenate = 0;
00158     char* wrap_str;
00159     int wrap_len;
00160     int len = strlen( str );
00161
00162     if( len == 0 )
00163         return VNULL;
00164
00165

```

```

00170     wrap_str = (char*)malloc( len * sizeof(char) );
00171     wrap_len = len;
00172
00173     do
00174     {
00175         if( str[i] == ' ' )
00176         {
00177             i++;
00178         }
00179         else
00180         {
00181             if( k + right_margin + 2 > wrap_len )
00182             {
00183                 wrap_len += right_margin + 2;
00184                 wrap_str = (char*)realloc( wrap_str, wrap_len * sizeof( char ) );
00185             }
00186
00187             if( i + span >= len )
00188             {
00189                 hyphenate = 0;
00190                 line_len = len - i;
00191             }
00192             else
00193             {
00194                 j = span;
00195                 do
00196                 {
00197                     if( str[ i + j ] == ' ' )
00198                     {
00199                         hyphenate = 0;
00200                         line_len = j;
00201                         break;
00202                     }
00203                     else if( j == 0 )
00204                     {
00205                         hyphenate = 1;
00206                         line_len = span - 1;
00207                         break;
00208                     }
00209                     else
00210                     {
00211                         j--;
00212                     }
00213                 } while( 1 );
00214
00215                 memset( wrap_str + k, ' ', left_padding * sizeof( char ) );
00216                 k += left_padding;
00217
00218                 memcpy( wrap_str + k, str + i, line_len * sizeof( char ) );
00219                 k += line_len;
00220                 i += line_len;
00221
00222                 if( hyphenate )
00223                     wrap_str[k++] = '-';
00224
00225                 wrap_str[k++] = '\n';
00226
00227                 wrap_str[k] = '\0';
00228             }
00229         } while( i < len );
00230
00231     return wrap_str;
00232 }

```

9.88 src/generic/vstring.h File Reference

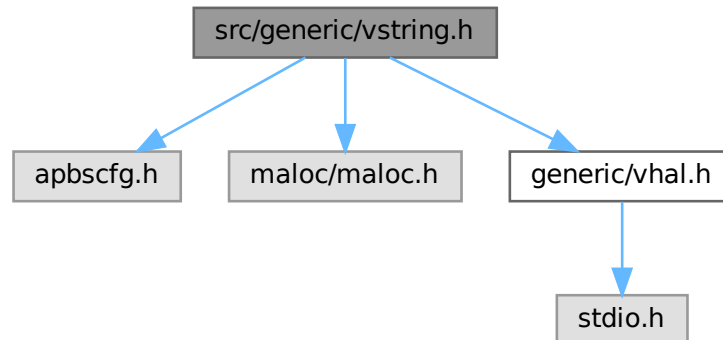
Contains declarations for class Vstring.

```

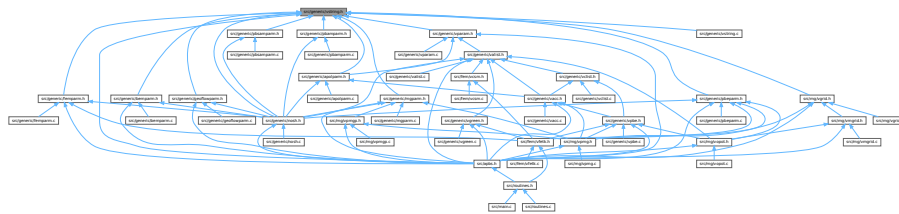
#include "apbscfg.h"
#include "malloc/malloc.h"
#include "generic/vhal.h"

```


Include dependency graph for vstring.h:



This graph shows which files directly or indirectly include this file:



Functions

- VEXTERNC int [Vstring_strcasecmp](#) (const char *s1, const char *s2)
Case-insensitive string comparison (BSD standard)
- VEXTERNC int [Vstring_isdigit](#) (const char *tok)
A modified sscanf that examines the complete string.
- char * [Vstring_wrappedtext](#) (const char *str, int right_margin, int left_padding)

9.88.1 Detailed Description

Contains declarations for class Vstring.

Version

\$Id\$

Author

Nathan A. Baker

Attention

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* Pacific Northwest National Laboratory
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```

Definition in file [vstring.h](#).

9.89 vstring.h

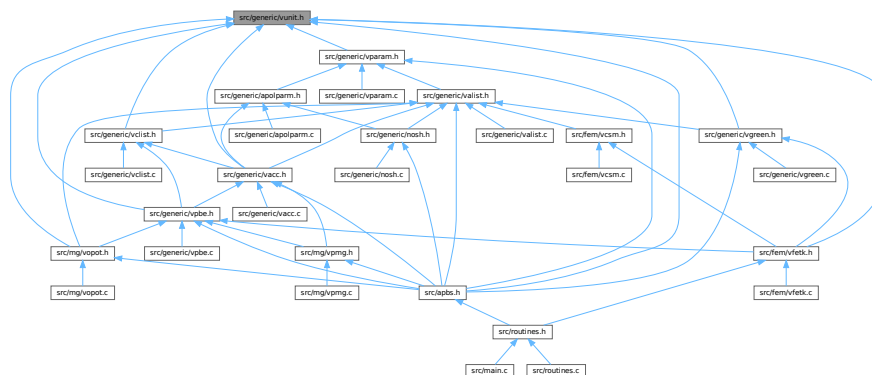
[Go to the documentation of this file.](#)

```
00001
00078 #ifndef _VSTRING_H_
00079 #define _VSTRING_H_
00080
00081 #include "apbscfg.h"
00082
00083 #include "malloc/malloc.h"
00084
00085 #include "generic/vhal.h"
00086
00099 VEXTERNC int Vstring_strcasecmp(const char *s1, const char *s2);
01000
01007 VEXTERNC int Vstring_isdigit(const char *tok);
01008
01014 VEXTERNC char* Vstring_wrappedtext (
01015     const char* str,
01016     int right_margin,
01017     int left_padding
01018 );
01019
01020 #endif /* ifndef _VSTRING_H_ */
```

9.90 src/generic/vunit.h File Reference

Contains a collection of useful constants and conversion factors.

This graph shows which files directly or indirectly include this file:



Macros

- #define **Vunit_J_to_cal** 4.1840000e+00
Multiply by this to convert J to cal.
- #define **Vunit_cal_to_J** 2.3900574e-01
Multiply by this to convert cal to J.
- #define **Vunit_amu_to_kg** 1.6605402e-27
Multiply by this to convert amu to kg.
- #define **Vunit_kg_to_amu** 6.0221367e+26
Multiply by this to convert kg to amu.
- #define **Vunit_ec_to_C** 1.6021773e-19
Multiply by this to convert ec to C.
- #define **Vunit_C_to_ec** 6.2415065e+18

- Multiply by this to convert C to ec .
 - #define `Vunit_ec` 1.6021773e-19
- Charge of an electron in C .
 - #define `Vunit_kb` 1.3806581e-23
- Boltzmann constant.
 - #define `Vunit_Na` 6.0221367e+23
- Avogadro's number.
 - #define `Vunit_pi` VPI
- π .
 - #define `Vunit_eps0` 8.8541878e-12
- Vacuum permittivity.
 - #define `Vunit_esu_ec2A` 3.3206364e+02
- $e_c^2 /$ in ESU units => kcal/mol
 - #define `Vunit_esu_kb` 1.9871913e-03
- k_b in ESU units => kcal/mol

9.90.1 Detailed Description

Contains a collection of useful constants and conversion factors.

Author

Nathan Baker

Nathan A. Baker

Version

\$Id\$

Attention

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* APBS -- Adaptive Poisson-Boltzmann Solver
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* Nathan A. Baker (nathan.baker@pnnl.gov)
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*
*

```

Definition in file [vunit.h](#).

9.91 vunit.h

[Go to the documentation of this file.](#)

```

00001
00063 #ifndef _VUNIT_H_
00064 #define _VUNIT_H_
00065
00068 #define Vunit_J_to_cal  4.1840000e+00
00069
00072 #define Vunit_cal_to_J  2.3900574e-01
00073
00076 #define Vunit_amu_to_kg  1.6605402e-27
00077
00080 #define Vunit_kg_to_amu  6.0221367e+26
00081
00084 #define Vunit_ec_to_C  1.6021773e-19
00085
00088 #define Vunit_C_to_ec  6.2415065e+18
00089
00092 #define Vunit_ec  1.6021773e-19
00093
00096 #define Vunit_kb  1.3806581e-23
00097
00100 #define Vunit_Na  6.0221367e+23
00101
00104 #define Vunit_pi  VPI
00105
00108 #define Vunit_eps0  8.8541878e-12
00109
00112 #define Vunit_esu_ec2A  3.3206364e+02
00113
00116 #define Vunit_esu_kb  1.9871913e-03
00117
00118 #endif /* ifndef _VUNIT_H_ */

```

9.92 src/main.c File Reference

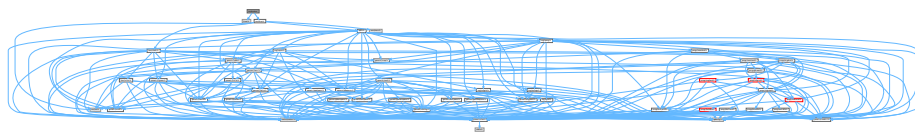
APBS "front end" program using formatted input files.

```

#include <time.h>
#include "routines.h"

```

Include dependency graph for main.c:



Functions

- `int main (int argc, char **argv)`
The main APBS function.

9.92.1 Detailed Description

APBS "front end" program using formatted input files.

Author

Nathan Baker

This driver program represents a mish-mash of instructions for calculating electrostatic potentials, as well as free energies of binding and solvation. It is invoked as:

```
apbs apbs.in
```

where apbs.in is a formatted input file (see documentation and examples).

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
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```

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*
*

```

Definition in file [main.c](#).

9.93 main.c

[Go to the documentation of this file.](#)

```

00001
00068 #include <time.h>
00069
00070 #include "routines.h"
00071
00072 VEMBED(rcsid="$Id$")
00073
00074
00080 int main(
00081     int argc,
00082     char **argv
00083 )
00084 {
00085     // PCE: Adding below variables temporarily
00086     clock_t ts, te;
00087     // End PCE
00088
00089     NOsh *nosh = VNULL;
00090
00091     MGparm *mgparm = VNULL;
00092     FEMparm *feparm = VNULL;
00093 #ifdef ENABLE_BEM
00094     BEMparm *beparm = VNULL;
00095 #endif
00096     GEOFLOWparm *geoflowparm = VNULL;
00097     PBEparm *pbeparm = VNULL;
00098     APOLparm *apolparm = VNULL;
00099     Vparam *param = VNULL;
00100 #if defined(ENABLE_PBAM) || defined(ENABLE_PBSAM)
00101     PBAMparm *pbamparm = VNULL;
00102 #endif
00103
00104 #ifdef ENABLE_PBSAM
00105     PBSAMparm *pbsamparm = VNULL;
00106 #endif
00107
00108     Vmem *mem = VNULL;
00109     Vcom *com = VNULL;
00110     Vio *sock = VNULL;
00111 #ifdef HAVE_MC_H
00112     Vfetc *fetc[NOSH_MAXCALC];
00113     Gem *gm[NOSH_MAXMOL];
00114     int isolve;
00115 #else
00116     void *fetc[NOSH_MAXCALC];
00117     void *gm[NOSH_MAXMOL];
00118 #endif

```

```

00119     Vpmg *pmg[NOSH_MAXCALC];
00120     Vpmgp *pmgp[NOSH_MAXCALC];
00121     Vpbe *pbe[NOSH_MAXCALC];
00122     Valist *alist[NOSH_MAXMOL];
00123     Vgrid *dielXMap[NOSH_MAXMOL],
00124           *dielYMap[NOSH_MAXMOL],
00125           *dielZMap[NOSH_MAXMOL],
00126           *kappaMap[NOSH_MAXMOL],
00127           *potMap[NOSH_MAXMOL],
00128           *chargeMap[NOSH_MAXMOL];
00129     char *input_path = VNULL,
00130          *output_path = VNULL;
00131     int i,
00132         rank,    // proc id
00133         size,    // total num of procs
00134         k;
00135     size_t bytesTotal,
00136           highWater;
00137     Voutput_Format outputformat;
00138
00139     int rc = 0;
00140
00141     /* The energy double arrays below store energies from various calculations. */
00142     double qfEnergy[NOSH_MAXCALC],
00143            qmEnergy[NOSH_MAXCALC];
00144     double dielEnergy[NOSH_MAXCALC],
00145            totEnergy[NOSH_MAXCALC];
00146     double *atomEnergy[NOSH_MAXCALC];
00147     AtomForce *atomForce[NOSH_MAXCALC]; /* Stores forces from various calculations. */
00148     int nenergy[NOSH_MAXCALC], /* Stores either a flag (0,1) displaying whether
00149                                * energies were calculated, or, if PCE_COMPS
00150                                * was used, the number of atom energies stored
00151                                * for the given calculation. */
00152         nforce[NOSH_MAXCALC]; /* Stores an integer which either says no
00153                                * calculation was performed (0) or gives the
00154                                * number of entries in the force array for each
00155                                * calculation. */
00156
00157     /* The real partition centers */
00158     double realCenter[3];
00159
00160     /* Instructions: */
00161     char header[] = {"\n\n\
00162 -----\n\
00163 APBS -- Adaptive Poisson-Boltzmann Solver\n\
00164 Version " PACKAGE_STRING "\n\
00165 \n\
00166 Nathan A. Baker (nathan.baker@pnnl.gov)\n\
00167 Pacific Northwest National Laboratory\n\
00168 \n\
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```



```

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00204      SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.\n\
00205      -----\n\
00206      APBS uses FETK (the Finite Element ToolKit) to solve the\n\
00207      Poisson-Boltzmann equation numerically. FETK is a portable collection\n\
00208      of finite element modeling class libraries developed by the Michael Holst\n\
00209      research group and written in an object-oriented form of C. FETk is\n\
00210      designed to solve general coupled systems of nonlinear partial differential\n\
00211      equations using adaptive finite element methods, inexact Newton methods,\n\
00212      and algebraic multilevel methods. More information about FETk may be found\n\
00213      at <http://www.FETk.ORG>.\n\
00214      -----\n\
00215      APBS also uses Aqua to solve the Poisson-Boltzmann equation numerically. \n\
00216      Aqua is a modified form of the Holst group PMG library <http://www.FETk.ORG>\n\
00217      which has been modified by Patrice Koehl\n\
00218      <http://koehllab.genomecenter.ucdavis.edu/> for improved efficiency and\n\
00219      memory usage when solving the Poisson-Boltzmann equation.\n\
00220      -----\n\
00221      Please cite your use of APBS as:\n\
00222      Baker NA, Sept D, Joseph S, Holst MJ, McCammon JA. Electrostatics of\n\
00223      nanosystems: application to microtubules and the ribosome. Proc.\n\
00224      Natl. Acad. Sci. USA 98, 10037-10041 2001.\n\
00225      \n\n");
00226      char *usage =
00227      {"\n\n\
00228      -----\n\
00229      This driver program calculates electrostatic potentials, energies,\n\
00230      and forces using both multigrid and finite element methods.\n\
00231      It is invoked as:\n\
00232      apbs [options] apbs.in\n\
00233      where apbs.in is a formatted input file and [options] are:\n\
00234      --output-file=<name>      Enables output logging to the path\n\
00235      listed in <name>. Uses flat-file\n\
00236      format is --output-format is not used.\n\
00237      --output-format=<type>    Specifies format for logging. Options\n\
00238      for type are either \"xml\" or \"flat\".\n\
00239      --help                    Display this help information.\n\
00240      --version                 Display the current APBS version.\n\
00241      -----\n\n\"};
00242
00243      /* ***** CHECK PARALLEL STATUS ***** */
00244      VASSERT(Vcom_init(&argc, &argv));
00245      com = Vcom_ctor(1);
00246      rank = Vcom_rank(com);
00247      size = Vcom_size(com);
00248      startVio();
00249      Vnm_setIoTag(rank, size);
00250      Vnm_tprintf( 0, "Hello world from PE %d\n", rank);
00251
00252      /* A bit of array/pointer initialization */
00253      mem = Vmem_ctor("MAIN");
00254      for (i=0; i<NOSH_MAXCALC; i++) {
00255          pmg[i] = VNULL;
00256          pmgp[i] = VNULL;
00257          fetk[i] = VNULL;
00258          pbe[i] = VNULL;
00259          qfEnergy[i] = 0;
00260          qmEnergy[i] = 0;
00261          dielEnergy[i] = 0;
00262          totEnergy[i] = 0;
00263          atomForce[i] = VNULL;
00264          nenergy[i] = 0;
00265          nforce[i] = 0;
00266      }
00267      for (i=0; i<NOSH_MAXMOL; i++) {
00268          alist[i] = VNULL;
00269          dielXMap[i] = VNULL;
00270          dielYMap[i] = VNULL;
00271          dielZMap[i] = VNULL;
00272          kappaMap[i] = VNULL;
00273          potMap[i] = VNULL;
00274          chargeMap[i] = VNULL;
00275      }
00276
00277      /* ***** CHECK INVOCATION AND OPTIONS ***** */
00278      Vnm_tstart(APBS_TIMER_WALL_CLOCK, "APBS WALL CLOCK");
00279      Vnm_tprintf( 1, "%s", header);
00280

```

```

00281 #ifdef APBS_FAST
00282     Vnm_tprint( 2, "WARNING: APBS was compiled with the --enable-fast option.\n"
00283     "WARNING: This mode is experimental and subject to change in future releases.\n"
00284     "WARNING: The fast mode enables: Gauss-Seidel Smoothing and \n"
00285     "WARNING: Conjugate Gradient Multigrid methods.\n\n");
00286 #endif
00287
00288     Vnm_tprint( 1, "This executable compiled on %s at %s\n\n", __DATE__, __TIME__);
00289
00290 #if defined(WITH_TINKER)
00291     Vnm_tprint( 2, "This executable was compiled with TINKER support and is not intended for stand-alone
    execution.\n");
00292     Vnm_tprint( 2, "Please compile another version without TINKER support.\n");
00293     exit(2);
00294 #endif
00295
00296     /* Process program arguments */
00297     i=0;
00298     outputformat = OUTPUT_NULL;
00299     while (i<argc){
00300         if (strcmp(argv[i], "--", 2) == 0) {
00301
00302             /* Long Options */
00303             if (Vstring_strcasecmp("--version", argv[i]) == 0){
00304                 Vnm_tprint(2, "%s\n", PACKAGE_STRING);
00305                 VJMPERR1(0);
00306             } else if (Vstring_strcasecmp("--help", argv[i]) == 0){
00307                 Vnm_tprint(2, "%s\n", usage);
00308                 VJMPERR1(0);
00309             } else if (strcmp(argv[i], "--output-format", 15) == 0) {
00310                 if (strstr(argv[i], "xml") != NULL) {
00311                     Vnm_tprint(2, "XML output format is now deprecated, please use --output-format=flat
instead!\n\n");
00312                     VJMPERR1(0);
00313                 }
00314                 else if (strstr(argv[i], "flat") != NULL) {
00315                     outputformat = OUTPUT_FLAT;
00316                 } else {
00317                     Vnm_tprint(2, "Invalid output-format type!\n");
00318                     VJMPERR1(0);
00319                 }
00320             } else if (strcmp(argv[i], "--output-file=", 14) == 0){
00321                 output_path = strstr(argv[i], "=");
00322                 ++output_path;
00323                 if (outputformat == OUTPUT_NULL) outputformat = OUTPUT_FLAT;
00324             } else {
00325                 Vnm_tprint(2, "UNRECOGNIZED COMMAND LINE OPTION %s!\n", argv[i]);
00326                 Vnm_tprint(2, "%s\n", usage);
00327                 VJMPERR1(0);
00328             }
00329         } else {
00330
00331             /* Set the path to the input file */
00332             if ((input_path == VNULL) && (i != 0))
00333                 input_path = argv[i];
00334             else if (i != 0) {
00335                 Vnm_tprint(2, "ERROR -- CALLED WITH TOO MANY ARGUMENTS!\n", \
00336                 argc);
00337                 Vnm_tprint(2, "%s\n", usage);
00338                 VJMPERR1(0);
00339             }
00340         }
00341         i++;
00342     }
00343
00344     /* If we set an output format but no path, error. */
00345     if ((outputformat != 0) && (output_path == NULL)) {
00346         Vnm_tprint(2, "The --output-path variable must be set when using --output-format!\n");
00347         VJMPERR1(0);
00348     }
00349
00350     /* If we failed to specify an input file, error. */
00351     if (input_path == NULL) {
00352         Vnm_tprint(2, "ERROR -- APBS input file not specified!\n", argc);
00353         Vnm_tprint(2, "%s\n", usage);
00354         VJMPERR1(0);
00355     }
00356
00357     /* Append rank info if a parallel run */
00358     if ((size > 1) && (output_path != NULL))
00359         printf(output_path, "%s%d", output_path, rank);

```

```
00360
00361 /* ***** PARSE INPUT FILE ***** */
00362 nosh = Nosh_ctor(rank, size);
00363 Vnm_tprint( 1, "Parsing input file %s...\n", input_path);
00364 Vnm_tprint( 1, "rank %d size %d...\n", rank, size);
00365 sock = Vio_ctor("FILE", "ASC", VNULL, input_path, "r");
00366 if (sock == VNULL) {
00367     Vnm_tprint(2, "Error while opening input file %s!\n", input_path);
00368     VJMPERR1(0);
00369 }
00370 if (!Nosh_parseInput(nosh, sock)) {
00371     Vnm_tprint( 2, "Error while parsing input file.\n");
00372     VJMPERR1(0);
00373 }
00374 else
00375     Vnm_tprint( 1, "Parsed input file.\n");
00376 Vio_dtor(&sock);
00377
00378 /* ***** LOAD PARAMETERS AND MOLECULES ***** */
00379 param = loadParameter(nosh);
00380 if (loadMolecules(nosh, param, alist) != 1) {
00381     Vnm_tprint(2, "Error reading molecules!\n");
00382     VJMPERR1(0);
00383 }
00384
00385 /* ***** SETUP CALCULATIONS ***** */
00386 if (Nosh_setupElecCalc(nosh, alist) != 1) {
00387     Vnm_tprint(2, "Error setting up ELEC calculations\n");
00388     VJMPERR1(0);
00389 }
00390
00391 if ((rc = Nosh_setupApolCalc(nosh, alist)) == ACD_ERROR) {
00392     Vnm_tprint(2, "Error setting up APOL calculations\n");
00393     VJMPERR1(0);
00394 }
00395
00396 /* ***** CHECK APOL***** */
00397 /* if((nosh->gotparm == 0) && (rc == ACD_YES)){
00398     Vnm_print(1, "\nError you must provide a parameter file if you\n" \
00399         "are performing an APOLAR calculation\n");
00400     VJMPERR1(0);
00401 } */
00402
00403 #if defined(DEBUG_MAC_OSX_OCL)
00404 #include "mach_chud.h"
00405 #include <stdint.h>
00406 uint64_t mbeg;
00407 machm_(&mbeg);
00408
00409 if (clFinish != NULL)
00410 {
00411     int ret = initOpenCL();
00412     printf("OpenCL runtime present - initialized = %i\n", ret);
00413 }
00414 else
00415 {
00416     setkOpenCLAvailable_(0);
00417     printf("OpenCL is not present!\n");
00418 }
00419 #endif
00420
00421 #if defined(DEBUG_MAC_OSX_STANDARD)
00422 #include "mach_chud.h"
00423 #include <stdint.h>
00424 uint64_t mbeg;
00425 machm_(&mbeg);
00426 #endif
00427
00428 /* ***** LOAD MAPS ***** */
00429 if (loadDielMaps(nosh, dielXMap, dielYMap, dielZMap) != 1) {
00430     Vnm_tprint(2, "Error reading dielectric maps!\n");
00431     VJMPERR1(0);
00432 }
00433 if (loadKappaMaps(nosh, kappaMap) != 1) {
00434     Vnm_tprint(2, "Error reading kappa maps!\n");
00435     VJMPERR1(0);
00436 }
00437 if (loadPotMaps(nosh, potMap) != 1) {
00438     Vnm_tprint(2, "Error reading potential maps!\n");
00439     VJMPERR1(0);
00440 }
```

```

00441     if (loadChargeMaps(nosh, chargeMap) != 1) {
00442         Vnm_tprint(2, "Error reading charge maps!\n");
00443         VJMPERR1(0);
00444     }
00445
00446     /* ***** DO THE CALCULATIONS ***** */
00447     Vnm_tprint( 1, "Preparing to run %d PBE calculations.\n",
00448         nosh->ncalc);
00449     for (i=0; i<nosh->ncalc; i++) {
00450         Vnm_tprint( 1, "-----\n");
00451
00452         switch (nosh->calc[i]->calctype) {
00453             /* Multigrid */
00454             case NCT_MG:
00455                 /* What is this? This seems like a very awkward way to find
00456                 the right ELEC statement... */
00457                 for (k=0; k<nosh->nelec; k++) {
00458                     if (nosh->elec2calc[k] >= i) {
00459                         break;
00460                     }
00461                 }
00462                 if (Vstring_strcasecmp(nosh->elecname[k], "") == 0) {
00463                     Vnm_tprint( 1, "CALCULATION #d: MULTIGRID\n", i+1);
00464                 } else {
00465                     Vnm_tprint( 1, "CALCULATION #d (%s): MULTIGRID\n",
00466                         i+1, nosh->elecname[k]);
00467                 }
00468                 /* Useful local variables */
00469                 mgparm = nosh->calc[i]->mgparm;
00470                 pbeparm = nosh->calc[i]->pbeparm;
00471
00472                 /* Set up problem */
00473                 Vnm_tprint( 1, "    Setting up problem...\n");
00474
00475                 if (!initMG(i, nosh, mgparm, pbeparm, realCenter, pbe,
00476                     alist, dielXMap, dielYMap, dielZMap, kappaMap,
00477                     chargeMap, pmgp, pmg, potMap)) {
00478                     Vnm_tprint( 2, "Error setting up MG calculation!\n");
00479                     VJMPERR1(0);
00480                 }
00481
00482                 /* Print problem parameters */
00483                 printMGPARM(mgparm, realCenter);
00484                 printPBEARM(pbeparm);
00485
00486                 /* Solve PDE */
00487                 if (solveMG(nosh, pmg[i], mgparm->type) != 1) {
00488                     Vnm_tprint(2, "Error solving PDE!\n");
00489                     VJMPERR1(0);
00490                 }
00491
00492                 /* Set partition information for observables and I/O */
00493                 if (setPartMG(nosh, mgparm, pmg[i]) != 1) {
00494                     Vnm_tprint(2, "Error setting partition info!\n");
00495                     VJMPERR1(0);
00496                 }
00497
00498                 /* Write out energies */
00499                 energyMG(nosh, i, pmg[i],
00500                     &(nenergy[i]), &(totEnergy[i]), &(qfEnergy[i]),
00501                     &(qmEnergy[i]), &(dielEnergy[i]));
00502
00503                 /* Write out forces */
00504                 forceMG(mem, nosh, pbeparm, mgparm, pmg[i], &(nforce[i]),
00505                     &(atomForce[i]), alist);
00506
00507                 /* Write out data folks might want */
00508                 writedataMG(rank, nosh, pbeparm, pmg[i]);
00509
00510                 /* Write matrix */
00511                 writematMG(rank, nosh, pbeparm, pmg[i]);
00512
00513                 /* If needed, cache atom energies */
00514                 nenergy[i] = 0;
00515                 if ((pbeparm->calcenergy == PCE_COMPS) && (outputformat != OUTPUT_NULL)){
00516                     storeAtomEnergy(pmg[i], i, &(atomEnergy[i]), &(nenergy[i]));
00517                 }
00518
00519                 fflush(stdout);
00520                 fflush(stderr);
00521

```

```

00522         break;
00523
00524         /* ***** Do FEM calculation ***** */
00525         case NCT_FEM:
00526 #ifdef HAVE_MC_H
00527         for (k=0; k<nosh->nelec; k++) {
00528             if (nosh->elec2calc[k] >= i) break;
00529         }
00530         if (Vstring_strcasecmp(nosh->elecname[i+1], "") == 0) {
00531             Vnm_tprint( 1, "CALCULATION #d: FINITE ELEMENT\n", i+1);
00532         } else {
00533             Vnm_tprint( 1, "CALCULATION #d (%s): FINITE ELEMENT\n", i+1, nosh->elecname[k+1]);
00534         }
00535
00536         /* Useful local variables */
00537         feparm = nosh->calc[i]->feparm;
00538         pbeparm = nosh->calc[i]->pbeparm;
00539
00540         /* Warn the user about some things */
00541         Vnm_tprint(2, "##### WARNING #####\n");
00542         Vnm_tprint(2, "## FE support is currently very experimental! ##\n");
00543         Vnm_tprint(2, "##### WARNING #####\n");
00544
00545         /* Set up problem */
00546         Vnm_tprint( 1, " Setting up problem...\n");
00547         /* Attempt to initialize and do an initial refinement of the mesh data. The mesh data
00548          * will be stored in the Vfetc object fetk, which contains the appropriate geometry
00549          * manager (Gem) object and Vcsm object describing the mesh structure. The mesh will
00550          * either be loaded from an external source or generated from scratch. */
00551         if (initFE(i, nosh, feparm, pbeparm, pbe, alist, fetk) != VRC_SUCCESS) {
00552             Vnm_tprint( 2, "Error setting up FE calculation!\n");
00553             VJMPErr(0);
00554         }
00555
00556         /* Print problem parameters */
00557         printFEPARM(i, nosh, feparm, fetk);
00558         printPBEPARM(pbeparm);
00559
00560         /* Refine mesh - this continues to run the AM_markRefine procedure already run
00561          * in initFE() to arrive at some initial refinement, but does checks of the
00562          * simplices so that it refines until the error or size tolerances are reached.
00563          * Once this is done, we have a mesh that has been refined to the point where
00564          * we can attempt to solve - further refinement may be needed in the loop
00565          * below. */
00566         if (!preRefineFE(i, feparm, fetk)) {
00567             Vnm_tprint( 2, "Error pre-refining mesh!\n");
00568             VJMPErr(0);
00569         }
00570
00571         /* Solve-estimate-refine */
00572         Vnm_tprint(2, "\n\nWARNING! DO NOT EXPECT PERFORMANCE OUT OF THE APBS/Fetc\n");
00573         Vnm_tprint(2, "INTERFACE AT THIS TIME. THE FINITE ELEMENT SOLVER IS\n");
00574         Vnm_tprint(2, "CURRENTLY NOT OPTIMIZED FOR THE PB EQUATION. IF YOU WANT\n");
00575         Vnm_tprint(2, "PERFORMANCE, PLEASE USE THE MULTIGRID-BASED METHODS, E.G.\n");
00576         Vnm_tprint(2, "MG-AUTO, MG-PARA, and MG-MANUAL (SEE DOCS.)\n\n");
00577         Vnm_tprint(1, " Beginning solve-estimate-refine cycle:\n");
00578
00579         for (isolve=0; isolve<feparm->maxsolve; isolve++) {
00580             Vnm_tprint(1, " Solve #d...\n", isolve);
00581
00582             /* Attempt to solve the mesh by using one of MC's solver types. */
00583             if (!solveFE(i, pbeparm, feparm, fetk)) {
00584                 Vnm_tprint(2, "ERROR SOLVING EQUATION!\n");
00585                 VJMPErr(0);
00586             }
00587
00588             /* Calculate the total electrostatic energy. */
00589             if (!energyFE(nosh, i, fetk, &(nenergy[i]),
00590                 &(totEnergy[i]), &(qfEnergy[i]),
00591                 &(qmEnergy[i]), &(dielEnergy[i]))) {
00592                 Vnm_tprint(2, "ERROR SOLVING EQUATION!\n");
00593                 VJMPErr(0);
00594             }
00595
00596             /* We're not going to refine if we've hit the max number
00597              * of solves */
00598             if (isolve < (feparm->maxsolve)-1) {
00599                 /* Do a final error estimation and mesh refinement. */
00600                 if (!postRefineFE(i, feparm, fetk)) {
00601                     break;
00602                 }
00603             }
00604         }

```

```

00603         }
00604         bytesTotal = Vmem_bytesTotal();
00605         highWater = Vmem_highWaterTotal();
00606         Vnm_tprint(1, "      Current memory use:      %g MB\n",
00607             ((double)bytesTotal/(1024.)/(1024.)));
00608         Vnm_tprint(1, "      High-water memory use: %g MB\n",
00609             ((double)highWater/(1024.)/(1024.)));
00610     }
00611
00612     Vnm_tprint(1, "  Writing FEM data to files.\n");
00613
00614     /* Save data. */
00615     if (!writedataFE(rank, nosh, pbeparm, fetk[i])) {
00616         Vnm_tprint(2, "  Error while writing FEM data!\n");
00617     }
00618 #else /* ifdef HAVE_MC_H */
00619     Vnm_print(2, "Error!  APBS not compiled with FEtk!\n");
00620     exit(2);
00621 #endif /* ifdef HAVE_MC_H */
00622     break;
00623
00624     /* Do an apolar calculation */
00625     case NCT_APOL:
00626         /* Copied from NCT_MG. See the note above (top of loop) for
00627            information about this loop.
00628         */
00629         for (k=0; k<nosh->napol; k++) {
00630             if (nosh->apol2calc[k] >= i) {
00631                 break;
00632             }
00633         }
00634
00635         if (Vstring_strcasecmp(nosh->apolname[k], "") == 0) {
00636             Vnm_tprint( 1, "CALCULATION #%d: APOLAR\n", i+1);
00637         } else {
00638             Vnm_tprint( 1, "CALCULATION #%d (%s): APOLAR\n",
00639                 i+1, nosh->apolname[k]);
00640         }
00641
00642         apolparm = nosh->calc[i]->apolparm;
00643         /* poor man's execution timer.
00644         ts = clock();
00645         rc = initAPOL(nosh, mem, param, apolparm, &(nforce[i]), &(atomForce[i]),
00646             alist[(apolparm->molid)-1]);
00647         Vnm_print(0, "initAPOL: Time elapsed: %f\n", ((double)clock() - ts) / CLOCKS_PER_SEC);
00648         if(rc == 0) {
00649             Vnm_tprint(2, "Error calculating apolar solvation quantities!\n");
00650             VJMPERR1(0);
00651         }
00652         break;
00653
00654     /* Boundary Element (tabi) */
00655     case NCT_BEM:
00656 #ifdef ENABLE_BEM
00657         /* What is this? This seems like a very awkward way to find
00658            the right ELEC statement... */
00659         for (k=0; k<nosh->nelec; k++) {
00660             if (nosh->elec2calc[k] >= i) {
00661                 break;
00662             }
00663         }
00664         if (Vstring_strcasecmp(nosh->elecname[k], "") == 0) {
00665             Vnm_tprint( 1, "CALCULATION #%d: BOUNDARY ELEMENT\n", i+1);
00666         } else {
00667             Vnm_tprint( 1, "CALCULATION #%d (%s): BOUNDARY ELEMENT\n",
00668                 i+1, nosh->elecname[k]);
00669         }
00670         /* Useful local variables */
00671         bemparm = nosh->calc[i]->bemparm;
00672         pbeparm = nosh->calc[i]->pbeparm;
00673
00674         /* Set up problem */
00675         Vnm_tprint( 1, "  Setting up problem...\n");
00676
00677         if (!initBEM(i,nosh, bemparm, pbeparm, pbe)) {
00678             Vnm_tprint( 2, "Error setting up BEM calculation!\n");
00679             VJMPERR1(0);
00680         }
00681
00682         /* Print problem parameters */
00683         printBEMPARM(bemparm);

```

```

00684         printPBEPARM(pbeparm);
00685
00686         /* Solve PDE */
00687         if (solveBEM(alist, nosh, pbeparm, bemparm, bemparm->type) != 1) {
00688             Vnm_tprint(2, "Error solving PDE!\n");
00689             VJMPERR1(0);
00690         }
00691
00692         /* Write out energies */
00693         energyBEM(nosh, i,
00694                 &(nenergy[i]), &(totEnergy[i]), &(qfEnergy[i]),
00695                 &(qmEnergy[i]), &(dielEnergy[i]));
00696
00697         /* Write out forces */
00698         forceBEM(nosh, pbeparm, bemparm, &(nforce[i]),
00699                 &(atomForce[i]), alist);
00700
00701         /* Write out data folks might want */
00702         writedataBEM(rank, nosh, pbeparm);
00703
00704         /* Write matrix */
00705         writematBEM(rank, nosh, pbeparm);
00706
00707         /* If needed, cache atom energies */
00708         nenergy[i] = 0;
00709         if ((pbeparm->calcenergy == PCE_COMPS) && (outputformat != OUTPUT_NULL)){
00710             storeAtomEnergy(pmg[i], i, &(atomEnergy[i]), &(nenergy[i]));
00711         }
00712
00713         fflush(stdout);
00714         fflush(stderr);
00715     #else /* ifdef ENABLE_BEM */
00716         Vnm_print(2, "Error! APBS not compiled with BEM!\n");
00717         exit(2);
00718     #endif
00719         break;
00720
00721         /* geometric flow */
00722         case NCT_GEOFLOW:
00723     #ifdef ENABLE_GEOFLOW
00724         /* What is this? This seems like a very awkward way to find
00725         the right ELEC statement... */
00726         for (k=0; k<nosh->nelec; k++) {
00727             if (nosh->elec2calc[k] >= i) {
00728                 break;
00729             }
00730         }
00731         if (Vstring_strcasecmp(nosh->elecname[k], "") == 0) {
00732             Vnm_tprint( 1, "CALCULATION #d: GEOMETRIC FLOW\n", i+1);
00733         } else {
00734             Vnm_tprint( 1, "CALCULATION #d (%s): GEOMETRIC FLOW\n",
00735                 i+1, nosh->elecname[k]);
00736         }
00737         /* Useful local variables */
00738         geoflowparm = nosh->calc[i]->geoflowparm;
00739         apolparm = nosh->calc[i]->apolparm;
00740         pbeparm = nosh->calc[i]->pbeparm;
00741
00742         /* Set up problem */
00743         Vnm_tprint( 1, " Setting up problem...\n");
00744
00745
00746         /* Solve PDE */
00747         if (solveGeometricFlow(alist, nosh, pbeparm, apolparm, geoflowparm) != 1) {
00748             Vnm_tprint(2, "Error solving GEOFLOW!\n");
00749             VJMPERR1(0);
00750         }
00751
00752         fflush(stdout);
00753         fflush(stderr);
00754         break;
00755     #else /* ifdef ENABLE_GEOFLOW */
00756         Vnm_print(2, "Error! APBS not compiled with GEOFLOW!\n");
00757         exit(2);
00758     #endif
00759
00760         /* Poisson-boltzmann analytical method */
00761         case NCT_PBAM:
00762     #ifdef ENABLE_PBAM
00763         /* What is this? This seems like a very awkward way to find
00764         the right ELEC statement... */

```

```

00765         //Vnm_tprint( 1, "Made it to start\n");
00766         for (k=0; k<nosh->nelec; k++) {
00767             if (nosh->elec2calc[k] >= i) {
00768                 break;
00769             }
00770         }
00771         if (Vstring_strcasecmp(nosh->elecname[k], "") == 0) {
00772             Vnm_tprint( 1, "CALCULATION #d: PBAM\n", i+1);
00773         } else {
00774             Vnm_tprint( 1, "CALCULATION #d (%s): PBAM\n",
00775                 i+1, nosh->elecname[k]);
00776         }
00777         /* Useful local variables */
00778         pbamparm = nosh->calc[i]->pbamparm;
00779         pbeparm = nosh->calc[i]->pbeparm;
00780
00781         /* Set up problem */
00782         Vnm_tprint( 1, "    Setting up problem...\n");
00783
00784         /* Solve LPBE with PBAM method */
00785         if (solvePBAM(alist, nosh, pbeparm, pbamparm) != 1) {
00786             Vnm_tprint(2, "Error solving PBAM!\n");
00787             VJMPERR1(0);
00788         }
00789
00790         fflush(stdout);
00791         fflush(stderr);
00792         break;
00793     #else /* ifdef ENABLE_PBAM */
00794         Vnm_print(2, "Error! APBS not compiled with PBAM!\n");
00795         exit(2);
00796     #endif
00797
00798     case NCT_PBSAM:
00799     #ifdef ENABLE_PBSAM
00800         Vnm_tprint( 1, "Made it to start\n");
00801         for (k=0; k<nosh->nelec; k++) {
00802             if (nosh->elec2calc[k] >= i) {
00803                 break;
00804             }
00805         }
00806         if (Vstring_strcasecmp(nosh->elecname[k], "") == 0) {
00807             Vnm_tprint( 1, "CALCULATION #d: PBSAM\n", i+1);
00808         } else {
00809             Vnm_tprint( 1, "CALCULATION #d (%s): PBSAM\n",
00810                 i+1, nosh->elecname[k]);
00811         }
00812         /* Useful local variables */
00813         pbamparm = nosh->calc[i]->pbamparm;
00814         pbsamparm = nosh->calc[i]->pbsamparm;
00815         pbeparm = nosh->calc[i]->pbeparm;
00816
00817         /* Set up problem */
00818         Vnm_tprint( 1, "    Setting up problem...\n");
00819
00820
00821         /* Solve LPBE with PBSAM method */
00822         if (solvePBSAM(alist, nosh, pbeparm, pbamparm, pbsamparm) != 1) {
00823             Vnm_tprint(2, "Error solving PBSAM!\n");
00824             VJMPERR1(0);
00825         }
00826
00827         fflush(stdout);
00828         fflush(stderr);
00829         break;
00830     #else /* ifdef ENABLE_PBSAM */
00831         Vnm_print(2, "Error! APBS not compiled with PBSAM!\n");
00832         exit(2);
00833     #endif
00834
00835     default:
00836         Vnm_tprint(2, "    Unknown calculation type (%d)!\n", nosh->calc[i]->calctype);
00837         exit(2);
00838         break;
00839     }
00840 }
00841 }
00842
00843 //Clear out the parameter file memory
00844 if(param != VNULL) Vparam_dtor(&param);
00845

```



```

00846  /* ***** HANDLE PRINT STATEMENTS ***** */
00847  if (nosh->nprint > 0) {
00848      Vnm_tprint( 1, "-----\n");
00849      Vnm_tprint( 1, "PRINT STATEMENTS\n");
00850  }
00851  for (i=0; i<nosh->nprint; i++) {
00852      /* Print energy */
00853      if (nosh->printwhat[i] == NPT_ENERGY) {
00854          printEnergy(com, nosh, totEnergy, i);
00855          /* Print force */
00856      } else if (nosh->printwhat[i] == NPT_FORCE) {
00857          printForce(com, nosh, nforce, atomForce, i);
00858      } else if (nosh->printwhat[i] == NPT_ELECENERGY) {
00859          printElecEnergy(com, nosh, totEnergy, i);
00860      } else if (nosh->printwhat[i] == NPT_ELECFORCE) {
00861          printElecForce(com, nosh, nforce, atomForce, i);
00862      } else if (nosh->printwhat[i] == NPT_APOLENERGY) {
00863          printApolEnergy(nosh, i);
00864      } else if (nosh->printwhat[i] == NPT_APOLFORCE) {
00865          printApolForce(com, nosh, nforce, atomForce, i);
00866      } else {
00867          Vnm_tprint( 2, "Undefined PRINT keyword!\n");
00868          break;
00869      }
00870  }
00871  Vnm_tprint( 1, "-----\n");
00872
00873  /* ***** HANDLE LOGGING ***** */
00874
00875  if (outputformat == OUTPUT_FLAT) {
00876      Vnm_tprint(2, " Writing data to flat file %s...\n\n", output_path);
00877      writedataFlat(nosh, com, output_path, totEnergy, qfEnergy, qmEnergy,
00878                  dielEnergy, nenergy, atomEnergy, nforce, atomForce);
00879  }
00880
00881  /* Destroy energy arrays if they still exist */
00882
00883  for (i=0; i<nosh->ncalc; i++) {
00884      if (nenergy[i] > 0) Vmem_free(mem, nenergy[i], sizeof(double),
00885                                  (void **)&(atomEnergy[i]));
00886  }
00887
00888  /* ***** GARBAGE COLLECTION ***** */
00889
00890  Vnm_tprint( 1, "CLEANING UP AND SHUTTING DOWN...\n");
00891  /* Clean up APBS structures */
00892  killForce(mem, nosh, nforce, atomForce);
00893  killEnergy();
00894  killMG(nosh, pbe, pmgp, pmg);
00895  #ifdef HAVE_MC_H
00896  killFE(nosh, pbe, fetk, gm);
00897  #endif
00898  killChargeMaps(nosh, chargeMap);
00899  killKappaMaps(nosh, kappaMap);
00900  killDielMaps(nosh, dielXMap, dielYMap, dielZMap);
00901  killMolecules(nosh, alist);
00902  NOsh_dtor(&nosh);
00903
00904  /* Memory statistics */
00905  bytesTotal = Vmem_bytesTotal();
00906  highWater = Vmem_highWaterTotal();
00907  Vnm_tprint( 1, "Final memory usage: %4.3f MB total, %4.3f MB high water\n",
00908              (double) (bytesTotal)/(1024.*1024.),
00909              (double) (highWater)/(1024.*1024.));
00910
00911  /* Clean up MALOC structures */
00912  Vcom_dtor(&com);
00913  Vmem_dtor(&mem);
00914
00915  /* And now it's time to so "so long"... */
00916  Vnm_tprint(1, "\n\n");
00917  Vnm_tprint( 1, "Thanks for using APBS!\n\n");
00918
00919  #if defined(DEBUG_MAC_OSX_OCL)
00920      mets_(&mbeg, "Main Program CL");
00921  #endif
00922  #if defined(DEBUG_MAC_OSX_STANDARD)
00923      mets_(&mbeg, "Main Program Standard");
00924  #endif
00925
00926  /* This should be last */

```

```

00927     Vnm_tstop(APBS_TIMER_WALL_CLOCK, "APBS WALL CLOCK");
00928     Vnm_flush(1);
00929     Vnm_flush(2);
00930     Vcom_finalize();
00931
00932     fflush(NULL);
00933
00934     return 0;
00935
00936     ERROR1:
00937     Vcom_finalize();
00938     Vcom_dtor(&com);
00939     Vmem_dtor(&mem);
00940     return APBSRC;
00941 }

```

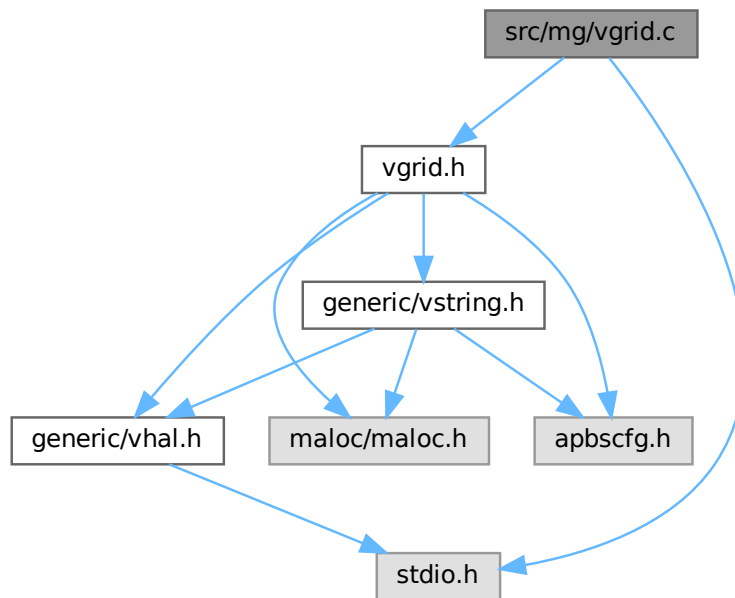
9.94 src/mg/vgrid.c File Reference

Class Vgrid methods.

```
#include "vgrid.h"
```

```
#include <stdio.h>
```

Include dependency graph for vgrid.c:



Macros

- #define **IJK**(i, j, k) (((k)*(nx)*(ny))+((j)*(nx))+i)

Functions

- VPUBLIC unsigned long int **Vgrid_memChk** (**Vgrid** *thee)
Return the memory used by this structure (and its contents) in bytes.

- VPUBLIC [Vgrid](#) * [Vgrid_ctor](#) (int nx, int ny, int nz, double hx, double hy, double hzed, double xmin, double ymin, double zmin, double *data)
Construct Vgrid object with values obtained from Vpmg_readDX (for example)
- VPUBLIC int [Vgrid_ctor2](#) ([Vgrid](#) *thee, int nx, int ny, int nz, double hx, double hy, double hzed, double xmin, double ymin, double zmin, double *data)
Initialize Vgrid object with values obtained from Vpmg_readDX (for example)
- VPUBLIC void [Vgrid_dtor](#) ([Vgrid](#) **thee)
Object destructor.
- VPUBLIC void [Vgrid_dtor2](#) ([Vgrid](#) *thee)
FORTTRAN stub object destructor.
- VPUBLIC int [Vgrid_value](#) ([Vgrid](#) *thee, double pt[3], double *value)
Get potential value (from mesh or approximation) at a point.
- VPUBLIC int [Vgrid_curvature](#) ([Vgrid](#) *thee, double pt[3], int cflag, double *value)
Get second derivative values at a point.
- VPUBLIC int [Vgrid_gradient](#) ([Vgrid](#) *thee, double pt[3], double grad[3])
Get first derivative values at a point.
- VPUBLIC int [Vgrid_readGZ](#) ([Vgrid](#) *thee, const char *fname)
Read in OpenDX data in GZIP format.
- VPUBLIC int [Vgrid_readDX](#) ([Vgrid](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname)
Read in data in OpenDX grid format.
- VPUBLIC int [Vgrid_readDXBIN](#) ([Vgrid](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname)
Read in binary data in OpenDX grid format.
- VPUBLIC void [Vgrid_writeGZ](#) ([Vgrid](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, char *title, double *pvec)
Write out OpenDX data in GZIP format.
- VPUBLIC void [Vgrid_writeDX](#) ([Vgrid](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, char *title, double *pvec)
Write out the data in OpenDX grid format.
- VPUBLIC void [Vgrid_writeDXBIN](#) ([Vgrid](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, char *title, double *pvec)
Write out the binary data in OpenDX grid format.
- VPUBLIC void [Vgrid_writeUHBD](#) ([Vgrid](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, char *title, double *pvec)
Write out the data in UHBD grid format.
- VPUBLIC double [Vgrid_integrate](#) ([Vgrid](#) *thee)
Get the integral of the data.
- VPUBLIC double [Vgrid_normL1](#) ([Vgrid](#) *thee)
Get the L_1 norm of the data. This returns the integral:
- VPUBLIC double [Vgrid_normL2](#) ([Vgrid](#) *thee)
Get the L_2 norm of the data. This returns the integral:
- VPUBLIC double [Vgrid_seminormH1](#) ([Vgrid](#) *thee)
Get the H_1 semi-norm of the data. This returns the integral:
- VPUBLIC double [Vgrid_normH1](#) ([Vgrid](#) *thee)
Get the H_1 norm (or energy norm) of the data. This returns the integral:
- VPUBLIC double [Vgrid_normLinf](#) ([Vgrid](#) *thee)
Get the L_∞ norm of the data. This returns the integral:

Variables

- VPRIVATE char * [MCwhiteChars](#) = " =,;\t\n"
- VPRIVATE char * [MCcommChars](#) = "#%"
- VPRIVATE double [Vcompare](#)
- VPRIVATE char [Vprecision](#) [26]

9.94.1 Detailed Description

Class Vgrid methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
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* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
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* CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE)
* ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF
* THE POSSIBILITY OF SUCH DAMAGE.
*
*
```

Definition in file [vgrid.c](#).

9.94.2 Macro Definition Documentation

9.94.2.1 IJK

```
#define IJK(
    i,
    j,
    k ) ( ((k)*(nx)*(ny)) + ((j)*(nx)) + (i) )
```

Definition at line 67 of file [vgrid.c](#).

9.94.3 Function Documentation

9.94.3.1 Vgrid_writeGZ()

```
VPUBLIC void Vgrid_writeGZ (
    Vgrid * thee,
    const char * iodev,
    const char * iofmt,
    const char * thost,
    const char * fname,
    char * title,
    double * pvec )
```

Write out OpenDX data in GZIP format.

Author

Dave Gohara

Parameters

<i>thee</i>	Object to hold new grid data
<i>iodev</i>	I/O device
<i>iofmt</i>	I/O format
<i>thost</i>	Remote host name
<i>fname</i>	File name
<i>title</i>	Data title
<i>pvec</i>	Masking vector (0 = not written)

Definition at line 1011 of file [vgrid.c](#).

9.94.4 Variable Documentation

9.94.4.1 MCcommChars

```
VPPRIVATE char* MCcommChars = "##"
```

Definition at line 78 of file [vgrid.c](#).

9.94.4.2 MCwhiteChars

VPRIVATE char* MCwhiteChars = " =,;\t\n"

Definition at line 77 of file [vgrid.c](#).

9.94.4.3 Vcompare

VPRIVATE double Vcompare

Definition at line 79 of file [vgrid.c](#).

9.94.4.4 Vprecision

VPRIVATE char Vprecision[26]

Definition at line 80 of file [vgrid.c](#).

9.95 vgrid.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "vgrid.h"
00058 #include <stdio.h>
00059
00060 VEMBED(rcsid="$Id$")
00061
00062 #if !defined(VINLINE_VGRID)
00063     VPUBLIC unsigned long int Vgrid_memChk(Vgrid *thee) {
00064         return Vmem_bytes(thee->mem);
00065     }
00066 #endif
00067 #define IJK(i, j, k) ((k)*(nx)*(ny)) + ((j)*(nx)) + (i)
00068
00069 #if defined(_WIN32) && (_MSC_VER < 1800)
00070 #include <float.h>
00071 int isnan(double d)
00072 {
00073     return _isnan(d);
00074 }
00075 #endif
00076
00077 VPRIVATE char *MCwhiteChars = " =,;\t\n";
00078 VPRIVATE char *MCcommChars = "#%";
00079 VPRIVATE double Vcompare;
00080 VPRIVATE char Vprecision[26];
00081
00082 /* ////////////////////////////////////////
00083 // Routine: Vgrid_ctor
00084 // Author:  Nathan Baker
00086 VPUBLIC Vgrid* Vgrid_ctor(int nx,
00087                           int ny,
00088                           int nz,
00089                           double hx,
00090                           double hy,
00091                           double hzed,
00092                           double xmin,
00093                           double ymin,
00094                           double zmin,
00095                           double *data
00096                           ) {
00097
00098     Vgrid *thee = VNULL;
00099
00100     thee = (Vgrid*)Vmem_malloc(VNULL, 1, sizeof(Vgrid));
00101     VASSERT(thee != VNULL);
00102     VASSERT(Vgrid_ctor2(thee, nx, ny, nz, hx, hy, hzed,
00103                        xmin, ymin, zmin, data));
00104

```

```

00105     return thee;
00106 }
00107
00108 /* ////////////////////////////////////////////////////////////////////
00109 // Routine:  Vgrid_ctor2
00110 // Author:   Nathan Baker
00112 VPUBLIC int Vgrid_ctor2(Vgrid *thee, int nx, int ny, int nz,
00113                        double hx, double hy, double hzed,
00114                        double xmin, double ymin, double zmin,
00115                        double *data) {
00116
00117     if (thee == VNULL) return 0;
00118     thee->nx = nx;
00119     thee->ny = ny;
00120     thee->nz = nz;
00121     thee->hx = hx;
00122     thee->hy = hy;
00123     thee->hzed = hzed;
00124     thee->xmin = xmin;
00125     thee->xmax = xmin + (nx-1)*hx;
00126     thee->ymin = ymin;
00127     thee->ymax = ymin + (ny-1)*hy;
00128     thee->zmin = zmin;
00129     thee->zmax = zmin + (nz-1)*hzed;
00130     if (data == VNULL) {
00131         thee->ctordata = 0;
00132         thee->readdata = 0;
00133     } else {
00134         thee->ctordata = 1;
00135         thee->readdata = 0;
00136         thee->data = data;
00137     }
00138
00139     thee->mem = Vmem_ctor("APBS:VGRID");
00140
00141     Vcompare = pow(10,-1*(VGRID_DIGITS - 2));
00142     sprintf(Vprecision,"%12.2de %12.2de %12.2de", VGRID_DIGITS,
00143           VGRID_DIGITS, VGRID_DIGITS);
00144
00145     return 1;
00146 }
00147
00148 /* ////////////////////////////////////////////////////////////////////
00149 // Routine:  Vgrid_dtor
00150 // Author:   Nathan Baker
00152 VPUBLIC void Vgrid_dtor(Vgrid **thee) {
00153
00154     if ((*thee) != VNULL) {
00155         Vgrid_dtor2(*thee);
00156         Vmem_free(VNULL, 1, sizeof(Vgrid), (void **)thee);
00157         (*thee) = VNULL;
00158     }
00159 }
00160
00161 /* ////////////////////////////////////////////////////////////////////
00162 // Routine:  Vgrid_dtor2
00163 // Author:   Nathan Baker
00165 VPUBLIC void Vgrid_dtor2(Vgrid *thee) {
00166
00167     if (thee->readdata) {
00168         Vmem_free(thee->mem, (thee->nx*thee->ny*thee->nz), sizeof(double),
00169             (void **)&(thee->data));
00170     }
00171     Vmem_dtor(&(thee->mem));
00172 }
00173 }
00174
00175 /* ////////////////////////////////////////////////////////////////////
00176 // Routine:  Vgrid_value
00177 // Author:   Nathan Baker
00179 VPUBLIC int Vgrid_value(Vgrid *thee, double pt[3], double *value) {
00180
00181     int nx, ny, nz;
00182     size_t ihi, jhi, khi, ilo, jlo, klo;
00183     double hx, hy, hzed, xmin, ymin, zmin, ifloat, jfloat, kfloat;
00184     double xmax, ymax, zmax;
00185     double u, dx, dy, dz;
00186
00187     if (thee == VNULL) {
00188         Vnm_print(2, "Vgrid_value:  Error -- got VNULL thee!\n");
00189         VASSERT(0);

```

```

00190     }
00191     if (!(thee->ctordata || thee->readdata)) {
00192         Vnm_print(2, "Vgrid_value: Error -- no data available!\n");
00193         VASSERT(0);
00194     }
00195
00196     nx = thee->nx;
00197     ny = thee->ny;
00198     nz = thee->nz;
00199     hx = thee->hx;
00200     hy = thee->hy;
00201     hzed = thee->hzed;
00202     xmin = thee->xmin;
00203     ymin = thee->ymin;
00204     zmin = thee->zmin;
00205     xmax = thee->xmax;
00206     ymax = thee->ymax;
00207     zmax = thee->zmax;
00208
00209     u = 0;
00210
00211     ifloat = (pt[0] - xmin)/hx;
00212     jfloat = (pt[1] - ymin)/hy;
00213     kfloat = (pt[2] - zmin)/hzed;
00214
00215     ihi = (int)ceil(ifloat);
00216     jhi = (int)ceil(jfloat);
00217     khi = (int)ceil(kfloat);
00218     ilo = (int)floor(ifloat);
00219     jlo = (int)floor(jfloat);
00220     klo = (int)floor(kfloat);
00221     if (VABS(pt[0] - xmin) < Vcompare) ilo = 0;
00222     if (VABS(pt[1] - ymin) < Vcompare) jlo = 0;
00223     if (VABS(pt[2] - zmin) < Vcompare) klo = 0;
00224     if (VABS(pt[0] - xmax) < Vcompare) ihi = nx-1;
00225     if (VABS(pt[1] - ymax) < Vcompare) jhi = ny-1;
00226     if (VABS(pt[2] - zmax) < Vcompare) khi = nz-1;
00227
00228     /* See if we're on the mesh */
00229     /*the condions starting with ilo>=0 seem unnecessary since they are of type size_t*/
00230     if ((ihi<nx) && (jhi<ny) && (khi<nz) /*&&
00231         (ilo>=0) && (jlo>=0) && (klo>=0)*/) {
00232
00233         dx = ifloat - (double)(ilo);
00234         dy = jfloat - (double)(jlo);
00235         dz = kfloat - (double)(klo);
00236         u = dx      *dy      *dz      *(thee->data[IJK(ihi, jhi, khi)])
00237           + dx      *(1.0-dy)*dz      *(thee->data[IJK(ihi, jlo, khi)])
00238           + dx      *dy      *(1.0-dz)*(thee->data[IJK(ihi, jhi, klo)])
00239           + dx      *(1.0-dy)*(1.0-dz)*(thee->data[IJK(ihi, jlo, klo)])
00240           + (1.0-dx)*dy      *dz      *(thee->data[IJK(ilo, jhi, khi)])
00241           + (1.0-dx)*(1.0-dy)*dz      *(thee->data[IJK(ilo, jlo, khi)])
00242           + (1.0-dx)*dy      *(1.0-dz)*(thee->data[IJK(ilo, jhi, klo)])
00243           + (1.0-dx)*(1.0-dy)*(1.0-dz)*(thee->data[IJK(ilo, jlo, klo)]);
00244
00245         *value = u;
00246
00247         if (isnan(u)) {
00248             Vnm_print(2, "Vgrid_value: Got NaN!\n");
00249             Vnm_print(2, "Vgrid_value: (x, y, z) = (%4.3f, %4.3f, %4.3f)\n",
00250                 pt[0], pt[1], pt[2]);
00251             Vnm_print(2, "Vgrid_value: (ihi, jhi, khi) = (%d, %d, %d)\n",
00252                 ihi, jhi, khi);
00253             Vnm_print(2, "Vgrid_value: (ilo, jlo, klo) = (%d, %d, %d)\n",
00254                 ilo, jlo, klo);
00255             Vnm_print(2, "Vgrid_value: (nx, ny, nz) = (%d, %d, %d)\n",
00256                 nx, ny, nz);
00257             Vnm_print(2, "Vgrid_value: (dx, dy, dz) = (%4.3f, %4.3f, %4.3f)\n",
00258                 dx, dy, dz);
00259             Vnm_print(2, "Vgrid_value: data[IJK(ihi, jhi, khi)] = %g\n",
00260                 thee->data[IJK(ihi, jhi, khi)]);
00261             Vnm_print(2, "Vgrid_value: data[IJK(ihi, jlo, khi)] = %g\n",
00262                 thee->data[IJK(ihi, jlo, khi)]);
00263             Vnm_print(2, "Vgrid_value: data[IJK(ihi, jhi, klo)] = %g\n",
00264                 thee->data[IJK(ihi, jhi, klo)]);
00265             Vnm_print(2, "Vgrid_value: data[IJK(ihi, jlo, klo)] = %g\n",
00266                 thee->data[IJK(ihi, jlo, klo)]);
00267             Vnm_print(2, "Vgrid_value: data[IJK(ilo, jhi, khi)] = %g\n",
00268                 thee->data[IJK(ilo, jhi, khi)]);
00269             Vnm_print(2, "Vgrid_value: data[IJK(ilo, jlo, khi)] = %g\n",
00270                 thee->data[IJK(ilo, jlo, khi)]);

```



```

00271         Vnm_print(2, "Vgrid_value:  data[IJK(ilo,jhi,klo)] = %g\n",
00272                   thee->data[IJK(ilo,jhi,klo)]);
00273         Vnm_print(2, "Vgrid_value:  data[IJK(ilo,jlo,klo)] = %g\n",
00274                   thee->data[IJK(ilo,jlo,klo)]);
00275     }
00276     return 1;
00277 } else {
00278
00279     *value = 0;
00280     return 0;
00281 }
00282
00283 return 0;
00284 }
00285
00286 //
00287 }
00288
00289 /* ////////////////////////////////////////////////////////////////////
00290 // Routine:  Vgrid_curvature
00291 //
00292 //  Notes:  cflag=0 ==> Reduced Maximal Curvature
00293 //          cflag=1 ==> Mean Curvature (Laplace)
00294 //          cflag=2 ==> Gauss Curvature
00295 //          cflag=3 ==> True Maximal Curvature
00296 //
00297 // Authors:  Stephen Bond and Nathan Baker
00298 //
00299 VPUBLIC int Vgrid_curvature(Vgrid *thee, double pt[3], int cflag,
00300 double *value) {
00301
00302     double hx, hy, hzed, curv;
00303     double dxx, dyy, dzz;
00304     double uleft, umid, uright, testpt[3];
00305
00306     if (thee == VNULL) {
00307         Vnm_print(2, "Vgrid_curvature:  Error -- got VNULL thee!\n");
00308         VASSERT(0);
00309     }
00310     if (!(thee->ctordata || thee->readdata)) {
00311         Vnm_print(2, "Vgrid_curvature:  Error -- no data available!\n");
00312         VASSERT(0);
00313     }
00314
00315     hx = thee->hx;
00316     hy = thee->hy;
00317     hzed = thee->hzed;
00318
00319     curv = 0.0;
00320
00321     testpt[0] = pt[0];
00322     testpt[1] = pt[1];
00323     testpt[2] = pt[2];
00324
00325     /* Compute 2nd derivative in the x-direction */
00326     VJMPERR1(Vgrid_value( thee, testpt, &umid));
00327     testpt[0] = pt[0] - hx;
00328     VJMPERR1(Vgrid_value( thee, testpt, &uleft));
00329     testpt[0] = pt[0] + hx;
00330     VJMPERR1(Vgrid_value( thee, testpt, &uright));
00331     testpt[0] = pt[0];
00332
00333     dxx = (uright - 2*umid + uleft)/(hx*hx);
00334
00335     /* Compute 2nd derivative in the y-direction */
00336     VJMPERR1(Vgrid_value( thee, testpt, &umid));
00337     testpt[1] = pt[1] - hy;
00338     VJMPERR1(Vgrid_value( thee, testpt, &uleft));
00339     testpt[1] = pt[1] + hy;
00340     VJMPERR1(Vgrid_value( thee, testpt, &uright));
00341     testpt[1] = pt[1];
00342
00343     dyy = (uright - 2*umid + uleft)/(hy*hy);
00344
00345     /* Compute 2nd derivative in the z-direction */
00346     VJMPERR1(Vgrid_value( thee, testpt, &umid));
00347     testpt[2] = pt[2] - hzed;
00348     VJMPERR1(Vgrid_value( thee, testpt, &uleft));
00349     testpt[2] = pt[2] + hzed;
00350     VJMPERR1(Vgrid_value( thee, testpt, &uright));
00351
00352     dzz = (uright - 2*umid + uleft)/(hzed*hzed);

```

```

00353
00354
00355     if ( cflag == 0 ) {
00356         curv = fabs(dxx);
00357         curv = ( curv > fabs(dyy) ) ? curv : fabs(dyy);
00358         curv = ( curv > fabs(dzz) ) ? curv : fabs(dzz);
00359     } else if ( cflag == 1 ) {
00360         curv = (dxx + dyy + dzz)/3.0;
00361     } else {
00362         Vnm_print(2, "Vgrid_curvature: support for cflag = %d not available!\n", cflag);
00363         VASSERT( 0 ); /* Feature Not Coded Yet! */
00364     }
00365
00366     *value = curv;
00367     return 1;
00368
00369     VERROR1:
00370     return 0;
00371
00372 }
00373
00374 /* ////////////////////////////////////////
00375 // Routine: Vgrid_gradient
00376 //
00377 // Authors: Nathan Baker and Stephen Bond
00379 VPUBLIC int Vgrid_gradient(Vgrid *thee, double pt[3], double grad[3]) {
00380
00381     double hx, hy, hzed;
00382     double uleft, umid, uright, testpt[3];
00383     int haveleft, haveright;
00384
00385     if (thee == VNULL) {
00386         Vnm_print(2, "Vgrid_gradient: Error -- got VNULL thee!\n");
00387         VASSERT(0);
00388     }
00389     if (!(thee->ctordata || thee->readdata)) {
00390         Vnm_print(2, "Vgrid_gradient: Error -- no data available!\n");
00391         VASSERT(0);
00392     }
00393
00394     hx = thee->hx;
00395     hy = thee->hy;
00396     hzed = thee->hzed;
00397
00398     /* Compute derivative in the x-direction */
00399     testpt[0] = pt[0];
00400     testpt[1] = pt[1];
00401     testpt[2] = pt[2];
00402     VJMPERR1( Vgrid_value( thee, testpt, &umid));
00403     testpt[0] = pt[0] - hx;
00404     if (Vgrid_value( thee, testpt, &uleft)) haveleft = 1;
00405     else haveleft = 0;
00406     testpt[0] = pt[0] + hx;
00407     if (Vgrid_value( thee, testpt, &uright)) haveright = 1;
00408     else haveright = 0;
00409     if (haveright && haveleft) grad[0] = (uright - uleft)/(2*hx);
00410     else if (haveright) grad[0] = (uright - umid)/hx;
00411     else if (haveleft) grad[0] = (umid - uleft)/hx;
00412     else VJMPERR1(0);
00413
00414     /* Compute derivative in the y-direction */
00415     testpt[0] = pt[0];
00416     testpt[1] = pt[1];
00417     testpt[2] = pt[2];
00418     VJMPERR1(Vgrid_value(thee, testpt, &umid));
00419     testpt[1] = pt[1] - hy;
00420     if (Vgrid_value( thee, testpt, &uleft)) haveleft = 1;
00421     else haveleft = 0;
00422     testpt[1] = pt[1] + hy;
00423     if (Vgrid_value( thee, testpt, &uright)) haveright = 1;
00424     else haveright = 0;
00425     if (haveright && haveleft) grad[1] = (uright - uleft)/(2*hy);
00426     else if (haveright) grad[1] = (uright - umid)/hy;
00427     else if (haveleft) grad[1] = (umid - uleft)/hy;
00428     else VJMPERR1(0);
00429
00430     /* Compute derivative in the z-direction */
00431     testpt[0] = pt[0];
00432     testpt[1] = pt[1];
00433     testpt[2] = pt[2];
00434     VJMPERR1(Vgrid_value(thee, testpt, &umid));

```

```

00435     testpt[2] = pt[2] - hzed;
00436     if (Vgrid_value( thee, testpt, &uleft)) haveleft = 1;
00437     else haveleft = 0;
00438     testpt[2] = pt[2] + hzed;
00439     if (Vgrid_value( thee, testpt, &uright)) haveright = 1;
00440     else haveright = 0;
00441     if (haveright && haveleft) grad[2] = (uright - uleft)/(2*hzed);
00442     else if (haveright) grad[2] = (uright - umid)/hzed;
00443     else if (haveleft) grad[2] = (umid - uleft)/hzed;
00444     else VJMPERR1(0);
00445
00446     return 1;
00447
00448     VERROR1:
00449     return 0;
00450
00451 }
00452
00453 /* ////////////////////////////////////////
00454 // Routine:  Vgrid_readGZ
00455 //
00456 // Author:   David Gohara
00457 #ifndef HAVE_ZLIB
00458 #define off_t long
00459 #include "zlib.h"
00460 #endif
00461 #endif
00462 VPUBLIC int Vgrid_readGZ(Vgrid *thee, const char *fname) {
00463
00464 #ifndef HAVE_ZLIB
00465     size_t i, j, k, u;
00466     size_t len; // Temporary counter variable for loop conditionals
00467     size_t header, incr;
00468     double *temp;
00469     double dtmpl, dtmp2, dtmp3;
00470     gzFile infile;
00471     char line[VMAX_ARGLEN];
00472
00473     header = 0;
00474
00475     /* Check to see if the existing data is null and, if not, clear it out */
00476     if (thee->data != VNULL) {
00477         Vnm_print(1, "%s:  destroying existing data!\n", __func__);
00478         Vmem_free(thee->mem, thee->nx * thee->ny * thee->nz, sizeof(double),
00479                 (void **)&(thee->data));
00480     }
00481
00482     thee->readdata = 1;
00483     thee->ctordata = 0;
00484
00485     infile = gzopen(fname, "rb");
00486     if (infile == Z_NULL) {
00487         Vnm_print(2, "%s:  Problem opening compressed file %s\n", __func__, fname);
00488         return VRC_FAILURE;
00489     }
00490
00491     thee->hx = 0.0;
00492     thee->hy = 0.0;
00493     thee->hzed = 0.0;
00494
00495     //read data here
00496     while (header < 7) {
00497         if(gzgets(infile, line, VMAX_ARGLEN) == Z_NULL){
00498             return VRC_FAILURE;
00499         }
00500
00501         // Skip comments and newlines
00502         if(strncmp(line, "#", 1) == 0) continue;
00503         if(line[0] == '\n') continue;
00504
00505         switch (header) {
00506             case 0:
00507                 sscanf(line, "object 1 class gridpositions counts %d %d %d",
00508                        &(thee->nx), &(thee->ny), &(thee->nz));
00509                 break;
00510             case 1:
00511                 sscanf(line, "origin %lf %lf %lf",
00512                        &(thee->xmin), &(thee->ymin), &(thee->zmin));
00513                 break;
00514             case 2:
00515             case 3:
00516             case 4:

```

```

00517         sscanf(line, "delta %lf %lf %lf", &dtmpl, &dtmp2, &dtmp3);
00518         thee->hx += dtmpl;
00519         thee->hy += dtmp2;
00520         thee->hzcd += dtmp3;
00521         break;
00522     default:
00523         break;
00524     }
00525
00526     header++;
00527 }
00528
00529 /* Allocate space for the data */
00530 Vnm_print(0, "%s: allocating %d x %d x %d doubles for storage\n",
00531     __func__, thee->nx, thee->ny, thee->nz);
00532 len = thee->nx * thee->ny * thee->nz;
00533
00534 thee->data = VNULL;
00535 thee->data = Vmem_malloc(thee->mem, len, sizeof(double));
00536 if (thee->data == VNULL) {
00537     Vnm_print(2, "%s: Unable to allocate space for data!\n", __func__);
00538     return 0;
00539 }
00540
00541 /* Allocate a temporary buffer to store the compressed
00542  * data into (column major order). Add 2 to ensure the buffer is
00543  * big enough to take extra data on the final read loop.
00544  */
00545 temp = (double *)malloc(len * (2 * sizeof(double)));
00546
00547 for (i = 0; i < len; i += 3){
00548     memset(&line, 0, sizeof(line));
00549     gzgets(infile, line, VMAX_ARGLEN);
00550     sscanf(line, "%lf %lf %lf", &temp[i], &temp[i+1], &temp[i+2]);
00551 }
00552
00553 /* Now move the data to row major order */
00554 incr = 0;
00555 for (i=0; i<thee->nx; i++) {
00556     for (j=0; j<thee->ny; j++) {
00557         for (k=0; k<thee->nz; k++) {
00558             u = k*(thee->nx)*(thee->ny)+j*(thee->nx)+i;
00559             (thee->data)[u] = temp[incr++];
00560         }
00561     }
00562 }
00563
00564 /* calculate grid maxima */
00565 thee->xmax = thee->xmin + (thee->nx-1)*thee->hx;
00566 thee->ymax = thee->ymin + (thee->ny-1)*thee->hy;
00567 thee->zmax = thee->zmin + (thee->nz-1)*thee->hzcd;
00568
00569 /* Close off the socket */
00570 gzclose(infile);
00571 free(temp);
00572 #else
00573
00574 Vnm_print(0, "WARNING\n");
00575 Vnm_print(0, "Vgrid_readGZ: gzip read/write support is disabled in this build\n");
00576 Vnm_print(0, "Vgrid_readGZ: configure and compile without the --disable-zlib flag.\n");
00577 Vnm_print(0, "WARNING\n");
00578 #endif
00579 return VRC_SUCCESS;
00580 }
00581
00582 VPUBLIC int Vgrid_readDX(Vgrid *thee,
00583     const char *iodev,
00584     const char *iofmt,
00585     const char *thost,
00586     const char *fname
00587 ) {
00588
00589     size_t i, j, k, itmp, u;
00590     double dtmp;
00591     char tok[VMAX_BUFSIZE];
00592     Vio *sock;
00593
00594     /* Check to see if the existing data is null and, if not, clear it out */
00595     if (thee->data != VNULL) {
00596         Vnm_print(1, "Vgrid_readDX: destroying existing data!\n");
00597         Vmem_free(thee->mem, (thee->nx*thee->ny*thee->nz), sizeof(double),

```

```

00602         (void **)&(thee->data)); }
00603     thee->readdata = 1;
00604     thee->ctordata = 0;
00605
00606     /* Set up the virtual socket */
00607     sock = Vio_ctor(iodev,iofmt,thost,fname,"r");
00608     if (sock == VNULL) {
00609         Vnm_print(2, "Vgrid_readDX: Problem opening virtual socket %s\n",
00610             fname);
00611         return 0;
00612     }
00613     if (Vio_accept(sock, 0) < 0) {
00614         Vnm_print(2, "Vgrid_readDX: Problem accepting virtual socket %s\n",
00615             fname);
00616         return 0;
00617     }
00618
00619     Vio_setWhiteChars(sock, MCwhiteChars);
00620     Vio_setCommChars(sock, MCcommChars);
00621
00622     /* Read in the DX regular positions */
00623     /* Get "object" */
00624     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00625     VJMPERR1(!strcmp(tok, "object"));
00626     /* Get "l" */
00627     VJMPERR2(1 == Vio_scanf(sock, "%d", &itmp));
00628     /* Get "class" */
00629     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00630     VJMPERR1(!strcmp(tok, "class"));
00631     /* Get "gridpositions" */
00632     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00633     VJMPERR1(!strcmp(tok, "gridpositions"));
00634     /* Get "counts" */
00635     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00636     VJMPERR1(!strcmp(tok, "counts"));
00637     /* Get nx */
00638     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00639     VJMPERR1(1 == sscanf(tok, "%d", &(thee->nx)));
00640     /* Get ny */
00641     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00642     VJMPERR1(1 == sscanf(tok, "%d", &(thee->ny)));
00643     /* Get nz */
00644     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00645     VJMPERR1(1 == sscanf(tok, "%d", &(thee->nz)));
00646     Vnm_print(0, "Vgrid_readDX: Grid dimensions %d x %d x %d grid\n",
00647         thee->nx, thee->ny, thee->nz);
00648     /* Get "origin" */
00649     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00650     VJMPERR1(!strcmp(tok, "origin"));
00651     /* Get xmin */
00652     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00653     VJMPERR1(1 == sscanf(tok, "%lf", &(thee->xmin)));
00654     /* Get ymin */
00655     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00656     VJMPERR1(1 == sscanf(tok, "%lf", &(thee->ymin)));
00657     /* Get zmin */
00658     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00659     VJMPERR1(1 == sscanf(tok, "%lf", &(thee->zmin)));
00660     Vnm_print(0, "Vgrid_readDX: Grid origin = (%g, %g, %g)\n",
00661         thee->xmin, thee->ymin, thee->zmin);
00662     /* Get "delta" */
00663     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00664     VJMPERR1(!strcmp(tok, "delta"));
00665     /* Get hx */
00666     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00667     VJMPERR1(1 == sscanf(tok, "%lf", &(thee->hx)));
00668     /* Get 0.0 */
00669     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00670     VJMPERR1(1 == sscanf(tok, "%lf", &dtmp));
00671     VJMPERR1(dtmp == 0.0);
00672     /* Get 0.0 */
00673     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00674     VJMPERR1(1 == sscanf(tok, "%lf", &dtmp));
00675     VJMPERR1(dtmp == 0.0);
00676     /* Get "delta" */
00677     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00678     VJMPERR1(!strcmp(tok, "delta"));
00679     /* Get 0.0 */
00680     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00681     VJMPERR1(1 == sscanf(tok, "%lf", &dtmp));
00682     VJMPERR1(dtmp == 0.0);

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```

00683      /* Get hy */
00684      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00685      VJMPERR1(1 == sscanf(tok, "%lf", &(thee->hy)));
00686      /* Get 0.0 */
00687      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00688      VJMPERR1(1 == sscanf(tok, "%lf", &dtmp));
00689      VJMPERR1(dtmp == 0.0);
00690      /* Get "delta" */
00691      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00692      VJMPERR1(!strcmp(tok, "delta"));
00693      /* Get 0.0 */
00694      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00695      VJMPERR1(1 == sscanf(tok, "%lf", &dtmp));
00696      VJMPERR1(dtmp == 0.0);
00697      /* Get 0.0 */
00698      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00699      VJMPERR1(1 == sscanf(tok, "%lf", &dtmp));
00700      VJMPERR1(dtmp == 0.0);
00701      /* Get hz */
00702      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00703      VJMPERR1(1 == sscanf(tok, "%lf", &(thee->hz)));
00704      Vnm_print(0, "Vgrid_readDX: Grid spacings = (%g, %g, %g)\n",
00705               thee->hx, thee->hy, thee->hz);
00706      /* Get "object" */
00707      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00708      VJMPERR1(!strcmp(tok, "object"));
00709      /* Get "2" */
00710      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00711      /* Get "class" */
00712      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00713      VJMPERR1(!strcmp(tok, "class"));
00714      /* Get "gridconnections" */
00715      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00716      VJMPERR1(!strcmp(tok, "gridconnections"));
00717      /* Get "counts" */
00718      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00719      VJMPERR1(!strcmp(tok, "counts"));
00720      /* Get the dimensions again */
00721      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00722      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00723      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00724      /* Get "object" */
00725      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00726      VJMPERR1(!strcmp(tok, "object"));
00727      /* Get # */
00728      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00729      /* Get "class" */
00730      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00731      VJMPERR1(!strcmp(tok, "class"));
00732      /* Get "array" */
00733      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00734      VJMPERR1(!strcmp(tok, "array"));
00735      /* Get "type" */
00736      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00737      VJMPERR1(!strcmp(tok, "type"));
00738      /* Get "double" */
00739      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00740      VJMPERR1(!strcmp(tok, "double"));
00741      /* Get "rank" */
00742      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00743      VJMPERR1(!strcmp(tok, "rank"));
00744      /* Get # */
00745      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00746      /* Get "items" */
00747      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00748      VJMPERR1(!strcmp(tok, "items"));
00749      /* Get # */
00750      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00751      VJMPERR1(1 == sscanf(tok, "%lu", &itmp));
00752      u = (size_t)thee->nx * thee->ny * thee->nz;
00753      VJMPERR1(u == itmp);
00754      /* Get "data" */
00755      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00756      VJMPERR1(!strcmp(tok, "data"));
00757      /* Get "follows" */
00758      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00759      VJMPERR1(!strcmp(tok, "follows"));
00760
00761      /* Allocate space for the data */
00762      Vnm_print(0, "Vgrid_readDX: allocating %d x %d x %d doubles for storage\n",
00763               thee->nx, thee->ny, thee->nz);

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```

00764     thee->data = VNULL;
00765     thee->data = (double*)Vmem_malloc(thee->mem, u, sizeof(double));
00766     if (thee->data == VNULL) {
00767         Vnm_print(2, "Vgrid_readDX: Unable to allocate space for data!\n");
00768         return 0;
00769     }
00770
00771     for (i=0; i<thee->nx; i++) {
00772         for (j=0; j<thee->ny; j++) {
00773             for (k=0; k<thee->nz; k++) {
00774                 u = k*(thee->nx)*(thee->ny)+j*(thee->nx)+i;
00775                 VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00776                 VJMPERR1(1 == sscanf(tok, "%lf", &dtmp));
00777                 (thee->data)[u] = dtmp;
00778             }
00779         }
00780     }
00781
00782     /* calculate grid maxima */
00783     thee->xmax = thee->xmin + (thee->nx-1)*thee->hx;
00784     thee->ymax = thee->ymin + (thee->ny-1)*thee->hy;
00785     thee->zmax = thee->zmin + (thee->nz-1)*thee->hz;
00786
00787     /* Close off the socket */
00788     Vio_acceptFree(sock);
00789     Vio_dtor(&sock);
00790
00791     return 1;
00792
00793 VERROR1:
00794     Vio_dtor(&sock);
00795     Vnm_print(2, "Vgrid_readDX: Format problem with input file <%=s>\n",
00796             fname);
00797     return 0;
00798
00799 VERROR2:
00800     Vio_dtor(&sock);
00801     Vnm_print(2, "Vgrid_readDX: I/O problem with input file <%=s>\n",
00802             fname);
00803     return 0;
00804 }
00805
00810 VPUBLIC int Vgrid_readDXBIN(Vgrid *thee, const char *iodev, const char *iofmt,
00811                             const char *thost, const char *fname) {
00812
00813     size_t i, j, k, itmp, u;
00814     double dtmp, dtmp2;
00815     char tok[VMAX_BUFSIZE];
00816     int isBinary = 0;
00817     //Vio *sock;
00818
00819     /* Check to see if the existing data is null and, if not, clear it out */
00820     if (thee->data != VNULL) {
00821         Vnm_print(1, "Vgrid_readDXBIN: destroying existing data!\n");
00822         Vmem_free(thee->mem, (thee->nx*thee->ny*thee->nz), sizeof(double),
00823                 (void **)&(thee->data)); }
00824     thee->readdata = 1;
00825     thee->ctordata = 0;
00826
00827     /*Open file fd for binary reading*/
00828     FILE *fd = fopen(fname, "rb");
00829     if (fd == NULL) {
00830         printf("Vgrid_readDXBIN: Problem opening file %s\n", fname);
00831         fclose(fd);
00832         return 0;
00833     }
00834
00835     /* Set up the virtual socket */
00836     // sock = Vio_ctor(iodev, iofmt, thost, fname, "r");
00837     // if (sock == VNULL) {
00838     //     Vnm_print(2, "Vgrid_readDX: Problem opening virtual socket %s\n",
00839     //             fname);
00840     //     return 0;
00841     // }
00842     // if (Vio_accept(sock, 0) < 0) {
00843     //     Vnm_print(2, "Vgrid_readDX: Problem accepting virtual socket %s\n",
00844     //             fname);
00845     //     return 0;
00846     // }
00847     //
00848     // Vio_setWhiteChars(sock, MCwhiteChars);

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```

00849 //      Vio_setCommChars(sock, MCommChars);
00850
00851 //skip comments
00852 do{
00853     fgets(tok, VMAX_BUFSIZE, fd);
00854 }
00855 while(tok[0]!='#');
00856
00857 //get counts
00858 if(sscanf(tok,"object 1 class gridpositions counts %i %i %i\n",&(thee->nx),&(thee->ny),&(thee->nz))!= 3){
00859     printf("Vgrid_readDXBIN: Failed to read dimensions.\n");
00860     fclose(fd);
00861     return 0;
00862 }
00863 printf("Vgrid_readDXBIN: Grid dimensions %d x %d x %d grid\n",thee->nx, thee->ny, thee->nz);
00864
00865     /* Read in the DX regular positions */
00866
00867     /* Get "object" */
00868     //      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00869     //      VJMPERR1(!strcmp(tok, "object"));
00870     //      /* Get "1" */
00871     //      VJMPERR2(1 == Vio_scanf(sock, "%d", &itmp));
00872     //      /* Get "class" */
00873     //      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00874     //      VJMPERR1(!strcmp(tok, "class"));
00875     //      /* Get "gridpositions" */
00876     //      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00877     //      VJMPERR1(!strcmp(tok, "gridpositions"));
00878     //      /* Get "counts" */
00879     //      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00880     //      VJMPERR1(!strcmp(tok, "counts"));
00881     //      /* Get nx */
00882     //      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00883     //      VJMPERR1(1 == sscanf(tok, "%d", &(thee->nx)));
00884     //      /* Get ny */
00885     //      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00886     //      VJMPERR1(1 == sscanf(tok, "%d", &(thee->ny)));
00887     //      /* Get nz */
00888     //      VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00889     //      VJMPERR1(1 == sscanf(tok, "%d", &(thee->nz)));
00890     //      Vnm_print(0, "Vgrid_readDX: Grid dimensions %d x %d x %d grid\n",
00891     //      thee->nx, thee->ny, thee->nz);
00892
00893     if(fgets(tok,VMAX_BUFSIZE, fd) == NULL){
00894         printf("Vgrid_readDXBIN: unexpected end of file.\n");
00895         fclose(fd);
00896         return 0;
00897     }
00898     if(sscanf(tok,"origin %lf %lf %lf",&(thee->xmin),&(thee->ymin),&(thee->zmin))!=3){
00899         printf("Vgrid_readDXBIN: Failed to read origin cell data.\n");
00900         fclose(fd);
00901         return 0;
00902     }
00903     printf("Vgrid_readDXBIN: Grid origin = (%g %g %g)\n",thee->xmin, thee->ymin, thee->zmin);
00904
00905     //get Delta x
00906     if(fgets(tok,VMAX_BUFSIZE, fd) == NULL){
00907         printf("Vgrid_readDXBIN: unexpected end of file.\n");
00908         fclose(fd);
00909         return 0;
00910     }
00911     if(sscanf(tok,"delta %lf %lf %lf",&(thee->hx),&dtmp,&dtmp2)!=3){
00912         printf("Vgrid_readDXBIN: Failed to read delta x data.\n");
00913         fclose(fd);
00914         return 0;
00915     }
00916     //get Delta y
00917     if(fgets(tok,VMAX_BUFSIZE, fd) == NULL){
00918         printf("Vgrid_readDXBIN: Unexpected end of file\n");
00919         fclose(fd);
00920         return 0;
00921     }
00922     if(sscanf(tok,"delta %lf %lf %lf",&dtmp,&(thee->hy),&dtmp2)!=3){
00923         printf("Vgrid_readDXBIN: Failed to read delta y data.\n");
00924         fclose(fd);
00925         return 0;
00926     }
00927     //get Delta z
00928     if(fgets(tok,VMAX_BUFSIZE, fd) == NULL){
00929         printf("Vgrid_readDXBIN: Unexpected end of file.\n");

```



```

00930     fclose(fd);
00931     return 0;
00932 }
00933 if(sscanf(tok,"delta %lf %lf %lf",&dtmp,&dtmp2,&(thee->hzd))!=3){
00934     printf("Vgrid_readDXBIN: Failed to read delta z data.\n");
00935     fclose(fd);
00936     return 0;
00937 }
00938 printf("Vgrid_readDXBIN: Grid spacings = (%g, %g, %g)\n",thee->hx, thee->hy, thee->hzd);
00939
00940 //skip a line
00941 if(fgets(tok,VMAX_BUFSIZE, fd) == NULL){
00942     printf("Vgrid_readDXBIN: Unexpected end of file.\n");
00943     fclose(fd);
00944     return 0;
00945 }
00946
00947 //scan the buffer for the word binary
00948 if(fgets(tok,VMAX_BUFSIZE, fd) == NULL){
00949     printf("Vgrid_readDXBIN: Unexpected end of file.\n");
00950     fclose(fd);
00951     return 0;
00952 }
00953 if(strstr(tok,"binary")){
00954     isBinary = 1;
00955 }
00956 else{
00957     printf("Vgrid_readDXBIN: Binary tag not found. Will continue to try to read binary data.");
00958 }
00959
00960 u = (size_t)thee->nx * thee->ny * thee->nz;
00961 int tot = thee->nx * thee->ny * thee->nz;
00962
00963 /*Allocate space for the data*/
00964 printf("Vgrid_readDXBIN: allocating %d x %d x %d doubled for storage\n", thee->nx, thee->ny, thee->nz);
00965 thee->data = NULL;
00966 thee->data = (double *)malloc(tot*sizeof(double));
00967
00968 if(thee->data == NULL){
00969     printf("Vgrid_readDXBIN: Unable to allocate space for data!\n");
00970     fclose(fd);
00971     return 0;
00972 }
00973
00974 int counter = 0, r;
00975
00976 for (i=0; i<thee->nx; i++) {
00977     for (j=0; j<thee->ny; j++) {
00978         for (k=0; k<thee->nz; k++) {
00979             u = k*(thee->nx)*(thee->ny)+j*(thee->nx)+i;
00980             r = fread(&dtmp,sizeof(double),1,fd);
00981             (thee->data)[u] = dtmp;
00982             if(r!= 1){
00983                 printf("Vgrid_readDXBIN: Failed to read doubles.\n");
00984                 return 0;
00985             }
00986             counter++;
00987         }
00988     }
00989 }
00990
00991 if(counter!=tot){
00992     printf("Vgrid_readDXBIN: Read double = %d not equal to items = %d\n",counter, tot);
00993 }
00994
00995 /* calculate grid maxima */
00996 thee->xmax = thee->xmin + (thee->nx-1)*thee->hx;
00997 thee->ymax = thee->ymin + (thee->ny-1)*thee->hy;
00998 thee->zmax = thee->zmin + (thee->nz-1)*thee->hzd;
00999
01000 fclose(fd);
01001
01002 return 1;
01003 }
01004
01005
01006 /* ////////////////////////////////////////
01007 // Routine:  Vgrid_writeGZ
01008 //
01009 // Author:   Nathan Baker
01011 VPUBLIC void Vgrid_writeGZ(Vgrid *thee, const char *iodev, const char *iofmt,

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```

01012             const char *thost, const char *fname, char *title, double *pvec) {
01013
01014 #ifndef HAVE_ZLIB
01015     double xmin, ymin, zmin, hx, hy, hzed;
01016
01017     int nx, ny, nz, nxPART, nyPART, nzPART;
01018     int usepart, gotit;
01019     size_t icol, i, j, k, u;
01020     double x, y, z, xminPART, yminPART, zminPART;
01021
01022     size_t txyz;
01023     double txmin, tymin, tzmin;
01024
01025     char header[8196];
01026     char footer[8196];
01027     char line[80];
01028     char newline[] = "\n";
01029     gzFile outfile;
01030     char precFormat[VMAX_BUFSIZE];
01031
01032     if (thee == VNULL) {
01033         Vnm_print(2, "Vgrid_writeGZ: Error -- got VNULL thee!\n");
01034         VASSERT(0);
01035     }
01036     if (!(thee->ctordata || thee->readdata)) {
01037         Vnm_print(2, "Vgrid_writeGZ: Error -- no data available!\n");
01038         VASSERT(0);
01039     }
01040
01041     hx = thee->hx;
01042     hy = thee->hy;
01043     hzed = thee->hzed;
01044     nx = thee->nx;
01045     ny = thee->ny;
01046     nz = thee->nz;
01047     xmin = thee->xmin;
01048     ymin = thee->ymin;
01049     zmin = thee->zmin;
01050
01051     if (pvec == VNULL) usepart = 0;
01052     else usepart = 1;
01053
01054     /* Set up the virtual socket */
01055     Vnm_print(0, "Vgrid_writeGZ: Opening file...\n");
01056     outfile = gzopen(fname, "wb");
01057
01058     if (usepart) {
01059         /* Get the lower corner and number of grid points for the local
01060          * partition */
01061         xminPART = VLARGE;
01062         yminPART = VLARGE;
01063         zminPART = VLARGE;
01064         nxPART = 0;
01065         nyPART = 0;
01066         nzPART = 0;
01067         /* First, search for the lower corner */
01068         for (k=0; k<nz; k++) {
01069             z = k*hzed + zmin;
01070             for (j=0; j<ny; j++) {
01071                 y = j*hy + ymin;
01072                 for (i=0; i<nx; i++) {
01073                     x = i*hx + xmin;
01074                     if (pvec[IJK(i,j,k)] > 0.0) {
01075                         if (x < xminPART) xminPART = x;
01076                         if (y < yminPART) yminPART = y;
01077                         if (z < zminPART) zminPART = z;
01078                     }
01079                 }
01080             }
01081         }
01082         /* Now search for the number of grid points in the z direction */
01083         for (k=0; k<nz; k++) {
01084             gotit = 0;
01085             for (j=0; j<ny; j++) {
01086                 for (i=0; i<nx; i++) {
01087                     if (pvec[IJK(i,j,k)] > 0.0) {
01088                         gotit = 1;
01089                         break;
01090                     }
01091                 }
01092             }
01093             if (gotit) break;

```

```

01093     }
01094     if (gotit) nzPART++;
01095 }
01096 /* Now search for the number of grid points in the y direction */
01097 for (j=0; j<ny; j++) {
01098     gotit = 0;
01099     for (k=0; k<nz; k++) {
01100         for (i=0; i<nx; i++) {
01101             if (pvec[IJK(i,j,k)] > 0.0) {
01102                 gotit = 1;
01103                 break;
01104             }
01105         }
01106         if (gotit) break;
01107     }
01108     if (gotit) nyPART++;
01109 }
01110 /* Now search for the number of grid points in the x direction */
01111 for (i=0; i<nx; i++) {
01112     gotit = 0;
01113     for (k=0; k<nz; k++) {
01114         for (j=0; j<ny; j++) {
01115             if (pvec[IJK(i,j,k)] > 0.0) {
01116                 gotit = 1;
01117                 break;
01118             }
01119         }
01120         if (gotit) break;
01121     }
01122     if (gotit) nxPART++;
01123 }
01124
01125 if ((nxPART != nx) || (nyPART != ny) || (nzPART != nz)) {
01126     Vnm_print(0, "Vgrid_writeGZ: printing only subset of domain\n");
01127 }
01128
01129 txyz = (nxPART*nyPART*nzPART);
01130 txmin = xminPART;
01131 tymin = yminPART;
01132 tzmin = zminPART;
01133
01134 }else {
01135
01136     txyz = (nx*ny*nz);
01137     txmin = xmin;
01138     tymin = ymin;
01139     tzmin = zmin;
01140
01141 }
01142
01143 /* Write off the title (if we're not XDR) */
01144 sprintf(header,
01145     "# Data from %s\n" \
01146     "# \n" \
01147     "# %s\n" \
01148     "# \n" \
01149     "object 1 class gridpositions counts %i %i %i\n" \
01150     "origin %12.6e %12.6e %12.6e\n" \
01151     "delta %12.6e 0.000000e+00 0.000000e+00\n" \
01152     "delta 0.000000e+00 %12.6e 0.000000e+00\n" \
01153     "delta 0.000000e+00 0.000000e+00 %12.6e\n" \
01154     "object 2 class gridconnections counts %i %i %i\n" \
01155     "object 3 class array type double rank 0 items %lu data follows\n",
01156     PACKAGE_STRING,title,nx,ny,nz,txmin,tymin,tzmin,
01157     hx,hy,hzed,nx,ny,nz,txyz);
01158 gzwrite(outfile, header, strlen(header)*sizeof(char));
01159
01160 /* Now write the data */
01161 icol = 0;
01162 for (i=0; i<nx; i++) {
01163     for (j=0; j<ny; j++) {
01164         for (k=0; k<nz; k++) {
01165             u = k*(nx)*(ny)+j*(nx)+i;
01166             if (pvec[u] > 0.0) {
01167                 sprintf(line, "%12.6e ", thee->data[u]);
01168                 gzwrite(outfile, line, strlen(line)*sizeof(char));
01169                 icol++;
01170                 if (icol == 3) {
01171                     icol = 0;
01172                     gzwrite(outfile, newline, strlen(newline)*sizeof(char));
01173                 }

```

```

01174         }
01175     }
01176 }
01177 }
01178 if(icol < 3){
01179     char newline[] = "\n";
01180     gzwrite(outfile, newline, strlen(newline)*sizeof(char));
01181 }
01182
01183 /* Create the field */
01184 sprintf(footer, "attribute \"dep\" string \"positions\"\n" \
01185           "object \"regular positions regular connections\" class field\n" \
01186           "component \"positions\" value 1\n" \
01187           "component \"connections\" value 2\n" \
01188           "component \"data\" value 3\n");
01189 gzwrite(outfile, footer, strlen(footer)*sizeof(char));
01190
01191 gzclose(outfile);
01192 #else
01193
01194     Vnm_print(0, "WARNING\n");
01195     Vnm_print(0, "Vgrid_readGZ:  gzip read/write support is disabled in this build\n");
01196     Vnm_print(0, "Vgrid_readGZ:  configure and compile without the --disable-zlib flag.\n");
01197     Vnm_print(0, "WARNING\n");
01198 #endif
01199 }
01200
01201 /* ////////////////////////////////////////
01202 // Routine:  Vgrid_writeDX
01203 //
01204 // Author:   Nathan Baker
01206 VPUBLIC void Vgrid_writeDX(Vgrid *thee, const char *iodev, const char *iofmt,
01207     const char *thost, const char *fname, char *title, double *pvec) {
01208
01209     double xmin, ymin, zmin, hx, hy, hzed;
01210     int nx, ny, nz, nxPART, nyPART, nzPART;
01211     int usepart, gotit;
01212     size_t icol, i, j, k, u;
01213     double x, y, z, xminPART, yminPART, zminPART;
01214     Vio *sock;
01215     char precFormat[VMAX_BUFSIZE];
01216
01217     if (thee == VNULL) {
01218         Vnm_print(2, "Vgrid_writeDX:  Error -- got VNULL thee!\n");
01219         VASSERT(0);
01220     }
01221     if (!(thee->ctordata || thee->readdata)) {
01222         Vnm_print(2, "Vgrid_writeDX:  Error -- no data available!\n");
01223         VASSERT(0);
01224     }
01225
01226     hx = thee->hx;
01227     hy = thee->hy;
01228     hzed = thee->hzed;
01229     nx = thee->nx;
01230     ny = thee->ny;
01231     nz = thee->nz;
01232     xmin = thee->xmin;
01233     ymin = thee->ymin;
01234     zmin = thee->zmin;
01235
01236     if (pvec == VNULL) usepart = 0;
01237     else usepart = 1;
01238
01239     /* Set up the virtual socket */
01240     Vnm_print(0, "Vgrid_writeDX:  Opening virtual socket...\n");
01241     sock = Vio_ctor(iodev, iofmt, thost, fname, "w");
01242     if (sock == VNULL) {
01243         Vnm_print(2, "Vgrid_writeDX:  Problem opening virtual socket %s\n",
01244             fname);
01245         return;
01246     }
01247     if (Vio_connect(sock, 0) < 0) {
01248         Vnm_print(2, "Vgrid_writeDX:  Problem connecting virtual socket %s\n",
01249             fname);
01250         return;
01251     }
01252
01253     Vio_setWhiteChars(sock, MCwhiteChars);
01254     Vio_setCommChars(sock, MCcommChars);
01255

```

```

01256     Vnm_print(0, "Vgrid_writeDX: Writing to virtual socket...\n");
01257
01258     if (usepart) {
01259         /* Get the lower corner and number of grid points for the local
01260          * partition */
01261         xminPART = VLARGE;
01262         yminPART = VLARGE;
01263         zminPART = VLARGE;
01264         nxPART = 0;
01265         nyPART = 0;
01266         nzPART = 0;
01267         /* First, search for the lower corner */
01268         for (k=0; k<nz; k++) {
01269             z = k*hzed + zmin;
01270             for (j=0; j<ny; j++) {
01271                 y = j*hy + ymin;
01272                 for (i=0; i<nx; i++) {
01273                     x = i*hx + xmin;
01274                     if (pvec[IJK(i,j,k)] > 0.0) {
01275                         if (x < xminPART) xminPART = x;
01276                         if (y < yminPART) yminPART = y;
01277                         if (z < zminPART) zminPART = z;
01278                     }
01279                 }
01280             }
01281         }
01282         /* Now search for the number of grid points in the z direction */
01283         for (k=0; k<nz; k++) {
01284             gotit = 0;
01285             for (j=0; j<ny; j++) {
01286                 for (i=0; i<nx; i++) {
01287                     if (pvec[IJK(i,j,k)] > 0.0) {
01288                         gotit = 1;
01289                         break;
01290                     }
01291                 }
01292                 if (gotit) break;
01293             }
01294             if (gotit) nzPART++;
01295         }
01296         /* Now search for the number of grid points in the y direction */
01297         for (j=0; j<ny; j++) {
01298             gotit = 0;
01299             for (k=0; k<nz; k++) {
01300                 for (i=0; i<nx; i++) {
01301                     if (pvec[IJK(i,j,k)] > 0.0) {
01302                         gotit = 1;
01303                         break;
01304                     }
01305                 }
01306                 if (gotit) break;
01307             }
01308             if (gotit) nyPART++;
01309         }
01310         /* Now search for the number of grid points in the x direction */
01311         for (i=0; i<nx; i++) {
01312             gotit = 0;
01313             for (k=0; k<nz; k++) {
01314                 for (j=0; j<ny; j++) {
01315                     if (pvec[IJK(i,j,k)] > 0.0) {
01316                         gotit = 1;
01317                         break;
01318                     }
01319                 }
01320                 if (gotit) break;
01321             }
01322             if (gotit) nxPART++;
01323         }
01324
01325         if ((nxPART != nx) || (nyPART != ny) || (nzPART != nz)) {
01326             Vnm_print(0, "Vgrid_writeDX: printing only subset of domain\n");
01327         }
01328
01329         /* Write off the title (if we're not XDR) */
01330         if (Vstring_strcasecmp(iofmt, "XDR") == 0) {
01331             Vnm_print(0, "Vgrid_writeDX: Skipping comments for XDR format.\n");
01332         } else {
01333             Vnm_print(0, "Vgrid_writeDX: Writing comments for %s format.\n",
01334                       iofmt);
01335             Vio_printf(sock, "# Data from %s\n", PACKAGE_STRING);
01336         }

```

```

01337         Vio_printf(sock, "# \n");
01338         Vio_printf(sock, "# %s\n", title);
01339         Vio_printf(sock, "# \n");
01340     }
01341
01342     /* Write off the DX regular positions */
01343     Vio_printf(sock, "object 1 class gridpositions counts %d %d %d\n",
01344         nxPART, nyPART, nzPART);
01345
01346     sprintf(precFormat, Vprecision, xminPART, yminPART, zminPART);
01347     Vio_printf(sock, "origin %s\n", precFormat);
01348     sprintf(precFormat, Vprecision, hx, 0.0, 0.0);
01349     Vio_printf(sock, "delta %s\n", precFormat);
01350     sprintf(precFormat, Vprecision, 0.0, hy, 0.0);
01351     Vio_printf(sock, "delta %s\n", precFormat);
01352     sprintf(precFormat, Vprecision, 0.0, 0.0, hzed);
01353     Vio_printf(sock, "delta %s\n", precFormat);
01354
01355     /* Write off the DX regular connections */
01356     Vio_printf(sock, "object 2 class gridconnections counts %d %d %d\n",
01357         nxPART, nyPART, nzPART);
01358
01359     /* Write off the DX data */
01360     Vio_printf(sock, "object 3 class array type double rank 0 items %lu \
01361 data follows\n", (nxPART*nyPART*nzPART));
01362     icol = 0;
01363     for (i=0; i<nx; i++) {
01364         for (j=0; j<ny; j++) {
01365             for (k=0; k<nz; k++) {
01366                 u = k*(nx)*(ny)+j*(nx)+i;
01367                 if (pvec[u] > 0.0) {
01368                     Vio_printf(sock, "%12.6e ", thee->data[u]);
01369                     icol++;
01370                     if (icol == 3) {
01371                         icol = 0;
01372                         Vio_printf(sock, "\n");
01373                     }
01374                 }
01375             }
01376         }
01377     }
01378
01379     if (icol != 0) Vio_printf(sock, "\n");
01380
01381     /* Create the field */
01382     Vio_printf(sock, "attribute \"dep\" string \"positions\"\n");
01383     Vio_printf(sock, "object \"regular positions regular connections\" \
01384 class field\n");
01385     Vio_printf(sock, "component \"positions\" value 1\n");
01386     Vio_printf(sock, "component \"connections\" value 2\n");
01387     Vio_printf(sock, "component \"data\" value 3\n");
01388
01389 } else {
01390     /* Write off the title (if we're not XDR) */
01391     if (Vstring_strcasecmp(iofmt, "XDR") == 0) {
01392         Vnm_print(0, "Vgrid_writeDX: Skipping comments for XDR format.\n");
01393     } else {
01394         Vnm_print(0, "Vgrid_writeDX: Writing comments for %s format.\n",
01395             iofmt);
01396         Vio_printf(sock, "# Data from %s\n", PACKAGE_STRING);
01397         Vio_printf(sock, "# \n");
01398         Vio_printf(sock, "# %s\n", title);
01399         Vio_printf(sock, "# \n");
01400     }
01401
01402     /* Write off the DX regular positions */
01403     Vio_printf(sock, "object 1 class gridpositions counts %d %d %d\n",
01404         nx, ny, nz);
01405
01406     sprintf(precFormat, Vprecision, xmin, ymin, zmin);
01407     Vio_printf(sock, "origin %s\n", precFormat);
01408     sprintf(precFormat, Vprecision, hx, 0.0, 0.0);
01409     Vio_printf(sock, "delta %s\n", precFormat);
01410     sprintf(precFormat, Vprecision, 0.0, hy, 0.0);
01411     Vio_printf(sock, "delta %s\n", precFormat);
01412     sprintf(precFormat, Vprecision, 0.0, 0.0, hzed);
01413     Vio_printf(sock, "delta %s\n", precFormat);
01414
01415     /* Write off the DX regular connections */
01416     Vio_printf(sock, "object 2 class gridconnections counts %d %d %d\n",

```

```

01418         nx, ny, nz);
01419
01420         /* Write off the DX data */
01421         Vio_printf(sock, "object 3 class array type double rank 0 items %lu \
01422 data follows\n", (nx*ny*nz));
01423         icol = 0;
01424         for (i=0; i<nx; i++) {
01425             for (j=0; j<ny; j++) {
01426                 for (k=0; k<nz; k++) {
01427                     u = k*(nx)*(ny)+j*(nx)+i;
01428                     Vio_printf(sock, "%12.6e ", thee->data[u]);
01429                     icol++;
01430                     if (icol == 3) {
01431                         icol = 0;
01432                         Vio_printf(sock, "\n");
01433                     }
01434                 }
01435             }
01436         }
01437         if (icol != 0) Vio_printf(sock, "\n");
01438
01439         /* Create the field */
01440         Vio_printf(sock, "attribute \"dep\" string \"positions\"\n");
01441         Vio_printf(sock, "object \"regular positions regular connections\" \
01442 class field\n");
01443         Vio_printf(sock, "component \"positions\" value 1\n");
01444         Vio_printf(sock, "component \"connections\" value 2\n");
01445         Vio_printf(sock, "component \"data\" value 3\n");
01446     }
01447
01448     /* Close off the socket */
01449     Vio_connectFree(sock);
01450     Vio_dtor(&sock);
01451 }
01452
01453 /* ////////////////////////////////////// */
01454 // Routine: Vgrid_writeDXBIN
01455 //
01456 // Author: Juan Brandi
01457 VPUBLIC void Vgrid_writeDXBIN(Vgrid *thee, const char *iodev, const char *iofmt,
01458 const char *thost, const char *fname, char *title, double *pvec){
01459
01460     double xmin, ymin, zmin, hx, hy, hzed;
01461     int nx, ny, nz, nxPART, nyPART, nzPART;
01462     int usepart, gotit;
01463     size_t icol, i, j, k, u;
01464     double x, y, z, xminPART, yminPART, zminPART;
01465     //Vio *sock;
01466     char precFormat[VMAX_BUFSIZE];
01467
01468     if (thee == VNULL) {
01469         Vnm_print(2, "Vgrid_writeDXBIN: Error -- got VNULL thee!\n");
01470         VASSERT(0);
01471     }
01472     if (!(thee->ctordata || thee->readdata)) {
01473         Vnm_print(2, "Vgrid_writeDXBIN: Error -- no data available!\n");
01474         VASSERT(0);
01475     }
01476
01477
01478
01479     hx = thee->hx;
01480     hy = thee->hy;
01481     hzed = thee->hzed;
01482     nx = thee->nx;
01483     ny = thee->ny;
01484     nz = thee->nz;
01485     xmin = thee->xmin;
01486     ymin = thee->ymin;
01487     zmin = thee->zmin;
01488
01489     if (pvec == VNULL) usepart = 0;
01490     else usepart = 1;
01491
01492     /*will not use vio methods to try to avoid using malloc.*/
01493     FILE *fd = fopen(fname, "wb");
01494
01495     //check to se if the file was created/open successfully.
01496     if (fd == NULL) {
01497         printf("Vgrid_writeDXBIN: Problem opening file %s for writing.\n", fname);
01498         return;
01499     }

```

```

01500
01501 printf("Vgrid_writeDXBIN: Writing to file...\n");
01502
01503 if (usepart) {
01504     /* Get the lower corner and number of grid points for the local
01505      * partition */
01506     xminPART = VLARGE;
01507     yminPART = VLARGE;
01508     zminPART = VLARGE;
01509     nxPART = 0;
01510     nyPART = 0;
01511     nzPART = 0;
01512     /* First, search for the lower corner */
01513     for (k=0; k<nz; k++) {
01514         z = k*hzed + zmin;
01515         for (j=0; j<ny; j++) {
01516             y = j*hy + ymin;
01517             for (i=0; i<nx; i++) {
01518                 x = i*hx + xmin;
01519                 if (pvec[IJK(i,j,k)] > 0.0) {
01520                     if (x < xminPART) xminPART = x;
01521                     if (y < yminPART) yminPART = y;
01522                     if (z < zminPART) zminPART = z;
01523                 }
01524             }
01525         }
01526     }
01527     /* Now search for the number of grid points in the z direction */
01528     for (k=0; k<nz; k++) {
01529         gotit = 0;
01530         for (j=0; j<ny; j++) {
01531             for (i=0; i<nx; i++) {
01532                 if (pvec[IJK(i,j,k)] > 0.0) {
01533                     gotit = 1;
01534                     break;
01535                 }
01536             }
01537             if (gotit) break;
01538         }
01539         if (gotit) nzPART++;
01540     }
01541     /* Now search for the number of grid points in the y direction */
01542     for (j=0; j<ny; j++) {
01543         gotit = 0;
01544         for (k=0; k<nz; k++) {
01545             for (i=0; i<nx; i++) {
01546                 if (pvec[IJK(i,j,k)] > 0.0) {
01547                     gotit = 1;
01548                     break;
01549                 }
01550             }
01551             if (gotit) break;
01552         }
01553         if (gotit) nyPART++;
01554     }
01555     /* Now search for the number of grid points in the x direction */
01556     for (i=0; i<nx; i++) {
01557         gotit = 0;
01558         for (k=0; k<nz; k++) {
01559             for (j=0; j<ny; j++) {
01560                 if (pvec[IJK(i,j,k)] > 0.0) {
01561                     gotit = 1;
01562                     break;
01563                 }
01564             }
01565             if (gotit) break;
01566         }
01567         if (gotit) nxPART++;
01568     }
01569
01570     if ((nxPART != nx) || (nyPART != ny) || (nzPART != nz)) {
01571         Vnm_print(0, "Vgrid_writeDXBIN: printing only subset of domain\n");
01572     }
01573
01574     /* Write title (we're in XDR and "wb") */
01575     //Vnm_print(0, "Vgrid_writeDXBIN: Writing comments for dxbin format.\n");
01576     printf("Vgrid_writeDXBIN: Writing comments for dxbin format\n");
01577     fprintf(fd, "# Data from %s\n", PACKAGE_STRING);
01578     fprintf(fd, "# \n");
01579     fprintf(fd, "# %s\n", title);
01580     fprintf(fd, "# \n");

```



```

01581
01582 /* Write off the DX regular positions */
01583 fprintf(fd, "object 1 class gridpositions counts %d %d %d\n", nxPART, nyPART, nzPART);
01584
01585 sprintf(precFormat, Vprecision, xminPART, yminPART, zminPART);
01586 fprintf(fd, "origin %s\n", precFormat);
01587
01588 sprintf(precFormat, Vprecision, hx, 0.0, 0.0);
01589 fprintf(fd, "delta %s\n", precFormat);
01590
01591 sprintf(precFormat, Vprecision, 0.0, hy, 0.0);
01592 fprintf(fd, "delta %s\n", precFormat);
01593
01594 sprintf(precFormat, Vprecision, 0.0, 0.0, hzed);
01595 fprintf(fd, "delta %s\n", precFormat);
01596
01597 /* Write off the DX regular connections */
01598 fprintf(fd, "object 2 class gridconnections counts %d %d %d\n", nxPART, nyPART, nzPART);
01599
01600 /* Write off the DX data */
01601 fprintf(fd, "object 3 class array type double rank 0 items %d binary data
follows\n", (nxPART*nyPART*nzPART));
01602
01603 icol = 0;
01604 for (i=0; i<nx; i++) {
01605     for (j=0; j<ny; j++) {
01606         for (k=0; k<nz; k++) {
01607             u = k*(nx)*(ny)+j*(nx)+i;
01608             if (pvec[u] > 0.0) {
01609                 fwrite(&(thee->data)[u], sizeof(double), 1, fd);
01610                 icol++;
01611                 /*don't need the column formatting to write binary doubles.*/
01612                 if (icol == 3) {
01613                     icol = 0;
01614                 }
01615             }
01616         }
01617     }
01618 }
01619
01620 fprintf(fd, "\n");
01621
01622 /* Create the field */
01623 fprintf(fd, "attribute \"dep\" string \"positions\\n\\n\"");
01624 fprintf(fd, "object \"regular positions regular connections\" class field\n");
01625 fprintf(fd, "component \"positions\" value 1\n");
01626 fprintf(fd, "component \"connections\" value 2\n");
01627 fprintf(fd, "component \"data\" value 3\n");
01628
01629 fclose(fd);
01630
01631 } else {
01632     /*write dx format title*/
01633     printf("Vgrid_writeDXBIN: Writing comments for %s format.\n", iofmt);
01634     fprintf(fd, "# Data from %s\n", PACKAGE_STRING);
01635     fprintf(fd, "# \n");
01636     fprintf(fd, "# %s\n", title);
01637     fprintf(fd, "# \n");
01638
01639     /* Write off the DX regular positions */
01640     fprintf(fd, "object 1 class gridpositions counts %d %d %d\n", nx, ny, nz);
01641
01642     sprintf(precFormat, Vprecision, xmin, ymin, zmin);
01643     fprintf(fd, "origin %s\n", precFormat);
01644
01645     sprintf(precFormat, Vprecision, hx, 0.0, 0.0);
01646     fprintf(fd, "delta %s\n", precFormat);
01647
01648     sprintf(precFormat, Vprecision, 0.0, hy, 0.0);
01649     fprintf(fd, "delta %s\n", precFormat);
01650
01651     sprintf(precFormat, Vprecision, 0.0, 0.0, hzed);
01652     fprintf(fd, "delta %s\n", precFormat);
01653
01654     /* Write off the DX regular connections */
01655     fprintf(fd, "object 2 class gridconnections counts %d %d %d\n", nx, ny, nz);
01656
01657     /* Write off the DX data */
01658     fprintf(fd, "object 3 class array type double rank 0 items %d binary data follows\n", (nx*ny*nz));
01659
01660     icol = 0;

```

```

01661     for (i=0; i<nx; i++) {
01662         for (j=0; j<ny; j++) {
01663             for (k=0; k<nz; k++) {
01664                 u = k*(nx)*(ny)+j*(nx)+i;
01665                 fwrite(&(thee->data)[u], sizeof(double), 1, fd);
01666                 icol++;
01667                 if (icol == 3) {
01668                     icol = 0;
01669                 }
01670             }
01671         }
01672     }
01673     fprintf(fd, "\n");
01674
01675     /* Create the field */
01676     fprintf(fd, "attribute \"dep\" string \"positions\"\n");
01677     fprintf(fd, "object \"regular positions regular connections\" class field\n");
01678     fprintf(fd, "component \"positions\" value 1\n");
01679     fprintf(fd, "component \"connections\" value 2\n");
01680     fprintf(fd, "component \"data\" value 3\n");
01681
01682     fclose(fd);
01683 }
01684 }
01685 }
01686
01687
01688 /* ////////////////////////////////////////
01689 // Routine: Vgrid_writeUHBD
01690 // Author:  Nathan Baker
01692 VPUBLIC void Vgrid_writeUHBD(Vgrid *thee, const char *iodev, const char *iofmt,
01693     const char *thost, const char *fname, char *title, double *pvec) {
01694
01695     size_t u, icol, i, j, k;
01696     size_t gotit, nx, ny, nz;
01697     double xmin, ymin, zmin, hzed, hy, hx;
01698     Vio *sock;
01699
01700     if (thee == VNULL) {
01701         Vnm_print(2, "Vgrid_writeUHBD: Error -- got VNULL thee!\n");
01702         VASSERT(0);
01703     }
01704     if (!(thee->ctordata || thee->readdata)) {
01705         Vnm_print(2, "Vgrid_writeUHBD: Error -- no data available!\n");
01706         VASSERT(0);
01707     }
01708
01709     if ((thee->hx!=thee->hy) || (thee->hy!=thee->hzed)
01710         || (thee->hx!=thee->hzed)) {
01711         Vnm_print(2, "Vgrid_writeUHBD: can't write UHBD mesh with non-uniform \
01712 spacing\n");
01713         return;
01714     }
01715
01716     /* Set up the virtual socket */
01717     sock = Vio_ctor(iodev, iofmt, thost, fname, "w");
01718     if (sock == VNULL) {
01719         Vnm_print(2, "Vgrid_writeUHBD: Problem opening virtual socket %s\n",
01720             fname);
01721         return;
01722     }
01723     if (Vio_connect(sock, 0) < 0) {
01724         Vnm_print(2, "Vgrid_writeUHBD: Problem connecting virtual socket %s\n",
01725             fname);
01726         return;
01727     }
01728
01729     /* Get the lower corner and number of grid points for the local
01730      * partition */
01731     hx = thee->hx;
01732     hy = thee->hy;
01733     hzed = thee->hzed;
01734     nx = thee->nx;
01735     ny = thee->ny;
01736     nz = thee->nz;
01737     xmin = thee->xmin;
01738     ymin = thee->ymin;
01739     zmin = thee->zmin;
01740
01741     /* Let interested folks know that partition information is ignored */
01742     if (pvec != VNULL) {

```

```

01743         gotit = 0;
01744         for (i=0; i<(nx*ny*nz); i++) {
01745             if (pvec[i] == 0) {
01746                 gotit = 1;
01747                 break;
01748             }
01749         }
01750         if (gotit) {
01751             Vnm_print(2, "Vgrid_writeUHBD:  IGNORING PARTITION INFORMATION!\n");
01752             Vnm_print(2, "Vgrid_writeUHBD:  This means I/O from parallel runs \
01753 will have significant overlap.\n");
01754         }
01755     }
01756
01757     /* Write out the header */
01758     Vio_printf(sock, "%72s\n", title);
01759     Vio_printf(sock, "%12.5e%12.5e%7d%7d%7d%7d\n", 1.0, 0.0, -1, 0,
01760 nz, 1, nz);
01761     Vio_printf(sock, "%7d%7d%7d%12.5e%12.5e%12.5e%12.5e\n", nx, ny, nz,
01762 hx, (xmin-hx), (ymin-hx), (zmin-hx));
01763     Vio_printf(sock, "%12.5e%12.5e%12.5e%12.5e\n", 0.0, 0.0, 0.0, 0.0);
01764     Vio_printf(sock, "%12.5e%12.5e%7d%7d", 0.0, 0.0, 0, 0);
01765
01766     /* Write out the entries */
01767     icol = 0;
01768     for (k=0; k<nz; k++) {
01769         Vio_printf(sock, "\n%7d%7d%7d\n", k+1, thee->nx, thee->ny);
01770         icol = 0;
01771         for (j=0; j<ny; j++) {
01772             for (i=0; i<nx; i++) {
01773                 u = k*(nx)*(ny)+j*(nx)+i;
01774                 icol++;
01775                 Vio_printf(sock, " %12.5e", thee->data[u]);
01776                 if (icol == 6) {
01777                     icol = 0;
01778                     Vio_printf(sock, "\n");
01779                 }
01780             }
01781         }
01782     }
01783     if (icol != 0) Vio_printf(sock, "\n");
01784
01785     /* Close off the socket */
01786     Vio_connectFree(sock);
01787     Vio_dtor(&sock);
01788 }
01789
01790 VPUBLIC double Vgrid_integrate(Vgrid *thee) {
01791
01792     size_t i, j, k;
01793     int nx, ny, nz;
01794     double sum, w;
01795
01796     if (thee == VNULL) {
01797         Vnm_print(2, "Vgrid_integrate:  Got VNULL thee!\n");
01798         VASSERT(0);
01799     }
01800
01801     nx = thee->nx;
01802     ny = thee->ny;
01803     nz = thee->nz;
01804
01805     sum = 0.0;
01806
01807     for (k=0; k<nz; k++) {
01808         w = 1.0;
01809         if ((k==0) || (k==(nz-1))) w = w * 0.5;
01810         for (j=0; j<ny; j++) {
01811             w = 1.0;
01812             if ((j==0) || (j==(ny-1))) w = w * 0.5;
01813             for (i=0; i<nx; i++) {
01814                 w = 1.0;
01815                 if ((i==0) || (i==(nx-1))) w = w * 0.5;
01816                 sum = sum + w*(thee->data[IJK(i,j,k)]);
01817             }
01818         }
01819     }
01820
01821     sum = sum*(thee->hx)*(thee->hy)*(thee->hz);
01822
01823     return sum;

```

```

01824
01825 }
01826
01827
01828 VPUBLIC double Vgrid_normL1(Vgrid *thee) {
01829
01830     size_t i, j, k;
01831     int nx, ny, nz;
01832     double sum;
01833
01834     if (thee == VNULL) {
01835         Vnm_print(2, "Vgrid_normL1: Got VNULL thee!\n");
01836         VASSERT(0);
01837     }
01838
01839     nx = thee->nx;
01840     ny = thee->ny;
01841     nz = thee->nz;
01842
01843     sum = 0.0;
01844     for (k=0; k<nz; k++) {
01845         for (j=0; j<ny; j++) {
01846             for (i=0; i<nx; i++) {
01847                 sum = sum + VABS(thee->data[IJK(i,j,k)]);
01848             }
01849         }
01850     }
01851
01852     sum = sum*(thee->hx)*(thee->hy)*(thee->hz);
01853
01854     return sum;
01855 }
01856
01857
01858 VPUBLIC double Vgrid_normL2(Vgrid *thee) {
01859
01860     size_t i, j, k;
01861     int nx, ny, nz;
01862     double sum;
01863
01864     if (thee == VNULL) {
01865         Vnm_print(2, "Vgrid_normL2: Got VNULL thee!\n");
01866         VASSERT(0);
01867     }
01868
01869     nx = thee->nx;
01870     ny = thee->ny;
01871     nz = thee->nz;
01872
01873     sum = 0.0;
01874     for (k=0; k<nz; k++) {
01875         for (j=0; j<ny; j++) {
01876             for (i=0; i<nx; i++) {
01877                 sum = sum + VSQR(thee->data[IJK(i,j,k)]);
01878             }
01879         }
01880     }
01881
01882     sum = sum*(thee->hx)*(thee->hy)*(thee->hz);
01883
01884     return VSQRT(sum);
01885 }
01886
01887
01888 VPUBLIC double Vgrid_seminormH1(Vgrid *thee) {
01889
01890     size_t i, j, k;
01891     int nx, ny, nz, d;
01892     double pt[3], grad[3], sum, hx, hy, hzed, xmin, ymin, zmin;
01893
01894     if (thee == VNULL) {
01895         Vnm_print(2, "Vgrid_seminormH1: Got VNULL thee!\n");
01896         VASSERT(0);
01897     }
01898
01899     nx = thee->nx;
01900     ny = thee->ny;
01901     nz = thee->nz;
01902     hx = thee->hx;
01903     hy = thee->hy;
01904     hzed = thee->hz;

```

```

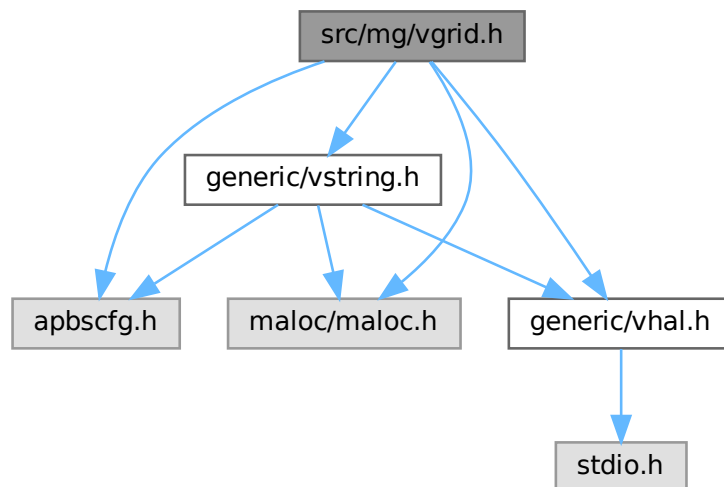
01905     xmin = thee->xmin;
01906     ymin = thee->ymin;
01907     zmin = thee->zmin;
01908
01909     sum = 0.0;
01910     for (k=0; k<nz; k++) {
01911         pt[2] = k*hzed + zmin;
01912         for (j=0; j<ny; j++) {
01913             pt[1] = j*hy + ymin;
01914             for (i=0; i<nx; i++) {
01915                 pt[0] = i*hx + xmin;
01916                 VASSERT(Vgrid_gradient(thee, pt, grad));
01917                 for (d=0; d<3; d++) sum = sum + VSQR(grad[d]);
01918             }
01919         }
01920     }
01921
01922     sum = sum*(hx)*(hy)*(hzed);
01923
01924     if (VABS(sum) < VSMALL) sum = 0.0;
01925     else sum = VSQRT(sum);
01926
01927     return sum;
01928 }
01929
01930
01931 VPUBLIC double Vgrid_normH1(Vgrid *thee) {
01932     double sum = 0.0;
01933
01934     if (thee == VNULL) {
01935         Vnm_print(2, "Vgrid_normH1: Got VNULL thee!\n");
01936         VASSERT(0);
01937     }
01938
01939     sum = VSQR(Vgrid_seminormH1(thee)) + VSQR(Vgrid_normL2(thee));
01940
01941     return VSQRT(sum);
01942 }
01943
01944
01945
01946 VPUBLIC double Vgrid_normLinf(Vgrid *thee) {
01947     size_t i, j, k;
01948     int nx, ny, nz, gotval;
01949     double sum, val;
01950
01951     if (thee == VNULL) {
01952         Vnm_print(2, "Vgrid_normLinf: Got VNULL thee!\n");
01953         VASSERT(0);
01954     }
01955
01956     nx = thee->nx;
01957     ny = thee->ny;
01958     nz = thee->nz;
01959
01960     sum = 0.0;
01961     gotval = 0;
01962     for (k=0; k<nz; k++) {
01963         for (j=0; j<ny; j++) {
01964             for (i=0; i<nx; i++) {
01965                 val = VABS(thee->data[IJK(i,j,k)]);
01966                 if (!gotval) {
01967                     gotval = 1;
01968                     sum = val;
01969                 }
01970                 if (val > sum) sum = val;
01971             }
01972         }
01973     }
01974
01975     return sum;
01976 }
01977
01978 }

```

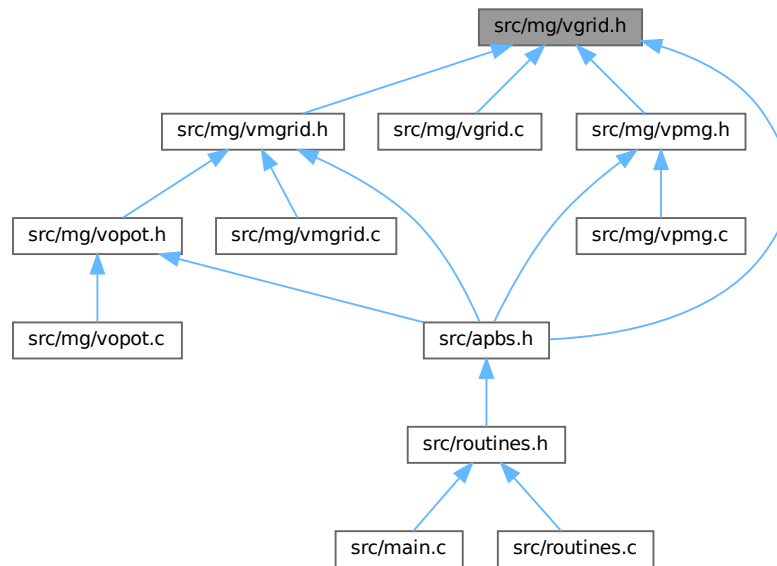
9.96 src/mg/vgrid.h File Reference

Potential oracle for Cartesian mesh data.

```
#include "apbscfg.h"  
#include "maloc/maloc.h"  
#include "generic/vhal.h"  
#include "generic/vstring.h"  
Include dependency graph for vgrid.h:
```



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVgrid](#)
Electrostatic potential oracle for Cartesian mesh data.

Macros

- #define [VGRID_DIGITS](#) 6
Number of decimal places for comparisons and formatting.

Typedefs

- typedef struct [sVgrid](#) [Vgrid](#)
Declaration of the Vgrid class as the sVgrid structure.

Functions

- VEXTERNC unsigned long int [Vgrid_memChk](#) ([Vgrid](#) *thee)
Return the memory used by this structure (and its contents) in bytes.
- VEXTERNC [Vgrid](#) * [Vgrid_ctor](#) (int nx, int ny, int nz, double hx, double hy, double hzed, double xmin, double ymin, double zmin, double *data)
Construct Vgrid object with values obtained from Vpmpg_readDX (for example)
- VEXTERNC int [Vgrid_ctor2](#) ([Vgrid](#) *thee, int nx, int ny, int nz, double hx, double hy, double hzed, double xmin, double ymin, double zmin, double *data)
Initialize Vgrid object with values obtained from Vpmpg_readDX (for example)
- VEXTERNC int [Vgrid_value](#) ([Vgrid](#) *thee, double x[3], double *value)

- Get potential value (from mesh or approximation) at a point.*

 - VEXTERNC void `Vgrid_dtor` (`Vgrid **thee`)

Object destructor.
- VEXTERNC void `Vgrid_dtor2` (`Vgrid *thee`)

FORTTRAN stub object destructor.
- VEXTERNC int `Vgrid_curvature` (`Vgrid *thee`, double `pt[3]`, int `cflag`, double `*curv`)

Get second derivative values at a point.
- VEXTERNC int `Vgrid_gradient` (`Vgrid *thee`, double `pt[3]`, double `grad[3]`)

Get first derivative values at a point.
- VEXTERNC int `Vgrid_readGZ` (`Vgrid *thee`, const char `*fname`)

Read in OpenDX data in GZIP format.
- VEXTERNC void `Vgrid_writeGZ` (`Vgrid *thee`, const char `*iodev`, const char `*iofmt`, const char `*thost`, const char `*fname`, char `*title`, double `*pvec`)

Write out OpenDX data in GZIP format.
- VEXTERNC void `Vgrid_writeUHBD` (`Vgrid *thee`, const char `*iodev`, const char `*iofmt`, const char `*thost`, const char `*fname`, char `*title`, double `*pvec`)

Write out the data in UHBD grid format.
- VEXTERNC void `Vgrid_writeDX` (`Vgrid *thee`, const char `*iodev`, const char `*iofmt`, const char `*thost`, const char `*fname`, char `*title`, double `*pvec`)

Write out the data in OpenDX grid format.
- VEXTERNC int `Vgrid_readDX` (`Vgrid *thee`, const char `*iodev`, const char `*iofmt`, const char `*thost`, const char `*fname`)

Read in data in OpenDX grid format.
- VEXTERNC void `Vgrid_writeDXBIN` (`Vgrid *thee`, const char `*iodev`, const char `*iofmt`, const char `*thost`, const char `*fname`, char `*title`, double `*pvec`)

Write out the binary data in OpenDX grid format.
- VEXTERNC int `Vgrid_readDXBIN` (`Vgrid *thee`, const char `*iodev`, const char `*iofmt`, const char `*thost`, const char `*fname`)

Read in binary data in OpenDX grid format.
- VEXTERNC double `Vgrid_integrate` (`Vgrid *thee`)

Get the integral of the data.
- VEXTERNC double `Vgrid_normL1` (`Vgrid *thee`)

Get the L_1 norm of the data. This returns the integral:
- VEXTERNC double `Vgrid_normL2` (`Vgrid *thee`)

Get the L_2 norm of the data. This returns the integral:
- VEXTERNC double `Vgrid_normLinf` (`Vgrid *thee`)

Get the L_∞ norm of the data. This returns the integral:
- VEXTERNC double `Vgrid_seminormH1` (`Vgrid *thee`)

Get the H_1 semi-norm of the data. This returns the integral:
- VEXTERNC double `Vgrid_normH1` (`Vgrid *thee`)

Get the H_1 norm (or energy norm) of the data. This returns the integral:

9.96.1 Detailed Description

Potential oracle for Cartesian mesh data.

Author

Nathan Baker and Steve Bond

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
*   Nathan A. Baker (nathan.baker@pnnl.gov)
*   Pacific Northwest National Laboratory
*
*   Additional contributing authors listed in the code documentation.
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*
*
```

Definition in file [vgrid.h](#).

9.96.2 Function Documentation

9.96.2.1 Vgrid_writeGZ()

```
VEXTERNC void Vgrid_writeGZ (
    Vgrid * thee,
    const char * iodev,
    const char * iofmt,
```

```

    const char * thost,
    const char * fname,
    char * title,
    double * pvec )

```

Write out OpenDX data in GZIP format.

Author

Dave Gohara

Parameters

<i>thee</i>	Object to hold new grid data
<i>iodev</i>	I/O device
<i>iofmt</i>	I/O format
<i>thost</i>	Remote host name
<i>fname</i>	File name
<i>title</i>	Data title
<i>pvec</i>	Masking vector (0 = not written)

Definition at line 1011 of file [vgrid.c](#).

9.97 vgrid.h

[Go to the documentation of this file.](#)

```

00001
00062 #ifndef _VGRID_H_
00063 #define _VGRID_H_
00064
00065 #include "apbscfg.h"
00066
00067 #include "malloc/malloc.h"
00068
00069 #include "generic/vhal.h"
00070 #include "generic/vstring.h"
00071
00074 #define VGRID_DIGITS 6
00075
00081 struct sVgrid {
00082
00083     int nx;
00084     int ny;
00085     int nz;
00086     double hx;
00087     double hy;
00088     double hzed;
00089     double xmin;
00090     double ymin;
00091     double zmin;
00092     double xmax;
00093     double ymax;
00094     double zmax;
00095     double *data;
00096     int readdata;
00097     int ctordata;
00099     Vmem *mem;
00100 };
00101
00106 typedef struct sVgrid Vgrid;
00107
00108 #if !defined(VINLINE_VGRID)
00109
00117     VEXTERNC unsigned long int Vgrid_memChk(Vgrid *thee);
00118
00119 #else /* if defined(VINLINE_VGRID) */
00120
00128 #define Vgrid_memChk(thee) (Vmem_bytes((thee)->vmem))

```

```

00129
00130 #endif /* if !defined(VINLINE_VPMG) */
00131
00149 VEXTERNC Vgrid* Vgrid_ctor(int nx, int ny, int nz,
00150                             double hx, double hy, double hzed,
00151                             double xmin, double ymin, double zmin,
00152                             double *data);
00153
00172 VEXTERNC int Vgrid_ctor2(Vgrid *thee, int nx, int ny, int nz,
00173                           double hx, double hy, double hzed,
00174                           double xmin, double ymin, double zmin,
00175                           double *data);
00176
00185 VEXTERNC int Vgrid_value(Vgrid *thee, double x[3], double *value);
00186
00192 VEXTERNC void Vgrid_dtor(Vgrid **thee);
00193
00199 VEXTERNC void Vgrid_dtor2(Vgrid *thee);
00200
00214 VEXTERNC int Vgrid_curvature(Vgrid *thee, double pt[3], int cflag,
00215                               double *curv);
00216
00225 VEXTERNC int Vgrid_gradient(Vgrid *thee, double pt[3], double grad[3] );
00226
00231 VEXTERNC int Vgrid_readGZ(
00232     Vgrid *thee,
00233     const char *fname
00234 );
00235
00239 VEXTERNC void Vgrid_writeGZ(
00240     Vgrid *thee,
00241     const char *iodev,
00242     const char *iofmt,
00243     const char *thost,
00244     const char *fname,
00245     char *title,
00246     double *pvec
00247 );
00248
00266 VEXTERNC void Vgrid_writeUHBD(Vgrid *thee, const char *iodev,
00267                                const char *iofmt, const char *thost, const char *fname, char *title,
00268                                double *pvec);
00269
00284 VEXTERNC void Vgrid_writeDX(Vgrid *thee, const char *iodev,
00285                                const char *iofmt, const char *thost, const char *fname, char *title,
00286                                double *pvec);
00287
00299 VEXTERNC int Vgrid_readDX(Vgrid *thee, const char *iodev, const char *iofmt,
00300                             const char *thost, const char *fname);
00301
00316 VEXTERNC void Vgrid_writeDXBIN(Vgrid *thee, const char *iodev,
00317                                const char *iofmt, const char *thost, const char *fname, char *title,
00318                                double *pvec);
00319
00320
00332 VEXTERNC int Vgrid_readDXBIN(Vgrid *thee, const char *iodev, const char *iofmt,
00333                                const char *thost, const char *fname);
00334
00341 VEXTERNC double Vgrid_integrate(Vgrid *thee);
00342
00351 VEXTERNC double Vgrid_normL1(Vgrid *thee);
00352
00361 VEXTERNC double Vgrid_normL2(Vgrid *thee);
00362
00371 VEXTERNC double Vgrid_normLinf(Vgrid *thee);
00372
00382 VEXTERNC double Vgrid_seminormH1(Vgrid *thee);
00383
00394 VEXTERNC double Vgrid_normH1(Vgrid *thee);
00395
00396 #endif

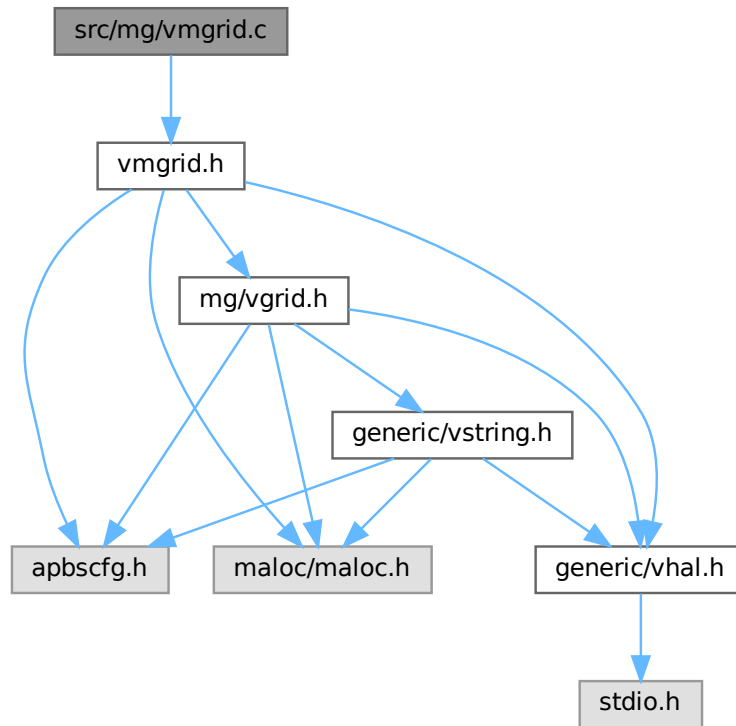
```

9.98 src/mg/vmgrid.c File Reference

Class Vmgrid methods.

```
#include "vmgrid.h"
```

Include dependency graph for vmgrid.c:



Functions

- `VPUBLIC Vmgrid * Vmgrid_ctor ()`
Construct Vmgrid object.
- `VPUBLIC int Vmgrid_ctor2 (Vmgrid *thee)`
Initialize Vmgrid object.
- `VPUBLIC void Vmgrid_dtor (Vmgrid **thee)`
Object destructor.
- `VPUBLIC void Vmgrid_dtor2 (Vmgrid *thee)`
FORTTRAN stub object destructor.
- `VPUBLIC int Vmgrid_value (Vmgrid *thee, double pt[3], double *value)`
Get potential value (from mesh or approximation) at a point.
- `VPUBLIC int Vmgrid_curvature (Vmgrid *thee, double pt[3], int cflag, double *value)`
Get second derivative values at a point.
- `VPUBLIC int Vmgrid_gradient (Vmgrid *thee, double pt[3], double grad[3])`
Get first derivative values at a point.
- `VPUBLIC int Vmgrid_addGrid (Vmgrid *thee, Vgrid *grid)`
Add a grid to the hierarchy.

9.98.1 Detailed Description

Class Vmgrid methods.

Author

Nathan Baker

Version

Id

[vmgrid.c](#) 1615 2010-10-20 19:16:35Z sobolevnm

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnl.gov)
* Pacific Northwest National Laboratory
*
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*
*
```

Definition in file [vmgrid.c](#).

9.99 vmgrid.c

[Go to the documentation of this file.](#)

```
00001
00049 #include "vmgrid.h"
```

```

00050
00051 VEMBED(rcsid="$Id: vmgrid.c 1615 2010-10-20 19:16:35Z sobolevnmr $")
00052
00053 /* ////////////////////////////////////////
00054 // Routine:  Vmgrid_ctor
00055 // Author:   Nathan Baker
00057 VPUBLIC Vmgrid* Vmgrid_ctor() {
00058
00059     Vmgrid *thee = VNULL;
00060
00061     thee = Vmem_malloc(VNULL, 1, sizeof(Vmgrid));
00062     VASSERT(thee != VNULL);
00063     VASSERT(Vmgrid_ctor2(thee));
00064
00065     return thee;
00066 }
00067
00068 /* ////////////////////////////////////////
00069 // Routine:  Vmgrid_ctor2
00070 // Author:   Nathan Baker
00072 VPUBLIC int Vmgrid_ctor2(Vmgrid *thee) {
00073
00074     int i;
00075
00076     if (thee == VNULL) return 0;
00077
00078     thee->ngrids = 0;
00079     for (i=0; i<VMGRIDMAX; i++) thee->grids[i] = VNULL;
00080
00081     return 1;
00082 }
00083
00084 /* ////////////////////////////////////////
00085 // Routine:  Vmgrid_dtor
00086 // Author:   Nathan Baker
00088 VPUBLIC void Vmgrid_dtor(Vmgrid **thee) {
00089
00090     if ((*thee) != VNULL) {
00091         Vmgrid_dtor2(*thee);
00092         Vmem_free(VNULL, 1, sizeof(Vmgrid), (void **)thee);
00093         (*thee) = VNULL;
00094     }
00095 }
00096
00097 /* ////////////////////////////////////////
00098 // Routine:  Vmgrid_dtor2
00099 // Author:   Nathan Baker
00101 VPUBLIC void Vmgrid_dtor2(Vmgrid *thee) { ; }
00102
00103 /* ////////////////////////////////////////
00104 // Routine:  Vmgrid_value
00105 // Author:   Nathan Baker
00107 VPUBLIC int Vmgrid_value(Vmgrid *thee, double pt[3], double *value) {
00108
00109     int i, rc;
00110     double tvalue;
00111
00112     VASSERT(thee != VNULL);
00113
00114     for (i=0; i<thee->ngrids; i++) {
00115         rc = Vgrid_value(thee->grids[i], pt, &tvalue);
00116         if (rc) {
00117             *value = tvalue;
00118             return 1;
00119         }
00120     }
00121
00122     Vnm_print(2, "Vmgrid_value: Point (%g, %g, %g) not found in \
00123 hierarchy!\n", pt[0], pt[1], pt[2]);
00124
00125     return 0;
00126 }
00127
00128 /* ////////////////////////////////////////
00129 // Routine:  Vmgrid_curvature
00130 //
00131 // Notes:  cflag=0 ==> Reduced Maximal Curvature
00132 //         cflag=1 ==> Mean Curvature (Laplace)
00133 //         cflag=2 ==> Gauss Curvature
00134 //         cflag=3 ==> True Maximal Curvature
00135 //

```

```

00136 // Authors:  Nathan Baker
00138 VPUBLIC int Vmgrid_curvature(Vmgrid *thee, double pt[3], int cflag,
00139     double *value) {
00140
00141     int i, rc;
00142     double tvalue;
00143
00144     VASSERT(thee != VNULL);
00145
00146     for (i=0; i<thee->ngrids; i++) {
00147         rc = Vgrid_curvature(thee->grids[i], pt, cflag, &tvalue);
00148         if (rc) {
00149             *value = tvalue;
00150             return 1;
00151         }
00152     }
00153
00154     Vnm_print(2, "Vmgrid_curvature:  Point (%g, %g, %g) not found in \
00155 hierarchy!\n", pt[0], pt[1], pt[2]);
00156
00157     return 0;
00158
00159 }
00160
00161 /* ////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////
00162 // Routine:  Vmgrid_gradient
00163 //
00164 // Authors:  Nathan Baker
00165 VPUBLIC int Vmgrid_gradient(Vmgrid *thee, double pt[3], double grad[3]) {
00166
00167     int i, j, rc;
00168     double tgrad[3];
00169
00170     VASSERT(thee != VNULL);
00171
00172     for (i=0; i<thee->ngrids; i++) {
00173         rc = Vgrid_gradient(thee->grids[i], pt, tgrad);
00174         if (rc) {
00175             for (j=0; j<3; j++) grad[j] = tgrad[j];
00176             return 1;
00177         }
00178     }
00179
00180     Vnm_print(2, "Vmgrid_gradient:  Point (%g, %g, %g) not found in \
00181 hierarchy!\n", pt[0], pt[1], pt[2]);
00182
00183     return 0;
00184
00185 }
00186
00187 // Routine:  Vmgrid_addGrid
00188 //
00189 // Authors:  Nathan Baker
00190 VPUBLIC int Vmgrid_addGrid(Vmgrid *thee, Vgrid *grid) {
00191
00192     int i, j, rc;
00193     double tgrad[3];
00194
00195     VASSERT(thee != VNULL);
00196
00197     if (grid == VNULL) {
00198         Vnm_print(2, "Vmgrid_addGrid:  Not adding VNULL grid!\n");
00199         return 0;
00200     }
00201
00202     if (thee->ngrids >= VMGRIDMAX) {
00203         Vnm_print(2, "Vmgrid_addGrid:  Too many grids in hierarchy (max = \
00204 %d)!\n", VMGRIDMAX);
00205         Vnm_print(2, "Vmgrid_addGrid:  Not adding grid!\n");
00206         return 0;
00207     }
00208
00209     thee->grids[thee->ngrids] = grid;
00210     (thee->ngrids)++;
00211
00212     return 1;
00213
00214 }
00215
00216 }

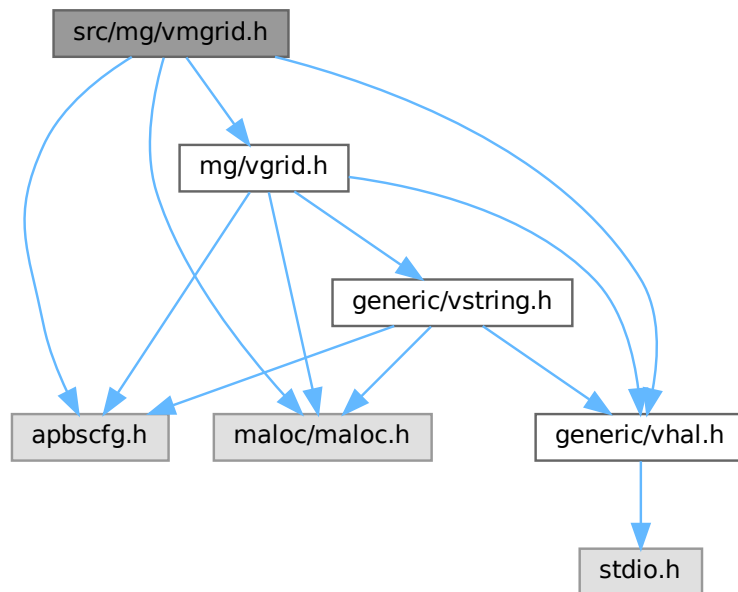
```

9.100 src/mg/vmgrid.h File Reference

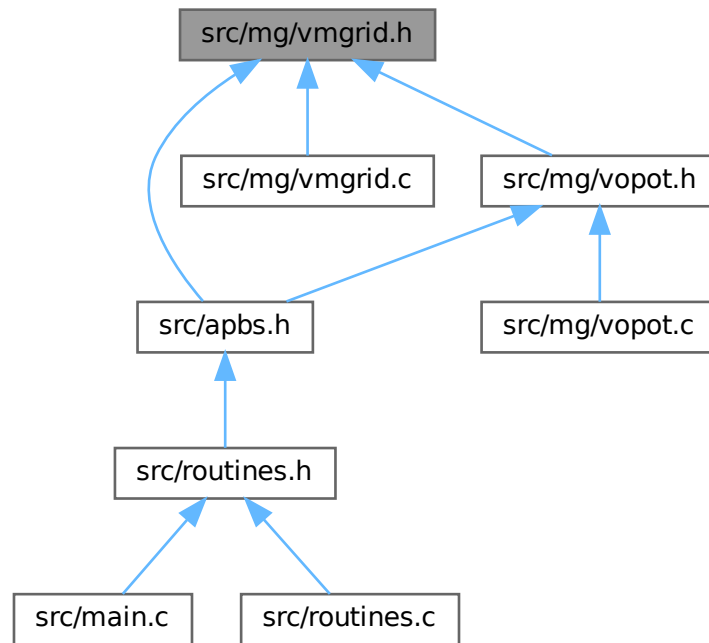
Multiresolution oracle for Cartesian mesh data.

```
#include "apbscfg.h"  
#include "maloc/maloc.h"  
#include "generic/vhal.h"  
#include "mg/vgrid.h"
```

Include dependency graph for vmgrid.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVmgrid](#)
Multiresolution oracle for Cartesian mesh data.

Macros

- #define [VMGRIDMAX](#) 20
The maximum number of levels in the grid hierarchy.

Typedefs

- typedef struct [sVmgrid](#) [Vmgrid](#)
Declaration of the Vmgrid class as the Vmgrid structure.

Functions

- VEXTERNC [Vmgrid](#) * [Vmgrid_ctor](#) ()
Construct Vmgrid object.
- VEXTERNC int [Vmgrid_ctor2](#) ([Vmgrid](#) *thee)
Initialize Vmgrid object.
- VEXTERNC int [Vmgrid_value](#) ([Vmgrid](#) *thee, double x[3], double *value)

- Get potential value (from mesh or approximation) at a point.*
- VEXTERNC void `Vmgrid_dtor` (`Vmgrid **thee`)
Object destructor.
- VEXTERNC void `Vmgrid_dtor2` (`Vmgrid *thee`)
FORTTRAN stub object destructor.
- VEXTERNC int `Vmgrid_addGrid` (`Vmgrid *thee`, `Vgrid *grid`)
Add a grid to the hierarchy.
- VEXTERNC int `Vmgrid_curvature` (`Vmgrid *thee`, double `pt[3]`, int `cflag`, double `*curv`)
Get second derivative values at a point.
- VEXTERNC int `Vmgrid_gradient` (`Vmgrid *thee`, double `pt[3]`, double `grad[3]`)
Get first derivative values at a point.
- VEXTERNC `Vgrid * Vmgrid_getGridByNum` (`Vmgrid *thee`, int `num`)
Get specific grid in hierarchy.
- VEXTERNC `Vgrid * Vmgrid_getGridByPoint` (`Vmgrid *thee`, double `pt[3]`)
Get grid in hierarchy which contains specified point or VNULL.

9.100.1 Detailed Description

Multiresolution oracle for Cartesian mesh data.

Author

Nathan Baker

Version

\$Id\$

Attention

```
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*
*

```

Definition in file [vmgrid.h](#).

9.101 vmgrid.h

[Go to the documentation of this file.](#)

```

00001
00062 #ifndef _VMGRID_H_
00063 #define _VMGRID_H_
00064
00065 #include "apbscfg.h"
00066
00067 #include "malloc/malloc.h"
00068
00069 #include "generic/vhal.h"
00070 #include "mg/vgrid.h"
00071
00076 #define VMGRIDMAX 20
00077
00078
00084 struct sVmgrid {
00085     int ngrids;
00087     Vgrid *grids[VMGRIDMAX];
00092 };
00093
00098 typedef struct sVmgrid Vmgrid;
00099
00105 VEXTERNC Vmgrid* Vmgrid_ctor();
00106
00113 VEXTERNC int Vmgrid_ctor2(Vmgrid *thee);
00114
00123 VEXTERNC int Vmgrid_value(Vmgrid *thee, double x[3], double *value);
00124
00130 VEXTERNC void Vmgrid_dtor(Vmgrid **thee);
00131
00137 VEXTERNC void Vmgrid_dtor2(Vmgrid *thee);
00138
00151 VEXTERNC int Vmgrid_addGrid(Vmgrid *thee, Vgrid *grid);
00152
00153
00167 VEXTERNC int Vmgrid_curvature(Vmgrid *thee, double pt[3], int cflag,
00168     double *curv);
00169
00178 VEXTERNC int Vmgrid_gradient(Vmgrid *thee, double pt[3], double grad[3] );
00179
00187 VEXTERNC Vgrid* Vmgrid_getGridByNum(Vmgrid *thee, int num);
00188
00196 VEXTERNC Vgrid* Vmgrid_getGridByPoint(Vmgrid *thee, double pt[3]);
00197
00198 #endif
00199

```

9.102 src/mg/vopot.c File Reference

Class Vopot methods.

Attention

```

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*
*

```

Definition in file [vopot.c](#).

9.102.2 Macro Definition Documentation**9.102.2.1 IJK**

```

#define IJK(
    i,
    j,
    k ) ((k)*(nx)*(ny)) + ((j)*(nx)) + (i)

```

Definition at line 113 of file [vopot.c](#).

9.103 vopot.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "vopot.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 /* ////////////////////////////////////// */
00062 // Routine: Vopot_ctor
00063 // Author: Nathan Baker
00065 VPUBLIC Vopot* Vopot_ctor(Vmgrid *mgrid, Vpbe *pbe, Vbcfl bcfl) {
00066
00067     Vopot *thee = VNULL;
00068
00069     thee = Vmem_malloc(VNULL, 1, sizeof(Vopot));
00070     VASSERT(thee != VNULL);
00071     VASSERT(Vopot_ctor2(thee, mgrid, pbe, bcfl));
00072
00073     return thee;
00074 }
00075
00076 /* ////////////////////////////////////// */
00077 // Routine: Vopot_ctor2
00078 // Author: Nathan Baker
00080 VPUBLIC int Vopot_ctor2(Vopot *thee, Vmgrid *mgrid, Vpbe *pbe, Vbcfl bcfl) {
00081
00082     if (thee == VNULL) return 0;
00083     thee->bcfl = bcfl;
00084     thee->mgrid = mgrid;
00085     thee->pbe = pbe;
00086
00087     return 1;
00088 }
00089
00090 /* ////////////////////////////////////// */
00091 // Routine: Vopot_dtor
00092 // Author: Nathan Baker
00094 VPUBLIC void Vopot_dtor(Vopot **thee) {
00095
00096     if ((*thee) != VNULL) {
00097         Vopot_dtor2(*thee);
00098         Vmem_free(VNULL, 1, sizeof(Vopot), (void **)thee);
00099         (*thee) = VNULL;
00100     }
00101 }
00102
00103 /* ////////////////////////////////////// */
00104 // Routine: Vopot_dtor2
00105 // Author: Nathan Baker
00107 VPUBLIC void Vopot_dtor2(Vopot *thee) { return; }
00108
00109 /* ////////////////////////////////////// */
00110 // Routine: Vopot_pot
00111 // Author: Nathan Baker
00113 #define IJK(i,j,k) ((k)*(nx)*(ny))+((j)*(nx))+((i))
00114 VPUBLIC int Vopot_pot(Vopot *thee, double pt[3], double *value) {
00115
00116     Vatom *atom;
00117     int i, iatom;
00118     double u, T, charge, eps_w, xkappa, dist, size, val, *position;
00119     Valist *alist;
00120
00121     VASSERT(thee != VNULL);
00122
00123     eps_w = Vpbe_getSolventDiel(thee->pbe);
00124     xkappa = (1.0e10)*Vpbe_getXkappa(thee->pbe);
00125     T = Vpbe_getTemperature(thee->pbe);
00126     alist = Vpbe_getValist(thee->pbe);
00127
00128     u = 0;
00129
00130     /* See if we're on the mesh */
00131     if (Vmgrid_value(thee->mgrid, pt, &u)) {
00132
00133         *value = u;
00134
00135     } else {
00136
00137         switch (thee->bcfl) {

```

```

00138
00139     case BCFL_ZERO:
00140         u = 0;
00141         break;
00142
00143     case BCFL_SDH:
00144         size = (1.0e-10)*Vpbe_getSoluteRadius(thee->pbe);
00145         position = Vpbe_getSoluteCenter(thee->pbe);
00146         charge = Vunit_ec*Vpbe_getSoluteCharge(thee->pbe);
00147         dist = 0;
00148         for (i=0; i<3; i++)
00149             dist += VSQR(position[i] - pt[i]);
00150         dist = (1.0e-10)*VSQRT(dist);
00151         val = (charge)/(4*VPI*Vunit_eps0*eps_w*dist);
00152         if (xkappa != 0.0)
00153             val = val*(exp(-xkappa*(dist-size))/(1+xkappa*size));
00154         val = val*Vunit_ec/(Vunit_kb*T);
00155         u = val;
00156         break;
00157
00158     case BCFL_MDH:
00159         u = 0;
00160         for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
00161             atom = Valist_getAtom(alist, iatom);
00162             position = Vatom_getPosition(atom);
00163             charge = Vunit_ec*Vatom_getCharge(atom);
00164             size = (1e-10)*Vatom_getRadius(atom);
00165             dist = 0;
00166             for (i=0; i<3; i++)
00167                 dist += VSQR(position[i] - pt[i]);
00168             dist = (1.0e-10)*VSQRT(dist);
00169             val = (charge)/(4*VPI*Vunit_eps0*eps_w*dist);
00170             if (xkappa != 0.0)
00171                 val = val*(exp(-xkappa*(dist-size))/(1+xkappa*size));
00172             val = val*Vunit_ec/(Vunit_kb*T);
00173             u = u + val;
00174         }
00175         break;
00176
00177     case BCFL_UNUSED:
00178         Vnm_print(2, "Vopot_pot: Invalid bcfl flag (%d)!\n",
00179             thee->bcfl);
00180         return 0;
00181
00182     case BCFL_FOCUS:
00183         Vnm_print(2, "Vopot_pot: Invalid bcfl flag (%d)!\n",
00184             thee->bcfl);
00185         return 0;
00186
00187     default:
00188         Vnm_print(2, "Vopot_pot: Bogus thee->bcfl flag (%d)!\n",
00189             thee->bcfl);
00190         return 0;
00191         break;
00192 }
00193
00194 *value = u;
00195
00196 }
00197
00198 return 1;
00199
00200 }
00201
00202 /* ////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////
00203 // Routine: Vopot_curvature
00204 //
00205 // Notes: cflag=0 ==> Reduced Maximal Curvature
00206 //        cflag=1 ==> Mean Curvature (Laplace)
00207 //        cflag=2 ==> Gauss Curvature
00208 //        cflag=3 ==> True Maximal Curvature
00209 // If we are off the grid, we can still evaluate the Laplacian; assuming, we
00210 // are away from the molecular surface, it is simply equal to the DH factor.
00211 //
00212 // Authors: Nathan Baker
00214 VPUBLIC int Vopot_curvature(Vopot *thee, double pt[3], int cflag,
00215     double *value) {
00216
00217     Vatom *atom;
00218     int i, iatom;
00219     double u, T, charge, eps_w, xkappa, dist, size, val, *position, zkappa2;

```

```

00220     Valist *alist;
00221
00222     VASSERT(thee != VNULL);
00223
00224     eps_w = Vpbe_getSolventDiel(thee->pbe);
00225     xkappa = (1.0e10)*Vpbe_getXkappa(thee->pbe);
00226     zkappa2 = Vpbe_getZkappa2(thee->pbe);
00227     T = Vpbe_getTemperature(thee->pbe);
00228     alist = Vpbe_getValist(thee->pbe);
00229
00230     u = 0;
00231
00232     if (Vmgrid_curvature(thee->mgrid, pt, cflag, value)) return 1;
00233     else if (cflag != 1) {
00234         Vnm_print(2, "Vopot_curvature: Off mesh!\n");
00235         return 1;
00236     } else {
00237
00238         switch (thee->bcfl) {
00239
00240             case BCFL_ZERO:
00241                 u = 0;
00242                 break;
00243
00244             case BCFL_SDH:
00245                 size = (1.0e-10)*Vpbe_getSoluteRadius(thee->pbe);
00246                 position = Vpbe_getSoluteCenter(thee->pbe);
00247                 charge = Vunit_ec*Vpbe_getSoluteCharge(thee->pbe);
00248                 dist = 0;
00249                 for (i=0; i<3; i++)
00250                     dist += VSQR(position[i] - pt[i]);
00251                 dist = (1.0e-10)*VSQRT(dist);
00252                 if (xkappa != 0.0)
00253                     u = zkappa2*(exp(-xkappa*(dist-size))/(1+xkappa*size));
00254                 break;
00255
00256             case BCFL_MDH:
00257                 u = 0;
00258                 for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
00259                     atom = Valist_getAtom(alist, iatom);
00260                     position = Vatom_getPosition(atom);
00261                     charge = Vunit_ec*Vatom_getCharge(atom);
00262                     size = (1e-10)*Vatom_getRadius(atom);
00263                     dist = 0;
00264                     for (i=0; i<3; i++)
00265                         dist += VSQR(position[i] - pt[i]);
00266                     dist = (1.0e-10)*VSQRT(dist);
00267                     if (xkappa != 0.0)
00268                         val = zkappa2*(exp(-xkappa*(dist-size))/(1+xkappa*size));
00269                     u = u + val;
00270                 }
00271                 break;
00272
00273             case BCFL_UNUSED:
00274                 Vnm_print(2, "Vopot_pot: Invlid bcfl (%d)!\n", thee->bcfl);
00275                 return 0;
00276
00277             case BCFL_FOCUS:
00278                 Vnm_print(2, "Vopot_pot: Invlid bcfl (%d)!\n", thee->bcfl);
00279                 return 0;
00280
00281             default:
00282                 Vnm_print(2, "Vopot_pot: Bogus thee->bcfl flag (%d)!\n",
00283                     thee->bcfl);
00284                 return 0;
00285                 break;
00286         }
00287
00288         *value = u;
00289     }
00290
00291     return 1;
00292 }
00293
00294
00295 /* ////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////
00296 // Routine: Vopot_gradient
00297 //
00298 // Authors: Nathan Baker
00300 VPUBLIC int Vopot_gradient(Vopot *thee, double pt[3], double grad[3]) {
00301

```



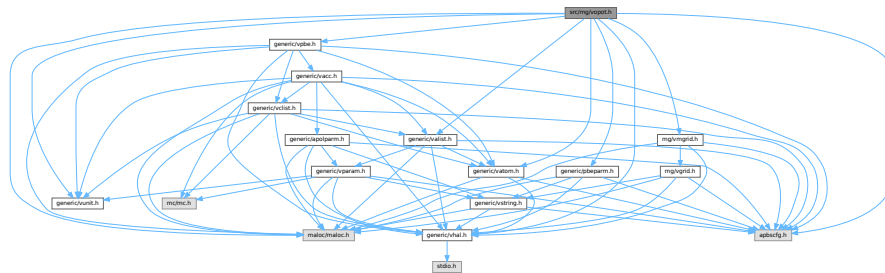
```

00302     Vatom *atom;
00303     int iatom;
00304     double T, charge, eps_w, xkappa, size, val, *position;
00305     double dx, dy, dz, dist;
00306     Valist *alist;
00307
00308     VASSERT(thee != VNULL);
00309
00310     eps_w = Vpbe_getSolventDiel(thee->pbe);
00311     xkappa = (1.0e10)*Vpbe_getXkappa(thee->pbe);
00312     T = Vpbe_getTemperature(thee->pbe);
00313     alist = Vpbe_getValist(thee->pbe);
00314
00315
00316     if (!Vmgrid_gradient(thee->mgrid, pt, grad)) {
00317
00318         switch (thee->bcfl) {
00319
00320             case BCFL_ZERO:
00321                 grad[0] = 0.0;
00322                 grad[1] = 0.0;
00323                 grad[2] = 0.0;
00324                 break;
00325
00326             case BCFL_SDH:
00327                 grad[0] = 0.0;
00328                 grad[1] = 0.0;
00329                 grad[2] = 0.0;
00330                 size = (1.0e-10)*Vpbe_getSoluteRadius(thee->pbe);
00331                 position = Vpbe_getSoluteCenter(thee->pbe);
00332                 charge = Vunit_ec*Vpbe_getSoluteCharge(thee->pbe);
00333                 dx = position[0] - pt[0];
00334                 dy = position[1] - pt[1];
00335                 dz = position[2] - pt[2];
00336                 dist = VSQR(dx) + VSQR(dy) + VSQR(dz);
00337                 dist = (1.0e-10)*VSQRT(dist);
00338                 val = (charge)/(4*VPI*Vunit_eps0*eps_w);
00339                 if (xkappa != 0.0)
00340                     val = val*(exp(-xkappa*(dist-size))/(1+xkappa*size));
00341                 val = val*Vunit_ec/(Vunit_kb*T);
00342                 grad[0] = val*dx/dist*(-1.0/dist/dist + xkappa/dist);
00343                 grad[1] = val*dy/dist*(-1.0/dist/dist + xkappa/dist);
00344                 grad[2] = val*dz/dist*(-1.0/dist/dist + xkappa/dist);
00345                 break;
00346
00347             case BCFL_MDH:
00348                 grad[0] = 0.0;
00349                 grad[1] = 0.0;
00350                 grad[2] = 0.0;
00351                 for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
00352                     atom = Valist_getAtom(alist, iatom);
00353                     position = Vatom_getPosition(atom);
00354                     charge = Vunit_ec*Vatom_getCharge(atom);
00355                     size = (1e-10)*Vatom_getRadius(atom);
00356                     dx = position[0] - pt[0];
00357                     dy = position[1] - pt[1];
00358                     dz = position[2] - pt[2];
00359                     dist = VSQR(dx) + VSQR(dy) + VSQR(dz);
00360                     dist = (1.0e-10)*VSQRT(dist);
00361                     val = (charge)/(4*VPI*Vunit_eps0*eps_w);
00362                     if (xkappa != 0.0)
00363                         val = val*(exp(-xkappa*(dist-size))/(1+xkappa*size));
00364                     val = val*Vunit_ec/(Vunit_kb*T);
00365                     grad[0] += (val*dx/dist*(-1.0/dist/dist + xkappa/dist));
00366                     grad[1] += (val*dy/dist*(-1.0/dist/dist + xkappa/dist));
00367                     grad[2] += (val*dz/dist*(-1.0/dist/dist + xkappa/dist));
00368                 }
00369                 break;
00370
00371             case BCFL_UNUSED:
00372                 Vnm_print(2, "Vopot: Invalid bcfl (%d)!\n", thee->bcfl);
00373                 return 0;
00374
00375             case BCFL_FOCUS:
00376                 Vnm_print(2, "Vopot: Invalid bcfl (%d)!\n", thee->bcfl);
00377                 return 0;
00378
00379             default:
00380                 Vnm_print(2, "Vopot_pot: Bogus thee->bcfl flag (%d)!\n",
00381                     thee->bcfl);
00382                 return 0;

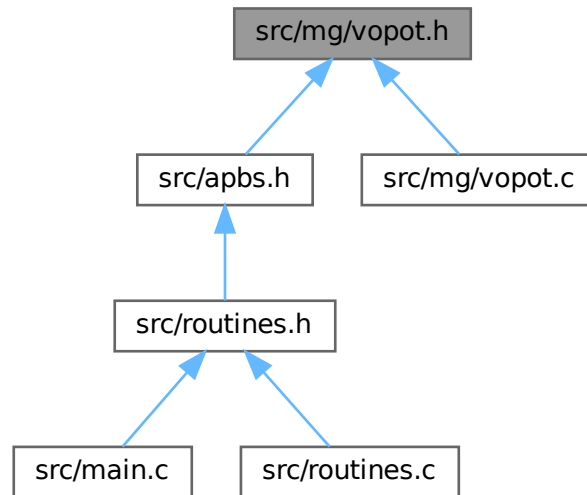
```

9.104 src/mg/vopot.h File Reference

Include dependency graph for vopot.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVopot](#)
Electrostatic potential oracle for Cartesian mesh data.

Typedefs

- typedef struct [sVopot](#) [Vopot](#)
Declaration of the Vopot class as the Vopot structure.

Functions

- VEXTERNC [Vopot](#) * [Vopot_ctor](#) ([Vmgrid](#) *mgrid, [Vpbe](#) *pbe, [Vbcfl](#) bcfl)
Construct Vopot object with values obtained from Vpmg_readDX (for example)
- VEXTERNC int [Vopot_ctor2](#) ([Vopot](#) *thee, [Vmgrid](#) *mgrid, [Vpbe](#) *pbe, [Vbcfl](#) bcfl)
Initialize Vopot object with values obtained from Vpmg_readDX (for example)
- VEXTERNC int [Vopot_pot](#) ([Vopot](#) *thee, double x[3], double *pot)
Get potential value (from mesh or approximation) at a point.
- VEXTERNC void [Vopot_dtor](#) ([Vopot](#) **thee)
Object destructor.
- VEXTERNC void [Vopot_dtor2](#) ([Vopot](#) *thee)
FORTTRAN stub object destructor.
- VEXTERNC int [Vopot_curvature](#) ([Vopot](#) *thee, double pt[3], int cflag, double *curv)
Get second derivative values at a point.
- VEXTERNC int [Vopot_gradient](#) ([Vopot](#) *thee, double pt[3], double grad[3])
Get first derivative values at a point.

9.104.1 Detailed Description

Potential oracle for Cartesian mesh data.

Author

Nathan Baker

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
*
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* THE POSSIBILITY OF SUCH DAMAGE.
*
*
```

Definition in file [vopot.h](#).

9.105 vopot.h

[Go to the documentation of this file.](#)

```

00001
00062 #ifndef _VOPOT_H_
00063 #define _VOPOT_H_
00064
00065 #include "apbscfg.h"
00066
00067 #include "malloc/malloc.h"
00068
00069 #include "generic/vhal.h"
00070 #include "generic/pbeparm.h"
00071 #include "generic/vatom.h"
00072 #include "generic/valist.h"
00073 #include "generic/vunit.h"
00074 #include "generic/vpbe.h"
00075 #include "generic/pbeparm.h"
00076 #include "mg/vmgrid.h"
00077
00083 struct sVopot {
00084     Vmgrid *mgrid;
00087     Vpbe *pbe;
00088     Vbcfl bcfl;
00090 };
00091
00096 typedef struct sVopot Vopot;
00097
00108 VEXTERNC Vopot* Vopot_ctor(Vmgrid *mgrid, Vpbe *pbe, Vbcfl bcfl);
00109
00121 VEXTERNC int Vopot_ctor2(Vopot *thee, Vmgrid *mgrid, Vpbe *pbe, Vbcfl bcfl);
00122
00131 VEXTERNC int Vopot_pot(Vopot *thee, double x[3], double *pot);
00132
00138 VEXTERNC void Vopot_dtor(Vopot **thee);
00139
00145 VEXTERNC void Vopot_dtor2(Vopot *thee);
00146
00160 VEXTERNC int Vopot_curvature(Vopot *thee, double pt[3], int cflag, double
00161 *curv);
00162
00171 VEXTERNC int Vopot_gradient(Vopot *thee, double pt[3], double grad[3] );
00172
00173
00174 #endif

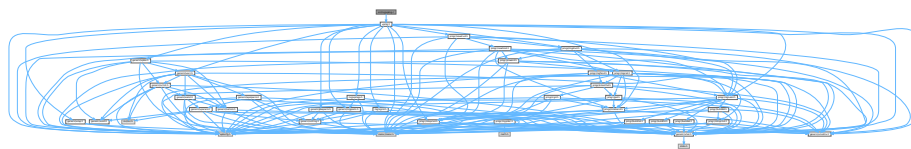
```

9.106 src/mg/vpmg.c File Reference

Class Vpmg methods.

#include "vpmg.h"

Include dependency graph for vpmg.c:



Functions

- VPUBLIC unsigned long int [Vpmg_memChk](#) ([Vpmg](#) *thee)
Return the memory used by this structure (and its contents) in bytes.
- VPUBLIC void [Vpmg_printColComp](#) ([Vpmg](#) *thee, char path[72], char title[72], char mxtype[3], int flag)
Print out a column-compressed sparse matrix in Harwell-Boeing format.
- VPUBLIC [Vpmg](#) * [Vpmg_ctor](#) ([Vpmgp](#) *pmg, [Vpbe](#) *pbe, int focusFlag, [Vpmg](#) *pmgOLD, [MGparm](#) *mgparm, [PBEparm_calcEnergy](#) energyFlag)
Constructor for the Vpmg class (allocates new memory)

- VPUBLIC int [Vpmg_ctor2](#) ([Vpmg](#) *thee, [Vpmgp](#) *pmgp, [Vpbe](#) *pbe, int focusFlag, [Vpmg](#) *pmgOLD, [MGparm](#) *mgparm, [PBEparm_calcEnergy](#) energyFlag)
FORTRAN stub constructor for the Vpmg class (uses previously-allocated memory)
- VPUBLIC int [Vpmg_solve](#) ([Vpmg](#) *thee)
Solve the PBE using PMG.
- VPUBLIC void [Vpmg_dtor](#) ([Vpmg](#) **thee)
Object destructor.
- VPUBLIC void [Vpmg_dtor2](#) ([Vpmg](#) *thee)
FORTRAN stub object destructor.
- VPUBLIC void [Vpmg_setPart](#) ([Vpmg](#) *thee, double lowerCorner[3], double upperCorner[3], int bflags[6])
Set partition information which restricts the calculation of observables to a (rectangular) subset of the problem domain.
- VPUBLIC void [Vpmg_unsetPart](#) ([Vpmg](#) *thee)
Remove partition restrictions.
- VPUBLIC int [Vpmg_fillArray](#) ([Vpmg](#) *thee, double *vec, [Vdata_Type](#) type, double parm, [Vhal_PBEType](#) pbetype, [PBEparm](#) *pbeparm)
Fill the specified array with accessibility values.
- VPRIVATE double [Vpmg_polarizEnergy](#) ([Vpmg](#) *thee, int extFlag)
Determines energy from polarizeable charge and interaction with fixed charges according to Rocchia et al.
- VPUBLIC double [Vpmg_energy](#) ([Vpmg](#) *thee, int extFlag)
Get the total electrostatic energy.
- VPUBLIC double [Vpmg_dielEnergy](#) ([Vpmg](#) *thee, int extFlag)
Get the "polarization" contribution to the electrostatic energy.
- VPUBLIC double [Vpmg_dielGradNorm](#) ([Vpmg](#) *thee)
Get the integral of the gradient of the dielectric function.
- VPUBLIC double [Vpmg_qmEnergy](#) ([Vpmg](#) *thee, int extFlag)
Get the "mobile charge" contribution to the electrostatic energy.
- VPRIVATE double [Vpmg_qmEnergyNONLIN](#) ([Vpmg](#) *thee, int extFlag)
- VPUBLIC double [Vpmg_qmEnergySMPBE](#) ([Vpmg](#) *thee, int extFlag)
Vpmg_qmEnergy for SMPBE.
- VPUBLIC double [Vpmg_qfEnergy](#) ([Vpmg](#) *thee, int extFlag)
Get the "fixed charge" contribution to the electrostatic energy.
- VPRIVATE double [Vpmg_qfEnergyPoint](#) ([Vpmg](#) *thee, int extFlag)
Calculates charge-potential energy using summation over delta function positions (i.e. something like an Linf norm)
- VPUBLIC double [Vpmg_qfAtomEnergy](#) ([Vpmg](#) *thee, [Vatom](#) *atom)
Get the per-atom "fixed charge" contribution to the electrostatic energy.
- VPRIVATE double [Vpmg_qfEnergyVolume](#) ([Vpmg](#) *thee, int extFlag)
Calculates charge-potential energy as integral over a volume.
- VPRIVATE void [Vpmg_splineSelect](#) (int srflm, [Vacc](#) *acc, double *gpos, double win, double infrad, [Vatom](#) *atom, double *force)
Selects a spline based surface method from either VSM_SPLINE, VSM_SPLINE5 or VSM_SPLINE7.
- VPRIVATE void [bcfl1](#) (double size, double *apos, double charge, double xkappa, double pre1, double *gxcf, double *gycf, double *gzcf, double *xf, double *yf, double *zf, int nx, int ny, int nz)
*Increment all boundary points by $pre1 * (charge/d) * (exp(-xkappa * (d-size)) / (1 + xkappa * size))$ to add the effect of the Debye-Huckel potential due to a single charge.*
- VPRIVATE void [bcCalcOrig](#) ([Vpmg](#) *thee)
- VPRIVATE int [gridPointsValid](#) (int i, int j, int k, int nx, int ny, int nz)
- VPRIVATE void [packAtoms](#) (double *ax, double *ay, double *az, double *charge, double *size, [Vpmg](#) *thee)

- VPRIVATE void [packUnpack](#) (int nx, int ny, int nz, int ngrid, double *gx, double *gy, double *gz, double *value, [Vpmg](#) *thee, int pack)
- VPRIVATE void [bcflnew](#) ([Vpmg](#) *thee)
- VPRIVATE void [multipolebc](#) (double r, double kappa, double eps_p, double eps_w, double rad, double tsr[3])
This routine serves bcfl2. It returns (in tsr) the contraction independent portion of the Debye-Huckel potential tensor for a spherical ion with a central charge, dipole and quadrupole. See the code for an in depth description.
- VPRIVATE void [bcfl_sdh](#) ([Vpmg](#) *thee)
- VPRIVATE void [bcfl_mdh](#) ([Vpmg](#) *thee)
- VPRIVATE void [bcfl_mem](#) (double zmem, double L, double eps_m, double eps_w, double V, double xkappa, double *gxcf, double *gycf, double *gzcf, double *xf, double *yf, double *zf, int nx, int ny, int nz)
- VPRIVATE void [bcfl_map](#) ([Vpmg](#) *thee)
- VPRIVATE void [bcCalc](#) ([Vpmg](#) *thee)
Fill boundary condition arrays.
- VPRIVATE void [fillcoCoefMap](#) ([Vpmg](#) *thee)
Fill operator coefficient arrays from pre-calculated maps.
- VPRIVATE void [fillcoCoefMol](#) ([Vpmg](#) *thee)
Fill operator coefficient arrays from a molecular surface calculation.
- VPRIVATE void [fillcoCoefMollon](#) ([Vpmg](#) *thee)
Fill ion (nonlinear) operator coefficient array from a molecular surface calculation.
- VPRIVATE void [fillcoCoefMolDiel](#) ([Vpmg](#) *thee)
Fill differential operator coefficient arrays from a molecular surface calculation.
- VPRIVATE void [fillcoCoefMolDielNoSmooth](#) ([Vpmg](#) *thee)
Fill differential operator coefficient arrays from a molecular surface calculation without smoothing.
- VPRIVATE void [fillcoCoefMolDielSmooth](#) ([Vpmg](#) *thee)
Fill differential operator coefficient arrays from a molecular surface calculation with smoothing.
- VPRIVATE void [fillcoCoefSpline](#) ([Vpmg](#) *thee)
Fill operator coefficient arrays from a spline-based surface calculation.
- VPRIVATE void [fillcoCoef](#) ([Vpmg](#) *thee)
Top-level driver to fill all operator coefficient arrays.
- VPRIVATE Vrc_Codes [fillcoCharge](#) ([Vpmg](#) *thee)
Top-level driver to fill source term charge array.
- VPRIVATE Vrc_Codes [fillcoChargeMap](#) ([Vpmg](#) *thee)
Fill source term charge array from a pre-calculated map.
- VPRIVATE void [fillcoChargeSpline1](#) ([Vpmg](#) *thee)
Fill source term charge array from linear interpolation.
- VPRIVATE double [bspline2](#) (double x)
Evaluate a cubic B-spline.
- VPRIVATE double [dbspline2](#) (double x)
Evaluate a cubic B-spline derivative.
- VPRIVATE void [fillcoChargeSpline2](#) ([Vpmg](#) *thee)
Fill source term charge array from cubic spline interpolation.
- VPUBLIC int [Vpmg_fillco](#) ([Vpmg](#) *thee, [Vsurf_Meth](#) surfMeth, double splineWin, [Vchrg_Meth](#) chargeMeth, int useDielXMap, [Vgrid](#) *dielXMap, int useDielYMap, [Vgrid](#) *dielYMap, int useDielZMap, [Vgrid](#) *dielZMap, int useKappaMap, [Vgrid](#) *kappaMap, int usePotMap, [Vgrid](#) *potMap, int useChargeMap, [Vgrid](#) *chargeMap)
Fill the coefficient arrays prior to solving the equation.
- VPUBLIC int [Vpmg_force](#) ([Vpmg](#) *thee, double *force, int atomID, [Vsurf_Meth](#) srfrm, [Vchrg_Meth](#) chgm)
Calculate the total force on the specified atom in units of $k_B T/AA$.
- VPUBLIC int [Vpmg_ibForce](#) ([Vpmg](#) *thee, double *force, int atomID, [Vsurf_Meth](#) srfrm)

- Calculate the osmotic pressure on the specified atom in units of $k_B T/AA$.*

 - VPUBLIC int [Vpmg_dbForce](#) ([Vpmg](#) *thee, double *dbForce, int atomID, [Vsurf_Meth](#) srfrm)
- Calculate the dielectric boundary forces on the specified atom in units of $k_B T/AA$.*

 - VPUBLIC int [Vpmg_qfForce](#) ([Vpmg](#) *thee, double *force, int atomID, [Vchrg_Meth](#) chgm)
- Calculate the "charge-field" force on the specified atom in units of $k_B T/AA$.*

 - VPRIVATE void [qfForceSpline1](#) ([Vpmg](#) *thee, double *force, int atomID)

Charge-field force due to a linear spline charge function.

 - VPRIVATE void [qfForceSpline2](#) ([Vpmg](#) *thee, double *force, int atomID)

Charge-field force due to a cubic spline charge function.

 - VPRIVATE void [qfForceSpline4](#) ([Vpmg](#) *thee, double *force, int atomID)

Charge-field force due to a quintic spline charge function.

 - VPRIVATE void [markFrac](#) (double rtot, double *tpos, int nx, int ny, int nz, double hx, double hy, double hzed, double xmin, double ymin, double zmin, double *xarray, double *yarray, double *zarray)
 - VPRIVATE void [markSphere](#) (double rtot, double *tpos, int nx, int ny, int nz, double hx, double hy, double hz, double xmin, double ymin, double zmin, double *array, double markVal)

Mark the grid points inside a sphere with a particular value. This marks by resetting the the grid points inside the sphere to the specified value.

 - VPRIVATE void [zlapSolve](#) ([Vpmg](#) *thee, double **solution, double **source, double **work1)

Calculate the solution to Poisson's equation with a simple Laplacian operator and zero-valued Dirichlet boundary conditions. Store the solution in thee->u.

 - VPUBLIC int [Vpmg_solveLaplace](#) ([Vpmg](#) *thee)

Solve Poisson's equation with a homogeneous Laplacian operator using the solvent dielectric constant. This solution is performed by a sine wave decomposition.

 - VPRIVATE double [VFCHI4](#) (int i, double f)

Return 2.5 plus difference of i - f.

 - VPRIVATE double [bspline4](#) (double x)

Evaluate a 5th Order B-Spline (4th order polynomial)

 - VPUBLIC double [dbspline4](#) (double x)

Evaluate a 5th Order B-Spline derivative (4th order polynomial)

 - VPUBLIC double [d2bspline4](#) (double x)

Evaluate the 2nd derivative of a 5th Order B-Spline.

 - VPUBLIC double [d3bspline4](#) (double x)

Evaluate the 3rd derivative of a 5th Order B-Spline.

 - VPUBLIC void [fillcoPermanentMultipole](#) ([Vpmg](#) *thee)

Fill source term charge array for the use of permanent multipoles.

 - VPRIVATE void [fillcoCoefSpline4](#) ([Vpmg](#) *thee)

Fill operator coefficient arrays from a 7th order polynomial based surface calculation.

 - VPUBLIC void [fillcoPermanentInduced](#) ([Vpmg](#) *thee)
 - VPRIVATE void [fillcoCoefSpline3](#) ([Vpmg](#) *thee)

Fill operator coefficient arrays from a 5th order polynomial based surface calculation.

 - VPRIVATE void [bcolcomp](#) (int *iparm, double *rparm, int *iwork, double *rwork, double *values, int *rowind, int *colptr, int *flag)

Build a column-compressed matrix in Harwell-Boeing format.

 - VPRIVATE void [bcolcomp2](#) (int *iparm, double *rparm, int *nx, int *ny, int *nz, int *iz, int *ipc, double *rpc, double *ac, double *cc, double *values, int *rowind, int *colptr, int *flag)

Build a column-compressed matrix in Harwell-Boeing format.

 - VPRIVATE void [bcolcomp3](#) (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac, double *cc, double *values, int *rowind, int *colptr, int *flag)

Build a column-compressed matrix in Harwell-Boeing format.

- VPRIVATE void `bcolcomp4` (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *oC, double *cc, double *oE, double *oN, double *uC, double *values, int *rowind, int *colptr, int *flag)

Build a column-compressed matrix in Harwell-Boeing format.

- VPRIVATE void `pcolcomp` (int *nrow, int *ncol, int *nnzero, double *values, int *rowind, int *colptr, char *path, char *title, char *mxtype)

Print a column-compressed matrix in Harwell-Boeing format.

9.106.1 Detailed Description

Class Vpmg methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
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```

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*
*

```

Definition in file [vpmg.c](#).

9.106.2 Function Documentation

9.106.2.1 bcCalc()

```

VPRIVATE void bcCalc (
    Vpmg * thee )

```

Fill boundary condition arrays.

Author

Nathan Baker

Definition at line [4382](#) of file [vpmg.c](#).

9.106.2.2 bcCalcOrig()

```

VPRIVATE void bcCalcOrig (
    Vpmg * thee )

```

Definition at line [2828](#) of file [vpmg.c](#).

9.106.2.3 bcfl1()

```

VPRIVATE void bcfl1 (
    double size,
    double * apos,
    double charge,
    double xkappa,
    double prel,
    double * gxcf,
    double * gycf,
    double * gzcf,
    double * xf,

```

```

double * yf,
double * zf,
int nx,
int ny,
int nz )

```

Increment all boundary points by $\text{pre1} * (\text{charge}/d) * (\exp(-x\kappa * (d - \text{size})) / (1 + x\kappa * \text{size}))$ to add the effect of the Debye-Huckel potential due to a single charge.

Author

Nathan Baker

Parameters

<i>apos</i>	Size of the ion
<i>charge</i>	Position of the ion
<i>xkappa</i>	Charge of the ion
<i>pre1</i>	Exponential screening factor
<i>gxcf</i>	Unit- and dielectric-dependent prefactor
<i>gycf</i>	Set to x-boundary values
<i>gzcf</i>	Set to y-boundary values
<i>xf</i>	Set to z-boundary values
<i>yf</i>	Boundary point x-coordinates
<i>zf</i>	Boundary point y-coordinates
<i>nx</i>	Boundary point z-coordinates
<i>ny</i>	Number of grid points in x-direction
<i>nz</i>	Number of grid points in y-direction Number of grid points in y-direction

Definition at line [2564](#) of file [vpmg.c](#).

9.106.2.4 bcfl_map()

```

VPRIVATE void bcfl_map (
    Vpmg * thee )

```

Definition at line [4174](#) of file [vpmg.c](#).

9.106.2.5 bcfl_mdh()

```

VPRIVATE void bcfl_mdh (
    Vpmg * thee )

```

Definition at line [3868](#) of file [vpmg.c](#).

9.106.2.6 bcfl_mem()

```

VPRIVATE void bcfl_mem (
    double zmem,
    double L,
    double eps_m,
    double eps_w,

```

```

double V,
double xkappa,
double * gxcf,
double * gycf,
double * gzcf,
double * xf,
double * yf,
double * zf,
int nx,
int ny,
int nz )

```

Definition at line 3995 of file [vpmg.c](#).

9.106.2.7 bcfl_sdh()

```

VPRIVATE void bcfl_sdh (
    Vpmg * thee )

```

Definition at line 3597 of file [vpmg.c](#).

9.106.2.8 bcflnew()

```

VPRIVATE void bcflnew (
    Vpmg * thee )

```

Definition at line 3407 of file [vpmg.c](#).

9.106.2.9 bspline2()

```

VPRIVATE double bspline2 (
    double x )

```

Evaluate a cubic B-spline.

Author

Nathan Baker

Returns

Cubic B-spline value

Parameters

<i>x</i>	Position
----------	----------

Definition at line 5496 of file [vpmg.c](#).

9.106.2.10 bspline4()

```

VPRIVATE double bspline4 (
    double x )

```

Evaluate a 5th Order B-Spline (4th order polynomial)

Author

: Michael Schnieders

Returns

5th Order B-Spline

Parameters

x	Position
-----	----------

Definition at line [7136](#) of file [vpmg.c](#).

9.106.2.11 d2bspline4()

```
VPUBLIC double d2bspline4 (  
    double  $x$  )
```

Evaluate the 2nd derivative of a 5th Order B-Spline.

Author

: Michael Schnieders

Returns

2nd derivative of a 5th Order B-Spline

Parameters

x	Position
-----	----------

Definition at line [7202](#) of file [vpmg.c](#).

9.106.2.12 d3bspline4()

```
VPUBLIC double d3bspline4 (  
    double  $x$  )
```

Evaluate the 3rd derivative of a 5th Order B-Spline.

Author

: Michael Schnieders

Returns

3rd derivative of a 5th Order B-Spline

Parameters

x	Position
-----	----------

Definition at line [7229](#) of file [vpmg.c](#).

9.106.2.13 db spline2()

```
VPRIVATE double db spline2 (  
    double x )
```

Evaluate a cubic B-spline derivative.

Author

Nathan Baker

Returns

Cubic B-spline derivative

Parameters

<i>x</i>	Position
----------	----------

Definition at line 5512 of file [vpmg.c](#).

9.106.2.14 db spline4()

```
VPUBLIC double db spline4 (  
    double x )
```

Evaluate a 5th Order B-Spline derivative (4th order polynomial)

Author

: Michael Schnieders

Returns

5th Order B-Spline derivative

Parameters

<i>x</i>	Position
----------	----------

Definition at line 7170 of file [vpmg.c](#).

9.106.2.15 fillcoCharge()

```
VPRIVATE Vrc_Codes fillcoCharge (  
    Vpmg * thee )
```

Top-level driver to fill source term charge array.

Returns

Success/failure status

Author

Nathan Baker

Definition at line 5287 of file [vpmg.c](#).

9.106.2.16 fillcoChargeMap()

```
VPRIVATE Vrc_Codes fillcoChargeMap (  
    Vpmg * thee )
```

Fill source term charge array from a pre-calculated map.

Returns

Success/failure status

Author

Nathan Baker

Definition at line 5343 of file [vpmg.c](#).

9.106.2.17 fillcoChargeSpline1()

```
VPRIVATE void fillcoChargeSpline1 (  
    Vpmg * thee )
```

Fill source term charge array from linear interpolation.

Author

Nathan Baker

Definition at line 5391 of file [vpmg.c](#).

9.106.2.18 fillcoChargeSpline2()

```
VPRIVATE void fillcoChargeSpline2 (  
    Vpmg * thee )
```

Fill source term charge array from cubic spline interpolation.

Author

Nathan Baker

Definition at line 5528 of file [vpmg.c](#).

9.106.2.19 fillcoCoef()

```
VPRIVATE void fillcoCoef (  
    Vpmg * thee )
```

Top-level driver to fill all operator coefficient arrays.

Author

Nathan Baker

Definition at line 5247 of file [vpmg.c](#).

9.106.2.20 fillcoCoefMap()

```
VPRIVATE void fillcoCoefMap (  
    Vpmg * thee )
```

Fill operator coefficient arrays from pre-calculated maps.

Author

Nathan Baker

Definition at line 4489 of file [vpmg.c](#).

9.106.2.21 fillcoCoefMol()

```
VPRIVATE void fillcoCoefMol (  
    Vpmg * thee )
```

Fill operator coefficient arrays from a molecular surface calculation.

Author

Nathan Baker

Definition at line 4612 of file [vpmg.c](#).

9.106.2.22 fillcoCoefMolDiel()

```
VPRIVATE void fillcoCoefMolDiel (  
    Vpmg * thee )
```

Fill differential operator coefficient arrays from a molecular surface calculation.

Author

Nathan Baker

Definition at line 4726 of file [vpmg.c](#).

9.106.2.23 fillcoCoefMolDielNoSmooth()

```
VPRIVATE void fillcoCoefMolDielNoSmooth (  
    Vpmg * thee )
```

Fill differential operator coefficient arrays from a molecular surface calculation without smoothing.

Author

Nathan Baker

Definition at line 4737 of file [vpmg.c](#).

9.106.2.24 fillcoCoefMolDielSmooth()

```
VPRIVATE void fillcoCoefMolDielSmooth (  
    Vpmg * thee )
```

Fill differential operator coefficient arrays from a molecular surface calculation with smoothing.

Molecular surface, dielectric smoothing following an implementation of Bruccoleri, et al. J Comput Chem 18 268-276 (1997).

This algorithm uses a 9 point harmonic smoothing technique - the point in question and all grid points 1/sqrt(2) grid spacings away.

Note

This uses thee->a1cf, thee->a2cf, thee->a3cf as temporary storage.

Author

Todd Dolinsky

Definition at line 4891 of file [vpmg.c](#).

9.106.2.25 fillcoCoefMolIon()

```
VPRIVATE void fillcoCoefMolIon (  
    Vpmg * thee )
```

Fill ion (nonlinear) operator coefficient array from a molecular surface calculation.

Author

Nathan Baker

Definition at line 4628 of file [vpmg.c](#).

9.106.2.26 fillcoCoefSpline()

```
VPRIVATE void fillcoCoefSpline (  
    Vpmg * thee )
```

Fill operator coefficient arrays from a spline-based surface calculation.

Author

Nathan Baker

Definition at line 5022 of file [vpmg.c](#).

9.106.2.27 fillcoCoefSpline3()

```
VPRIVATE void fillcoCoefSpline3 (  
    Vpmg * thee )
```

Fill operator coefficient arrays from a 5th order polynomial based surface calculation.

Author

Michael Schnieders

Definition at line 10430 of file [vpmg.c](#).

9.106.2.28 fillcoCoefSpline4()

```
VPRIVATE void fillcoCoefSpline4 (  
    Vpmg * thee )
```

Fill operator coefficient arrays from a 7th order polynomial based surface calculation.

Author

Michael Schnieders

Definition at line 9939 of file [vpmg.c](#).

9.106.2.29 fillcoPermanentInduced()

```
VPUBLIC void fillcoPermanentInduced (  
    Vpmg * thee )
```

Definition at line 10260 of file [vpmg.c](#).

9.106.2.30 fillcoPermanentMultipole()

```
VPUBLIC void fillcoPermanentMultipole (  
    Vpmg * thee )
```

Fill source term charge array for the use of permanent multipoles.

Author

Michael Schnieders

Definition at line 7240 of file [vpmg.c](#).

9.106.2.31 gridPointIsValid()

```
VPRIVATE int gridPointIsValid (  
    int i,  
    int j,  
    int k,  
    int nx,  
    int ny,  
    int nz )
```

Definition at line 3130 of file [vpmg.c](#).

9.106.2.32 markFrac()

```
VPRIVATE void markFrac (  
    double rtot,  
    double * tpos,  
    int nx,  
    int ny,  
    int nz,  
    double hx,  
    double hy,  
    double hzed,  
    double xmin,  
    double ymin,  
    double zmin,  
    double * xarray,  
    double * yarray,  
    double * zarray )
```

Definition at line 6684 of file [vpmg.c](#).

9.106.2.33 markSphere()

```
VPRIVATE void markSphere (  
    double rtot,
```

```
double * tpos,  
int nx,  
int ny,  
int nz,  
double hx,  
double hy,  
double hzed,  
double xmin,  
double ymin,  
double zmin,  
double * array,  
double markVal )
```

Mark the grid points inside a sphere with a particular value. This marks by resetting the the grid points inside the sphere to the specified value.

Author

Nathan Baker

Parameters

<i>tpos</i>	Sphere radius
<i>nx</i>	Sphere position
<i>ny</i>	Number of grid points
<i>nz</i>	Number of grid points
<i>hx</i>	Number of grid points
<i>hy</i>	Grid spacing
<i>hz</i>	Grid spacing
<i>xmin</i>	Grid spacing
<i>ymin</i>	Grid lower corner
<i>zmin</i>	Grid lower corner
<i>array</i>	Grid lower corner
<i>markVal</i>	Grid values Value to mark with

Definition at line [6849](#) of file [vpmg.c](#).

9.106.2.34 multipolebc()

```
VPRIVATE void multipolebc (  
double r,  
double kappa,  
double eps_p,  
double eps_w,  
double rad,  
double tsr[3] )
```

This routine serves bcf12. It returns (in tsr) the contraction independent portion of the Debye-Huckel potential tensor for a spherical ion with a central charge, dipole and quadrupole. See the code for an in depth description.

Author

Michael Schnieders

Parameters

<i>kappa</i>	Distance to the boundary
<i>eps</i> ↔ <i>_p</i>	Exponential screening factor
<i>eps</i> ↔ <i>_w</i>	Solute dielectric
<i>rad</i>	Solvent dielectric
<i>tsr</i>	Radius of the sphere Contraction-independent portion of each tensor

Definition at line 3487 of file [vpmg.c](#).

9.106.2.35 packAtoms()

```
VPRIVATE void packAtoms (
    double * ax,
    double * ay,
    double * az,
    double * charge,
    double * size,
    Vpmg * thee )
```

Definition at line 3313 of file [vpmg.c](#).

9.106.2.36 packUnpack()

```
VPRIVATE void packUnpack (
    int nx,
    int ny,
    int nz,
    int ngrid,
    double * gx,
    double * gy,
    double * gz,
    double * value,
    Vpmg * thee,
    int pack )
```

Definition at line 3338 of file [vpmg.c](#).

9.106.2.37 qfForceSpline1()

```
VPRIVATE void qfForceSpline1 (
    Vpmg * thee,
    double * force,
    int atomID )
```

Charge-field force due to a linear spline charge function.

Author

Nathan Baker

Parameters

<i>atomID</i>	Set to force Valist atom ID
---------------	-----------------------------

Definition at line 6311 of file [vpmg.c](#).

9.106.2.38 qfForceSpline2()

```
VPRIVATE void qfForceSpline2 (  
    Vpmg * thee,  
    double * force,  
    int atomID )
```

Charge-field force due to a cubic spline charge function.

Author

Nathan Baker

Parameters

<i>atomID</i>	Set to force Valist atom ID
---------------	-----------------------------

Definition at line 6448 of file [vpmg.c](#).

9.106.2.39 qfForceSpline4()

```
VPRIVATE void qfForceSpline4 (  
    Vpmg * thee,  
    double * force,  
    int atomID )
```

Charge-field force due to a quintic spline charge function.

Author

Michael Schnieders

Parameters

<i>atomID</i>	Set to force Valist atom ID
---------------	-----------------------------

Definition at line 6561 of file [vpmg.c](#).

9.106.2.40 VFCHI4()

```
VPRIVATE double VFCHI4 (  
    int i,  
    double f )
```

Return 2.5 plus difference of i - f.

Author

Michael Schnieders

Returns

$(2.5 + ((\text{double})(i) - (f)))$

Definition at line 7132 of file [vpmg.c](#).

9.106.2.41 Vpmg_polarizEnergy()

```
VPRIVATE double Vpmg_polarizEnergy (  
    Vpmg * thee,  
    int extFlag )
```

Determines energy from polarizeable charge and interaction with fixed charges according to Rocchia et al.

Author

Nathan Baker

Returns

Energy in kT

Parameters

<i>extFlag</i>	If 1, add external energy contributions to result
----------------	---

Definition at line 1148 of file [vpmg.c](#).

9.106.2.42 Vpmg_qfEnergyPoint()

```
VPRIVATE double Vpmg_qfEnergyPoint (  
    Vpmg * thee,  
    int extFlag )
```

Calculates charge-potential energy using summation over delta function positions (i.e. something like an Linf norm)

Author

Nathan Baker

Returns

Energy in kT

Parameters

<i>extFlag</i>	If 1, add external energy contributions to result
----------------	---

Definition at line 1704 of file [vpmg.c](#).

9.106.2.43 Vpmg_qfEnergyVolume()

```
VPRIVATE double Vpmg_qfEnergyVolume (
    Vpmg * thee,
    int extFlag )
```

Calculates charge-potential energy as integral over a volume.

Author

Nathan Baker

Returns

Energy in kT

Parameters

<i>extFlag</i>	If 1, add external energy contributions to result
----------------	---

Definition at line 1861 of file [vpmg.c](#).

9.106.2.44 Vpmg_qmEnergyNONLIN()

```
VPRIVATE double Vpmg_qmEnergyNONLIN (
    Vpmg * thee,
    int extFlag )
```

Definition at line 1401 of file [vpmg.c](#).

9.106.2.45 Vpmg_qmEnergySMPBE()

```
VPUBLIC double Vpmg_qmEnergySMPBE (
    Vpmg * thee,
    int extFlag )
```

Vpmg_qmEnergy for SMPBE.

Author

Vincent Chu

Definition at line 1490 of file [vpmg.c](#).

9.106.2.46 Vpmg_splineSelect()

```
VPRIVATE void Vpmg_splineSelect (
    int srfm,
    Vacc * acc,
    double * gpos,
    double win,
    double infrad,
    Vatom * atom,
    double * force )
```

Selects a spline based surface method from either VSM_SPLINE, VSM_SPLINE5 or VSM_SPLINE7.

Author

David Gohara

Parameters

<i>acc</i>	Surface method, currently VSM_SPLINE, VSM_SPLINE5, or VSM_SPLINE7
<i>gpos</i>	Accessibility object
<i>win</i>	Position array -> array[3]
<i>infrad</i>	Spline window
<i>atom</i>	Inflation radius
<i>force</i>	Atom object Force array -> array[3]

Definition at line 1893 of file [vpmg.c](#).**9.106.2.47 zlapSolve()**

```
VPRIVATE void zlapSolve (
    Vpmg * thee,
    double ** solution,
    double ** source,
    double ** work1 )
```

Calculate the solution to Poisson's equation with a simple Laplacian operator and zero-valued Dirichlet boundary conditions. Store the solution in thee->u.

Author

Nathan Baker

Note

Vpmg_fillco must be called first

Parameters

<i>source</i>	Solution term vector
<i>work1</i>	Source term vector Work vector

Definition at line 6898 of file [vpmg.c](#).**9.107 vpmg.c**

[Go to the documentation of this file.](#)

```
00001
00073 #include "vpmg.h"
00074
00075 VEMBED(rcsid="$Id$")
00076
00077 #if !defined(VINLINE_VPMG)
00078
00079 VPUBLIC unsigned long int Vpmg_memChk(Vpmg *thee) {
00080     if (thee == VNULL) return 0;
00081     return Vmem_bytes(thee->vmem);
00082 }
00083
00084 #endif /* if !defined(VINLINE_VPMG) */
```



```

00085
00086
00087 VPUBLIC void Vpmg_printColComp(Vpmg *thee, char path[72], char title[72],
00088     char mxtype[3], int flag) {
00089
00090     int nn, nxm2, nym2, nzm2, ncol, nrow, nonz;
00091     double *nzval;
00092     int *colptr, *rowind;
00093
00094     /* Calculate the total number of unknowns */
00095     nxm2 = thee->pmgp->nx - 2;
00096     nym2 = thee->pmgp->ny - 2;
00097     nzm2 = thee->pmgp->nz - 2;
00098     nn = nxm2*ny + nym2*nzm2;
00099     ncol = nn;
00100     nrow = nn;
00101
00102     /* Calculate the number of non-zero matrix entries:
00103     *   nn      nonzeros on diagonal
00104     *   nn-1    nonzeros on first off-diagonal
00105     *   nn-nx   nonzeros on second off-diagonal
00106     *   nn-nx*ny nonzeros on third off-diagonal
00107     *
00108     *   7*nn-2*nx*ny-2*nx-2 TOTAL non-zeros
00109     */
00110     nonz = 7*nn - 2*nxm2*ny + 2*nym2 - 2*nxm2 - 2;
00111     nzval = (double*)Vmem_malloc(thee->vmem, nonz, sizeof(double));
00112     rowind = (int*)Vmem_malloc(thee->vmem, nonz, sizeof(int));
00113     colptr = (int*)Vmem_malloc(thee->vmem, (ncol+1), sizeof(int));
00114
00115 #ifndef VAPBSQUIET
00116     Vnm_print(1, "Vpmg_printColComp: Allocated space for %d nonzeros\n",
00117         nonz);
00118 #endif
00119
00120     bcolcomp(thee->iparm, thee->rparm, thee->iwork, thee->rwork,
00121         nzval, rowind, colptr, &flag);
00122
00123
00124 #if 0
00125     for (i=0; i<nn; i++) {
00126         Vnm_print(1, "nnz(%d) = %g\n", i, nzval[i]);
00127     }
00128 #endif
00129
00130     /* I do not understand why I need to pass nzval in this way, but it
00131     * works... */
00132     pcolcomp(&nrow, &ncol, &nonz, &(nzval[0]), rowind, colptr, path, title,
00133         mxtype);
00134
00135     Vmem_free(thee->vmem, (ncol+1), sizeof(int), (void **)&colptr);
00136     Vmem_free(thee->vmem, nonz, sizeof(int), (void **)&rowind);
00137     Vmem_free(thee->vmem, nonz, sizeof(double), (void **)&nzval);
00138
00139 }
00140
00141 VPUBLIC Vpmg* Vpmg_ctor(Vpmgp *pmgp, Vpbe *pbe, int focusFlag,
00142     Vpmg *pmgOLD, MGparm *mgparm, PBEparm_calcEnergy energyFlag) {
00143
00144     Vpmg *thee = VNULL;
00145
00146     thee = (Vpmg*)Vmem_malloc(VNULL, 1, sizeof(Vpmg));
00147     VASSERT(thee != VNULL);
00148     VASSERT( Vpmg_ctor2(thee, pmgp, pbe, focusFlag, pmgOLD, mgparm,
00149         energyFlag) );
00150     return thee;
00151 }
00152
00153 VPUBLIC int Vpmg_ctor2(Vpmg *thee, Vpmgp *pmgp, Vpbe *pbe, int focusFlag,
00154     Vpmg *pmgOLD, MGparm *mgparm, PBEparm_calcEnergy energyFlag) {
00155
00156     int i, j, nion;
00157     double ionConc[MAXION], ionQ[MAXION], ionRadii[MAXION], zkappa2, zks2;
00158     double ionstr, partMin[3], partMax[3];
00159     size_t size;
00160
00161     /* Get the parameters */
00162     VASSERT(pmgp != VNULL);
00163     VASSERT(pbe != VNULL);
00164     thee->pmgp = pmgp;
00165     thee->pbe = pbe;

```

```

00166
00167 /* Set up the memory */
00168 thee->vmem = Vmem_ctor("APBS:VPMG");
00169
00170
00171
00173 /* Initialize ion concentrations and valencies in PMG routines */
00174 zkappa2 = Vpbe_getZkappa2(thee->pbe);
00175 ionstr = Vpbe_getBulkIonicStrength(thee->pbe);
00176 if (ionstr > 0.0) zks2 = 0.5/ionstr;
00177 else zks2 = 0.0;
00178 Vpbe_getIons(thee->pbe, &union, ionConc, ionRadii, ionQ);
00179
00180 /* TEMPORARY USEAQUA */
00181 /* Calculate storage requirements */
00182 if (mgparm->useAqua == 0) {
00183     Vpmgp_size(thee->pmgp);
00184 } else {
00185     VABORT_MSG0("Aqua is currently disabled");
00186 }
00187
00188 /* We need some additional storage if: nonlinear & newton OR cgm */
00189 /* SMPBE Added - nonlin = 2 added since it mimics NPBE */
00190 if ( ( ((thee->pmgp->nonlin == NONLIN_NPBE) || (thee->pmgp->nonlin == NONLIN_SMPBE))
00191      && (thee->pmgp->meth == VSOL_Newton) ) || (thee->pmgp->meth == VSOL_CGM) )
00192 {
00193     thee->pmgp->nrwk += (2*(thee->pmgp->nf));
00194 }
00195
00196
00197 if (thee->pmgp->iinfo > 1) {
00198     Vnm_print(2, "Vpmg_ctor2: PMG chose nx = %d, ny = %d, nz = %d\n",
00199               thee->pmgp->nx, thee->pmgp->ny, thee->pmgp->nz);
00200     Vnm_print(2, "Vpmg_ctor2: PMG chose nlev = %d\n",
00201               thee->pmgp->nlev);
00202     Vnm_print(2, "Vpmg_ctor2: PMG chose nxc = %d, nyc = %d, nzc = %d\n",
00203               thee->pmgp->nxc, thee->pmgp->nyc, thee->pmgp->nzc);
00204     Vnm_print(2, "Vpmg_ctor2: PMG chose nf = %d, nc = %d\n",
00205               thee->pmgp->nf, thee->pmgp->nc);
00206     Vnm_print(2, "Vpmg_ctor2: PMG chose narr = %d, narrc = %d\n",
00207               thee->pmgp->narr, thee->pmgp->narrc);
00208     Vnm_print(2, "Vpmg_ctor2: PMG chose n_rpc = %d, n_iz = %d, n_ipc = %d\n",
00209               thee->pmgp->n_rpc, thee->pmgp->n_iz, thee->pmgp->n_ipc);
00210     Vnm_print(2, "Vpmg_ctor2: PMG chose nrwk = %d, niwk = %d\n",
00211               thee->pmgp->nrwk, thee->pmgp->niwk);
00212 }
00213
00214
00215
00216 /* Allocate boundary storage */
00217 thee->gxcf = (double *)Vmem_malloc(
00218     thee->vmem,
00219     10*(thee->pmgp->ny)*(thee->pmgp->nz),
00220     sizeof(double)
00221 );
00222
00223 thee->gycf = (double *)Vmem_malloc(
00224     thee->vmem,
00225     10*(thee->pmgp->nx)*(thee->pmgp->nz),
00226     sizeof(double)
00227 );
00228
00229 thee->gzcf = (double *)Vmem_malloc(
00230     thee->vmem,
00231     10*(thee->pmgp->nx)*(thee->pmgp->ny),
00232     sizeof(double)
00233 );
00234
00235
00236
00237 /* Warn users if they are using BCFL_MAP that
00238 we do not include external energies */
00239 if (thee->pmgp->bcfl == BCFL_MAP)
00240     Vnm_print(2, "Vpmg_ctor2: \nWarning: External energies are not used in BCFL_MAP calculations!\n");
00241
00242 if (focusFlag) {
00243
00244     /* Overwrite any default or user-specified boundary condition
00245      * arguments; we are now committed to a calculation via focusing */
00246     if (thee->pmgp->bcfl != BCFL_FOCUS) {
00247         Vnm_print(2,

```

```

00248         "Vpmg_ctor2: reset boundary condition flag to BCFL_FOCUS!\n");
00249     thee->pmgp->bcfl = BCFL_FOCUS;
00250 }
00251
00252 /* Fill boundaries */
00253 Vnm_print(0, "Vpmg_ctor2: Filling boundary with old solution!\n");
00254 focusFillBound(thee, pmgOLD);
00255
00256 /* Calculate energetic contributions from region outside focusing
00257  * domain */
00258 if (energyFlag != PCE_NO) {
00259
00260     if (mgparm->type == MCT_PARALLEL) {
00261
00262         for (j=0; j<3; j++) {
00263             partMin[j] = mgparm->partDisjCenter[j]
00264                 - 0.5*mgparm->partDisjLength[j];
00265             partMax[j] = mgparm->partDisjCenter[j]
00266                 + 0.5*mgparm->partDisjLength[j];
00267         }
00268
00269     } else {
00270         for (j=0; j<3; j++) {
00271             partMin[j] = mgparm->center[j] - 0.5*mgparm->glen[j];
00272             partMax[j] = mgparm->center[j] + 0.5*mgparm->glen[j];
00273         }
00274
00275         extEnergy(thee, pmgOLD, energyFlag, partMin, partMax,
00276                 mgparm->partDisjOwnSide);
00277     }
00278
00279 } else {
00280
00281     /* Ignore external energy contributions */
00282     thee->extQmEnergy = 0;
00283     thee->extDiEnergy = 0;
00284     thee->extQfEnergy = 0;
00285 }
00286
00287 /* Allocate partition vector storage */
00288 size = (thee->pmgp->nx)*(thee->pmgp->ny)*(thee->pmgp->nz);
00289 thee->pvec = (double *)Vmem_malloc(
00290     thee->vmem,
00291     size,
00292     sizeof(double)
00293 );
00294
00295 /* Allocate remaining storage */
00296 thee->iparm = (int *)Vmem_malloc(thee->vmem, 100, sizeof(int));
00297 thee->rparm = (double *)Vmem_malloc(thee->vmem, 100, sizeof(double));
00298 thee->iwork = (int *)Vmem_malloc(thee->vmem, thee->pmgp->niwk, sizeof(int));
00299 thee->rwork = (double *)Vmem_malloc(thee->vmem, thee->pmgp->nrwk, sizeof(double));
00300 thee->charge = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00301 thee->kappa = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00302 thee->pot = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00303 thee->epsx = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00304 thee->epsy = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00305 thee->epsz = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00306 thee->alcf = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00307 thee->a2cf = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00308 thee->a3cf = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00309 thee->ccf = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00310 thee->fcf = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00311 thee->tcf = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00312 thee->u = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00313 thee->xf = (double *)Vmem_malloc(thee->vmem, 5*(thee->pmgp->nx), sizeof(double));
00314 thee->yf = (double *)Vmem_malloc(thee->vmem, 5*(thee->pmgp->ny), sizeof(double));
00315 thee->zf = (double *)Vmem_malloc(thee->vmem, 5*(thee->pmgp->nz), sizeof(double));
00316
00317
00318
00319 /* Packs parameters into the iparm and rparm arrays */
00320 Vpackmg(thee->iparm, thee->rparm, &(thee->pmgp->nrwk), &(thee->pmgp->niwk),
00321     &(thee->pmgp->nx), &(thee->pmgp->ny), &(thee->pmgp->nz),
00322     &(thee->pmgp->nlev), &(thee->pmgp->nu1), &(thee->pmgp->nu2),
00323     &(thee->pmgp->mgkey), &(thee->pmgp->itmax), &(thee->pmgp->istop),
00324     &(thee->pmgp->ipcon), &(thee->pmgp->nonlin), &(thee->pmgp->mgsmoo),
00325     &(thee->pmgp->mgprol), &(thee->pmgp->mgcoar), &(thee->pmgp->mgsovl),
00326     &(thee->pmgp->mgdisc), &(thee->pmgp->iinfo), &(thee->pmgp->errtol),
00327     &(thee->pmgp->ipkey), &(thee->pmgp->omegal), &(thee->pmgp->omegan),
00328     &(thee->pmgp->irite), &(thee->pmgp->iperf));

```

```

00329
00330
00331
00332     /* Currently for SMPBE type calculations we do not want to apply a scale
00333        factor to the ionConc */
00340     switch(pmgp->ipkey) {
00341
00342         case IPKEY_SMPBE:
00343
00344             Vmvpdefinitmpbe(&nion, ionQ, ionConc, &pbe->smvolume, &pbe->smsize);
00345
00346             break;
00347
00348
00349         case IPKEY_NPBE:
00350
00351             /* Else adjust the inoConc by scaling factor zks2 */
00352             for (i=0; i<nion; i++)
00353                 ionConc[i] = zks2 * ionConc[i];
00354
00355             Vmvpdefinitnpbe(&nion, ionQ, ionConc);
00356
00357             break;
00358
00359
00360         case IPKEY_LPBE:
00361
00362             /* Else adjust the inoConc by scaling factor zks2 */
00363             for (i=0; i<nion; i++)
00364                 ionConc[i] = zks2 * ionConc[i];
00365
00366             Vmvpdefinitlpbe(&nion, ionQ, ionConc);
00367
00368             break;
00369
00370
00371         default:
00372             Vnm_print(2, "PMG: Warning: PBE structure not initialized!\n");
00373             /* Else adjust the inoConc by scaling factor zks2 */
00374             for (i=0; i<nion; i++)
00375                 ionConc[i] = zks2 * ionConc[i];
00376
00377             break;
00378     }
00379
00380     /* Set the default chargeSrc for 5th order splines */
00381     thee->chargeSrc = mgparm->chgs;
00382
00383     /* Turn off restriction of observable calculations to a specific
00384        * partition */
00385     Vpmg_unsetPart(thee);
00386
00387     /* The coefficient arrays have not been filled */
00388     thee->filled = 0;
00389
00390     /*
00391     * TODO: Move the dtor out of here. The current ctor is done in routines.C,
00392     *       This was originally moved out to kill a memory leak. The dtor has
00393     *       has been removed from initMG and placed back here to keep memory
00394     *       usage low. killMG has been modified accordingly.
00395     */
00396     Vpmg_dtor(&pmgOLD);
00397
00398     return 1;
00399 }
00400
00401 VPUBLIC int Vpmg_solve(Vpmg *thee) {
00402
00403     int i,
00404         nx,
00405         ny,
00406         nz,
00407         n;
00408     double zkappa2;
00409
00410     nx = thee->pmgp->nx;
00411     ny = thee->pmgp->ny;
00412     nz = thee->pmgp->nz;
00413     n = nx*ny*nz;
00414
00415     if (!(thee->filled)) {

```

```

00416         Vnm_print(2, "Vpmg_solve: Need to call Vpmg_fillco()!\n");
00417         return 0;
00418     }
00419
00420     /* Fill the "true solution" array */
00421     for (i=0; i<n; i++) {
00422         thee->tcf[i] = 0.0;
00423     }
00424
00425     /* Fill the RHS array */
00426     for (i=0; i<n; i++) {
00427         thee->fcf[i] = thee->charge[i];
00428     }
00429
00430     /* Fill the operator coefficient array. */
00431     for (i=0; i<n; i++) {
00432         thee->a1cf[i] = thee->epsx[i];
00433         thee->a2cf[i] = thee->epsy[i];
00434         thee->a3cf[i] = thee->epsz[i];
00435     }
00436
00437     /* Fill the nonlinear coefficient array by multiplying the kappa
00438      * accessibility array (containing values between 0 and 1) by zkappa2. */
00439     zkappa2 = Vpbe_getZkappa2(thee->pbe);
00440     if (zkappa2 > VPMGSMALL) {
00441         for (i=0; i<n; i++) {
00442             thee->ccf[i] = zkappa2*thee->kappa[i];
00443         }
00444     } else {
00445         for (i=0; i<n; i++) {
00446             thee->ccf[i] = 0.0;
00447         }
00448     }
00449
00450     switch(thee->pmgp->meth) {
00451         /* CGMG (linear) */
00452         case VSOL_CGMG:
00453
00454             if (thee->pmgp->iinfo > 1)
00455                 Vnm_print(2, "Driving with CGMGDRIV\n");
00456
00457             VABORT_MSG0("CGMGDRIV is not currently supported");
00458             break;
00459
00460         /* Newton (nonlinear) */
00461         case VSOL_Newton:
00462
00463             if (thee->pmgp->iinfo > 1)
00464                 Vnm_print(2, "Driving with NEWDRIV\n");
00465
00466             Vnewdriv
00467                 (thee->iparm, thee->rparm, thee->iwork, thee->rwork,
00468                  thee->u, thee->xf, thee->yf, thee->zf, thee->gxcf, thee->gycf,
00469                  thee->gzcf, thee->a1cf, thee->a2cf, thee->a3cf, thee->ccf,
00470                  thee->fcf, thee->tcf);
00471             break;
00472
00473         /* MG (linear/nonlinear) */
00474         case VSOL_MG:
00475
00476             if (thee->pmgp->iinfo > 1)
00477                 Vnm_print(2, "Driving with MGDRIV\n");
00478
00479             Vmgdriv(thee->iparm, thee->rparm, thee->iwork, thee->rwork,
00480                    thee->u, thee->xf, thee->yf, thee->zf, thee->gxcf, thee->gycf,
00481                    thee->gzcf, thee->a1cf, thee->a2cf, thee->a3cf, thee->ccf,
00482                    thee->fcf, thee->tcf);
00483             break;
00484
00485         /* CGHS (linear/nonlinear) */
00486         case VSOL_CG:
00487
00488             if (thee->pmgp->iinfo > 1)
00489                 Vnm_print(2, "Driving with NCGHSDRIV\n");
00490
00491             VABORT_MSG0("NCGHSDRIV is not currently supported");
00492             break;
00493
00494         /* SOR (linear/nonlinear) */
00495         case VSOL_SOR:
00496

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```

00497         if (thee->pmgp->iinfo > 1)
00498             Vnm_print(2, "Driving with NSORDRIV\n");
00499
00500         VABORT_MSG0("NSORDRIV is not currently supported");
00501         break;
00502
00503     /* GSRB (linear/nonlinear) */
00504     case VSOL_RBGS:
00505
00506         if (thee->pmgp->iinfo > 1)
00507             Vnm_print(2, "Driving with NGSRBDRIV\n");
00508
00509         VABORT_MSG0("NGSRBDRIV is not currently supported");
00510         break;
00511
00512     /* WJAC (linear/nonlinear) */
00513     case VSOL_WJ:
00514
00515         if (thee->pmgp->iinfo > 1)
00516             Vnm_print(2, "Driving with NWJACDRIV\n");
00517
00518         VABORT_MSG0("NWJACDRIV is not currently supported");
00519         break;
00520
00521     /* RICH (linear/nonlinear) */
00522     case VSOL_Richardson:
00523
00524         if (thee->pmgp->iinfo > 1)
00525             Vnm_print(2, "Driving with NRICHDRIV\n");
00526
00527         VABORT_MSG0("NRICHDRIV is not currently supported");
00528         break;
00529
00530     /* CGMG (linear) TEMPORARY USEAQUA */
00531     case VSOL_CGMGAqua:
00532
00533         if (thee->pmgp->iinfo > 1)
00534             Vnm_print(2, "Driving with CGMGDRIVAQUA\n");
00535
00536         VABORT_MSG0("CGMGDRIVAQUA is not currently supported");
00537         break;
00538
00539     /* Newton (nonlinear) TEMPORARY USEAQUA */
00540     case VSOL_NewtonAqua:
00541
00542         if (thee->pmgp->iinfo > 1)
00543             Vnm_print(2, "Driving with NEWDRIVAQUA\n");
00544
00545         VABORT_MSG0("NEWDRIVAQUA is not currently supported");
00546         break;
00547
00548     /* Error handling */
00549     default:
00550         Vnm_print(2, "Vpmg_solve: invalid solver method key (%d)\n",
00551             thee->pmgp->key);
00552         return 0;
00553         break;
00554 }
00555
00556 return 1;
00557
00558 }
00559
00560
00561 VPUBLIC void Vpmg_dtor(Vpmg **thee) {
00562
00563     if ((*thee) != VNULL) {
00564         Vpmg_dtor2(*thee);
00565         Vmem_free(VNULL, 1, sizeof(Vpmg), (void **)thee);
00566         (*thee) = VNULL;
00567     }
00568
00569 }
00570
00571 VPUBLIC void Vpmg_dtor2(Vpmg *thee) {
00572
00573     /* Clean up the storage */
00574
00575     Vmem_free(thee->vmem, 100, sizeof(int),
00576         (void *)&(thee->iparm));
00577     Vmem_free(thee->vmem, 100, sizeof(double),

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00578     (void *)&(thee->rparm));
00579     Vmem_free(thee->vmem, thee->pmgp->niwk, sizeof(int),
00580     (void *)&(thee->iwork));
00581     Vmem_free(thee->vmem, thee->pmgp->nrvk, sizeof(double),
00582     (void *)&(thee->rwork));
00583     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00584     (void *)&(thee->charge));
00585     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00586     (void *)&(thee->kappa));
00587     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00588     (void *)&(thee->pot));
00589     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00590     (void *)&(thee->epsx));
00591     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00592     (void *)&(thee->epsy));
00593     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00594     (void *)&(thee->epsz));
00595     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00596     (void *)&(thee->alcf));
00597     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00598     (void *)&(thee->a2cf));
00599     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00600     (void *)&(thee->a3cf));
00601     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00602     (void *)&(thee->ccf));
00603     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00604     (void *)&(thee->fcf));
00605     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00606     (void *)&(thee->tcf));
00607     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00608     (void *)&(thee->u));
00609     Vmem_free(thee->vmem, 5*(thee->pmgp->nx), sizeof(double),
00610     (void *)&(thee->xf));
00611     Vmem_free(thee->vmem, 5*(thee->pmgp->ny), sizeof(double),
00612     (void *)&(thee->yf));
00613     Vmem_free(thee->vmem, 5*(thee->pmgp->nz), sizeof(double),
00614     (void *)&(thee->zf));
00615     Vmem_free(thee->vmem, 10*(thee->pmgp->ny)*(thee->pmgp->nz), sizeof(double),
00616     (void *)&(thee->gxcf));
00617     Vmem_free(thee->vmem, 10*(thee->pmgp->nx)*(thee->pmgp->nz), sizeof(double),
00618     (void *)&(thee->gycf));
00619     Vmem_free(thee->vmem, 10*(thee->pmgp->nx)*(thee->pmgp->ny), sizeof(double),
00620     (void *)&(thee->gzcf));
00621     Vmem_free(thee->vmem, (thee->pmgp->nx)*(thee->pmgp->ny)*(thee->pmgp->nz),
00622     sizeof(double), (void *)&(thee->pvec));
00623
00624     Vmem_dtor(&(thee->vmem));
00625 }
00626
00627 VPUBLIC void Vpmg_setPart(Vpmg *thee, double lowerCorner[3],
00628     double upperCorner[3], int bflags[6]) {
00629
00630     Valist *alist;
00631     Vatom *atom;
00632     int i, j, k, nx, ny, nz;
00633     double xmin, ymin, zmin, x, y, z, hx, hy, hzed, xok, yok, zok;
00634     double x0,x1,y0,y1,z0,z1;
00635
00636     nx = thee->pmgp->nx;
00637     ny = thee->pmgp->ny;
00638     nz = thee->pmgp->nz;
00639     hx = thee->pmgp->hx;
00640     hy = thee->pmgp->hy;
00641     hzed = thee->pmgp->hzed;
00642     xmin = thee->pmgp->xcent - 0.5*hx*(nx-1);
00643     ymin = thee->pmgp->ycent - 0.5*hy*(ny-1);
00644     zmin = thee->pmgp->zcent - 0.5*hzed*(nz-1);
00645
00646     xok = 0;
00647     yok = 0;
00648     zok = 0;
00649
00650     /* We need have called Vpmg_fillco first */
00651
00652     alist = thee->pbe->alist;
00653
00654     Vnm_print(0, "Vpmg_setPart: lower corner = (%g, %g, %g)\n",
00655     lowerCorner[0], lowerCorner[1], lowerCorner[2]);
00656     Vnm_print(0, "Vpmg_setPart: upper corner = (%g, %g, %g)\n",
00657     upperCorner[0], upperCorner[1], upperCorner[2]);
00658     Vnm_print(0, "Vpmg_setPart: actual minima = (%g, %g, %g)\n",

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00659     xmin, ymin, zmin);
00660     Vnm_print(0, "Vpmg_setPart: actual maxima = (%g, %g, %g)\n",
00661     xmin+hx*(nx-1), ymin+hy*(ny-1), zmin+hzed*(nz-1));
00662     Vnm_print(0, "Vpmg_setPart: bflag[FRONT] = %d\n",
00663     bflags[VAPBS_FRONT]);
00664     Vnm_print(0, "Vpmg_setPart: bflag[BACK] = %d\n",
00665     bflags[VAPBS_BACK]);
00666     Vnm_print(0, "Vpmg_setPart: bflag[LEFT] = %d\n",
00667     bflags[VAPBS_LEFT]);
00668     Vnm_print(0, "Vpmg_setPart: bflag[RIGHT] = %d\n",
00669     bflags[VAPBS_RIGHT]);
00670     Vnm_print(0, "Vpmg_setPart: bflag[UP] = %d\n",
00671     bflags[VAPBS_UP]);
00672     Vnm_print(0, "Vpmg_setPart: bflag[DOWN] = %d\n",
00673     bflags[VAPBS_DOWN]);
00674
00675     /* Identify atoms as inside, outside, or on the border
00676     If on the border, use the bflags to determine if there
00677     is an adjacent processor - if so, this atom should be equally
00678     shared. */
00679
00680     for (i=0; i<Valist_getNumberAtoms(alist); i++) {
00681         atom = Valist_getAtom(alist, i);
00682
00683         if ((atom->position[0] < upperCorner[0]) &&
00684             (atom->position[0] > lowerCorner[0])) xok = 1;
00685         else {
00686             if ((VABS(atom->position[0] - lowerCorner[0]) < VPMGSMALL) &&
00687                 (bflags[VAPBS_LEFT] == 0)) xok = 1;
00688             else if ((VABS(atom->position[0] - lowerCorner[0]) < VPMGSMALL) &&
00689                 (bflags[VAPBS_LEFT] == 1)) xok = 0.5;
00690             else if ((VABS(atom->position[0] - upperCorner[0]) < VPMGSMALL) &&
00691                 (bflags[VAPBS_RIGHT] == 0)) xok = 1;
00692             else if ((VABS(atom->position[0] - upperCorner[0]) < VPMGSMALL) &&
00693                 (bflags[VAPBS_RIGHT] == 1)) xok = 0.5;
00694             else xok = 0;
00695         }
00696         if ((atom->position[1] < upperCorner[1]) &&
00697             (atom->position[1] > lowerCorner[1])) yok = 1;
00698         else {
00699             if ((VABS(atom->position[1] - lowerCorner[1]) < VPMGSMALL) &&
00700                 (bflags[VAPBS_BACK] == 0)) yok = 1;
00701             else if ((VABS(atom->position[1] - lowerCorner[1]) < VPMGSMALL) &&
00702                 (bflags[VAPBS_BACK] == 1)) yok = 0.5;
00703             else if ((VABS(atom->position[1] - upperCorner[1]) < VPMGSMALL) &&
00704                 (bflags[VAPBS_FRONT] == 0)) yok = 1;
00705             else if ((VABS(atom->position[1] - upperCorner[1]) < VPMGSMALL) &&
00706                 (bflags[VAPBS_FRONT] == 1)) yok = 0.5;
00707             else yok = 0;
00708         }
00709         if ((atom->position[2] < upperCorner[2]) &&
00710             (atom->position[2] > lowerCorner[2])) zok = 1;
00711         else {
00712             if ((VABS(atom->position[2] - lowerCorner[2]) < VPMGSMALL) &&
00713                 (bflags[VAPBS_DOWN] == 0)) zok = 1;
00714             else if ((VABS(atom->position[2] - lowerCorner[2]) < VPMGSMALL) &&
00715                 (bflags[VAPBS_DOWN] == 1)) zok = 0.5;
00716             else if ((VABS(atom->position[2] - upperCorner[2]) < VPMGSMALL) &&
00717                 (bflags[VAPBS_UP] == 0)) zok = 1;
00718             else if ((VABS(atom->position[2] - upperCorner[2]) < VPMGSMALL) &&
00719                 (bflags[VAPBS_UP] == 1)) zok = 0.5;
00720             else zok = 0;
00721         }
00722
00723         atom->partID = xok*yok*zok;
00724         /*
00725         Vnm_print(1, "DEBUG (%s, %d): atom->position[0] - upperCorner[0] = %g\n",
00726         __FILE__, __LINE__, atom->position[0] - upperCorner[0]);
00727         Vnm_print(1, "DEBUG (%s, %d): atom->position[0] - lowerCorner[0] = %g\n",
00728         __FILE__, __LINE__, atom->position[0] - lowerCorner[0]);
00729         Vnm_print(1, "DEBUG (%s, %d): atom->position[1] - upperCorner[1] = %g\n",
00730         __FILE__, __LINE__, atom->position[1] - upperCorner[1]);
00731         Vnm_print(1, "DEBUG (%s, %d): atom->position[1] - lowerCorner[1] = %g\n",
00732         __FILE__, __LINE__, atom->position[1] - lowerCorner[1]);
00733         Vnm_print(1, "DEBUG (%s, %d): atom->position[2] - upperCorner[2] = %g\n",
00734         __FILE__, __LINE__, atom->position[2] - upperCorner[2]);
00735         Vnm_print(1, "DEBUG (%s, %d): atom->position[2] - lowerCorner[0] = %g\n",
00736         __FILE__, __LINE__, atom->position[2] - lowerCorner[2]);
00737         Vnm_print(1, "DEBUG (%s, %d): xok = %g, yok = %g, zok = %g\n",
00738         __FILE__, __LINE__, xok, yok, zok);
00739     }
00740     */

```



```

00740
00741     }
00742
00743     /* Load up pvec -
00744     For all points within h{axis}/2 of a border - use a gradient
00745     to determine the pvec weight.
00746     Points on the boundary depend on the presence of an adjacent
00747     processor. */
00748
00749     for (i=0; i<(nx*ny*nz); i++) three->pvec[i] = 0.0;
00750
00751     for (i=0; i<nx; i++) {
00752         xok = 0.0;
00753         x = i*hx + xmin;
00754         if ( (x < (upperCorner[0]-hx/2)) &&
00755              (x > (lowerCorner[0]+hx/2))
00756             ) xok = 1.0;
00757         else if ( (VABS(x - lowerCorner[0]) < VPMGSMALL) &&
00758                  (bflags[VAPBS_LEFT] == 0) ) xok = 1.0;
00759         else if ( (VABS(x - lowerCorner[0]) < VPMGSMALL) &&
00760                  (bflags[VAPBS_LEFT] == 1) ) xok = 0.5;
00761         else if ( (VABS(x - upperCorner[0]) < VPMGSMALL) &&
00762                  (bflags[VAPBS_RIGHT] == 0) ) xok = 1.0;
00763         else if ( (VABS(x - upperCorner[0]) < VPMGSMALL) &&
00764                  (bflags[VAPBS_RIGHT] == 1) ) xok = 0.5;
00765         else if ((x > (upperCorner[0] + hx/2)) || (x < (lowerCorner[0] - hx/2))) xok = 0.0;
00766         else if ((x < (upperCorner[0] + hx/2)) || (x > (lowerCorner[0] - hx/2))) {
00767             x0 = VMAX2(x - hx/2, lowerCorner[0]);
00768             x1 = VMIN2(x + hx/2, upperCorner[0]);
00769             xok = VABS(x1-x0)/hx;
00770
00771             if (xok < 0.0) {
00772                 if (VABS(xok) < VPMGSMALL) xok = 0.0;
00773                 else {
00774                     Vnm_print(2, "Vpmg_setPart: fell off x-interval (%1.12E)!\n",
00775                               xok);
00776                     VASSERT(0);
00777                 }
00778             }
00779             if (xok > 1.0) {
00780                 if (VABS(xok - 1.0) < VPMGSMALL) xok = 1.0;
00781                 else {
00782                     Vnm_print(2, "Vpmg_setPart: fell off x-interval (%1.12E)!\n",
00783                               xok);
00784                     VASSERT(0);
00785                 }
00786             }
00787         }
00788     } else xok = 0.0;
00789
00790     for (j=0; j<ny; j++) {
00791         yok = 0.0;
00792         y = j*hy + ymin;
00793         if ( (y < (upperCorner[1]-hy/2)) && (y > (lowerCorner[1]+hy/2)) ) yok = 1.0;
00794         else if ( (VABS(y - lowerCorner[1]) < VPMGSMALL) &&
00795                  (bflags[VAPBS_BACK] == 0) ) yok = 1.0;
00796         else if ( (VABS(y - lowerCorner[1]) < VPMGSMALL) &&
00797                  (bflags[VAPBS_BACK] == 1) ) yok = 0.5;
00798         else if ( (VABS(y - upperCorner[1]) < VPMGSMALL) &&
00799                  (bflags[VAPBS_FRONT] == 0) ) yok = 1.0;
00800         else if ( (VABS(y - upperCorner[1]) < VPMGSMALL) &&
00801                  (bflags[VAPBS_FRONT] == 1) ) yok = 0.5;
00802         else if ((y > (upperCorner[1] + hy/2)) || (y < (lowerCorner[1] - hy/2))) yok=0.0;
00803         else if ((y < (upperCorner[1] + hy/2)) || (y > (lowerCorner[1] - hy/2))) {
00804             y0 = VMAX2(y - hy/2, lowerCorner[1]);
00805             y1 = VMIN2(y + hy/2, upperCorner[1]);
00806             yok = VABS(y1-y0)/hy;
00807
00808             if (yok < 0.0) {
00809                 if (VABS(yok) < VPMGSMALL) yok = 0.0;
00810                 else {
00811                     Vnm_print(2, "Vpmg_setPart: fell off y-interval (%1.12E)!\n",
00812                               yok);
00813                     VASSERT(0);
00814                 }
00815             }
00816             if (yok > 1.0) {
00817                 if (VABS(yok - 1.0) < VPMGSMALL) yok = 1.0;
00818                 else {
00819                     Vnm_print(2, "Vpmg_setPart: fell off y-interval (%1.12E)!\n",
00820                               yok);
00821                 }
00822             }
00823         }
00824     }

```

```

00821             VASSERT(0);
00822         }
00823     }
00824 }
00825 else yok=0.0;
00826
00827 for (k=0; k<nz; k++) {
00828     zok = 0.0;
00829     z = k*hzed + zmin;
00830     if ((z < (upperCorner[2]-hzed/2)) && (z > (lowerCorner[2]+hzed/2))) zok = 1.0;
00831     else if ((VABS(z - lowerCorner[2]) < VPMGSMALL) &&
00832             (bflags[VAPBS_DOWN] == 0)) zok = 1.0;
00833     else if ((VABS(z - lowerCorner[2]) < VPMGSMALL) &&
00834             (bflags[VAPBS_DOWN] == 1)) zok = 0.5;
00835     else if ((VABS(z - upperCorner[2]) < VPMGSMALL) &&
00836             (bflags[VAPBS_UP] == 0)) zok = 1.0;
00837     else if ((VABS(z - upperCorner[2]) < VPMGSMALL) &&
00838             (bflags[VAPBS_UP] == 1)) zok = 0.5;
00839     else if ((z > (upperCorner[2] + hzed/2)) || (z < (lowerCorner[2] - hzed/2))) zok=0.0;
00840     else if ((z < (upperCorner[2] + hzed/2)) || (z > (lowerCorner[2] - hzed/2))) {
00841         z0 = VMAX2(z - hzed/2, lowerCorner[2]);
00842         z1 = VMIN2(z + hzed/2, upperCorner[2]);
00843         zok = VABS(z1-z0)/hzed;
00844
00845         if (zok < 0.0) {
00846             if (VABS(zok) < VPMGSMALL) zok = 0.0;
00847             else {
00848                 Vnm_print(2, "Vpmg_setPart: fell off z-interval (%1.12E)!\n",
00849                     zok);
00850                 VASSERT(0);
00851             }
00852         }
00853         if (zok > 1.0) {
00854             if (VABS(zok - 1.0) < VPMGSMALL) zok = 1.0;
00855             else {
00856                 Vnm_print(2, "Vpmg_setPart: fell off z-interval (%1.12E)!\n",
00857                     zok);
00858                 VASSERT(0);
00859             }
00860         }
00861     }
00862     else zok = 0.0;
00863
00864     if (VABS(xok*yok*zok) < VPMGSMALL) thee->pvec[IJK(i,j,k)] = 0.0;
00865     else thee->pvec[IJK(i,j,k)] = xok*yok*zok;
00866 }
00867 }
00868 }
00869 }
00870 }
00871
00872 VPUBLIC void Vpmg_unsetPart(Vpmg *thee) {
00873     int i, nx, ny, nz;
00874     Vatom *atom;
00875     Valist *alist;
00876
00877     VASSERT(thee != VNULL);
00878
00879     nx = thee->pmgp->nx;
00880     ny = thee->pmgp->ny;
00881     nz = thee->pmgp->nz;
00882     alist = thee->pbe->alist;
00883
00884     for (i=0; i<(nx*ny*nz); i++) thee->pvec[i] = 1;
00885     for (i=0; i<Valist_getNumberAtoms(alist); i++) {
00886         atom = Valist_getAtom(alist, i);
00887         atom->partID = 1;
00888     }
00889 }
00890 }
00891
00892 VPUBLIC int Vpmg_fillArray(Vpmg *thee, double *vec, Vdata_Type type,
00893     double parm, Vhal_PBEType pbetype, PBEparm *pbeparm) {
00894     Vacc *acc = VNULL;
00895     Vpbe *pbe = VNULL;
00896     Vgrid *grid = VNULL;
00897     Vatom *atoms = VNULL;
00898     Valist *alist = VNULL;
00899     double position[3], hx, hy, hzed, xmin, ymin, zmin;
00900     double grad[3], eps, epsp, epss, zmagic, u;

```

```

00902     int i, j, k, l, nx, ny, nz, ichop;
00903
00904     pbe = thee->pbe;
00905     acc = Vpbe_getVacc(pbe);
00906     nx = thee->pmgp->nx;
00907     ny = thee->pmgp->ny;
00908     nz = thee->pmgp->nz;
00909     hx = thee->pmgp->hx;
00910     hy = thee->pmgp->hy;
00911     hzed = thee->pmgp->hzed;
00912     xmin = thee->pmgp->xmin;
00913     ymin = thee->pmgp->ymin;
00914     zmin = thee->pmgp->zmin;
00915     epsp = Vpbe_getSoluteDiel(pbe);
00916     epss = Vpbe_getSolventDiel(pbe);
00917     zmagic = Vpbe_getZmagic(pbe);
00918
00919     if (!(thee->filled)) {
00920         Vnm_print(2, "Vpmg_fillArray: need to call Vpmg_fillco first!\n");
00921         return 0;
00922     }
00923
00924     switch (type) {
00925
00926     case VDT_CHARGE:
00927
00928         for (i=0; i<nx*ny*nz; i++) vec[i] = thee->charge[i]/zmagic;
00929         break;
00930
00931     case VDT_DIELX:
00932
00933         for (i=0; i<nx*ny*nz; i++) vec[i] = thee->epsx[i];
00934         break;
00935
00936     case VDT_DIELY:
00937
00938         for (i=0; i<nx*ny*nz; i++) vec[i] = thee->epsy[i];
00939         break;
00940
00941     case VDT_DIELZ:
00942
00943         for (i=0; i<nx*ny*nz; i++) vec[i] = thee->epsz[i];
00944         break;
00945
00946     case VDT_KAPPA:
00947
00948         for (i=0; i<nx*ny*nz; i++) vec[i] = thee->kappa[i];
00949         break;
00950
00951     case VDT_POT:
00952
00953         for (i=0; i<nx*ny*nz; i++) vec[i] = thee->u[i];
00954         break;
00955
00956     case VDT_ATOMPOT:
00957         alist = thee->pbe->alist;
00958         atoms = alist[pbeparm->molid-1].atoms;
00959         grid = Vgrid_ctor(nx, ny, nz, hx, hy,
00960                          hzed, xmin, ymin, zmin, thee->u);
00961         for (i=0; i<alist[pbeparm->molid-1].number; i++) {
00962             position[0] = atoms[i].position[0];
00963             position[1] = atoms[i].position[1];
00964             position[2] = atoms[i].position[2];
00965
00966             Vgrid_value(grid, position, &vec[i]);
00967         }
00968         Vgrid_dtor(&grid);
00969         break;
00970
00971     case VDT_SMOL:
00972
00973         for (k=0; k<nz; k++) {
00974             for (j=0; j<ny; j++) {
00975                 for (i=0; i<nx; i++) {
00976
00977                     position[0] = i*hx + xmin;
00978                     position[1] = j*hy + ymin;
00979                     position[2] = k*hzed + zmin;
00980
00981                     vec[IJK(i,j,k)] = (Vacc_molAcc(acc, position, parm));
00982                 }

```

```

00983     }
00984     }
00985     break;
00986
00987     case VDT_SSPL:
00988
00989         for (k=0; k<nz; k++) {
00990             for (j=0; j<ny; j++) {
00991                 for (i=0; i<nx; i++) {
00992
00993                     position[0] = i*hx + xmin;
00994                     position[1] = j*hy + ymin;
00995                     position[2] = k*hzed + zmin;
00996
00997                     vec[IJK(i,j,k)] = Vacc_splineAcc(acc,position,parm,0);
00998                 }
00999             }
01000         }
01001     break;
01002
01003     case VDT_VDW:
01004
01005         for (k=0; k<nz; k++) {
01006             for (j=0; j<ny; j++) {
01007                 for (i=0; i<nx; i++) {
01008
01009                     position[0] = i*hx + xmin;
01010                     position[1] = j*hy + ymin;
01011                     position[2] = k*hzed + zmin;
01012
01013                     vec[IJK(i,j,k)] = Vacc_vdwAcc(acc,position);
01014                 }
01015             }
01016         }
01017     break;
01018
01019     case VDT_IVDW:
01020
01021         for (k=0; k<nz; k++) {
01022             for (j=0; j<ny; j++) {
01023                 for (i=0; i<nx; i++) {
01024
01025                     position[0] = i*hx + xmin;
01026                     position[1] = j*hy + ymin;
01027                     position[2] = k*hzed + zmin;
01028
01029                     vec[IJK(i,j,k)] = Vacc_ivdwAcc(acc,position,parm);
01030                 }
01031             }
01032         }
01033     break;
01034
01035     case VDT_LAP:
01036
01037         grid = Vgrid_ctor(nx, ny, nz, hx, hy, hzed, xmin, ymin, zmin,
01038             thee->u);
01039         for (k=0; k<nz; k++) {
01040             for (j=0; j<ny; j++) {
01041                 for (i=0; i<nx; i++) {
01042
01043                     if ((k==0) || (k==(nz-1)) ||
01044                         (j==0) || (j==(ny-1)) ||
01045                         (i==0) || (i==(nx-1))) {
01046
01047                         vec[IJK(i,j,k)] = 0;
01048                     }
01049                     else {
01050                         position[0] = i*hx + xmin;
01051                         position[1] = j*hy + ymin;
01052                         position[2] = k*hzed + zmin;
01053                         VASSERT(Vgrid_curvature(grid,position, 1,
01054                             &(vec[IJK(i,j,k)])));
01055                     }
01056                 }
01057             }
01058         }
01059         Vgrid_dtor(&grid);
01060     break;
01061
01062     case VDT_EDENS:
01063

```

```

01064     grid = Vgrid_ctor(nx, ny, nz, hx, hy, hzed, xmin, ymin, zmin,
01065                      thee->u);
01066     for (k=0; k<nz; k++) {
01067         for (j=0; j<ny; j++) {
01068             for (i=0; i<nx; i++) {
01069
01070                 position[0] = i*hx + xmin;
01071                 position[1] = j*hy + ymin;
01072                 position[2] = k*hzed + zmin;
01073                 VASSERT(Vgrid_gradient(grid, position, grad));
01074                 eps = epsp + (epss-epsp)*Vacc_molAcc(acc, position,
01075                pbe->solventRadius);
01076                 vec[IJK(i,j,k)] = 0.0;
01077                 for (l=0; l<3; l++)
01078                     vec[IJK(i,j,k)] += eps*VSQR(grad[l]);
01079             }
01080         }
01081     }
01082     Vgrid_dtor(&grid);
01083     break;
01084
01085 case VDT_NDENS:
01086
01087     for (k=0; k<nz; k++) {
01088         for (j=0; j<ny; j++) {
01089             for (i=0; i<nx; i++) {
01090
01091                 position[0] = i*hx + xmin;
01092                 position[1] = j*hy + ymin;
01093                 position[2] = k*hzed + zmin;
01094                 vec[IJK(i,j,k)] = 0.0;
01095                 u = thee->u[IJK(i,j,k)];
01096                 if ( VABS(Vacc_ivdwAcc(acc,
01097                position, pbe->maxIonRadius) - 1.0) < VSMALL) {
01098                     for (l=0; l<pbe->numIon; l++) {
01099                         double q = pbe->ionQ[l];
01100                         if (patype == PBE_NPBE || patype == PBE_SMPBE /* SMPBE Added */) {
01101                             vec[IJK(i,j,k)] += pbe->ionConc[l]*Vcap_exp(-q*u, &ichop);
01102                         } else if (patype == PBE_LPBE) {
01103                             vec[IJK(i,j,k)] += pbe->ionConc[l]*(1 - q*u + 0.5*q*q*u*u);
01104                         }
01105                     }
01106                 }
01107             }
01108         }
01109     }
01110     break;
01111
01112 case VDT_QDENS:
01113
01114     for (k=0; k<nz; k++) {
01115         for (j=0; j<ny; j++) {
01116             for (i=0; i<nx; i++) {
01117                 position[0] = i*hx + xmin;
01118                 position[1] = j*hy + ymin;
01119                 position[2] = k*hzed + zmin;
01120                 vec[IJK(i,j,k)] = 0.0;
01121                 u = thee->u[IJK(i,j,k)];
01122                 if ( VABS(Vacc_ivdwAcc(acc,
01123                position, pbe->maxIonRadius) - 1.0) < VSMALL) {
01124                     for (l=0; l<pbe->numIon; l++) {
01125                         double q = pbe->ionQ[l];
01126                         if (patype == PBE_NPBE || patype == PBE_SMPBE /* SMPBE Added */) {
01127                             vec[IJK(i,j,k)] += pbe->ionConc[l]*q*Vcap_exp(-q*u, &ichop);
01128                         } else if (patype == PBE_LPBE) {
01129                             vec[IJK(i,j,k)] += pbe->ionConc[l]*q*(1 - q*u + 0.5*q*q*u*u);
01130                         }
01131                     }
01132                 }
01133             }
01134         }
01135     }
01136     break;
01137
01138 default:
01139     Vnm_print(2, "main: Bogus data type (%d)!\n", type);
01140     return 0;
01141     break;
01142 }
01143
01144 return 1;

```

```

01145
01146 }
01147
01148 VPRIVATE double Vpmg_polarizEnergy(Vpmg *thee,
01149                                     int extFlag
01150                                     ) {
01151
01152     int i,
01153         j,
01154         k,
01155         ijk,
01156         nx,
01157         ny,
01158         nz,
01159         iatom;
01160     double xmin,
01161            ymin,
01162            zmin,
01163            //x, // gcc: not used
01164            //y,
01165            //z,
01166            hx,
01167            hy,
01168            hzed,
01169            epsp,
01170            lap,
01171            pt[3],
01172            T,
01173            pre,
01174            polq,
01175            dist2,
01176            dist,
01177            energy,
01178            q,
01179            *charge,
01180            *pos,
01181            eps_w;
01182     Vgrid *potgrid;
01183     Vpbe *pbe;
01184     Valist *alist;
01185     Vatom *atom;
01186
01187     xmin = thee->pmgp->xmin;
01188     ymin = thee->pmgp->ymin;
01189     zmin = thee->pmgp->zmin;
01190     hx = thee->pmgp->hx;
01191     hy = thee->pmgp->hy;
01192     hzed = thee->pmgp->hzed;
01193     nx = thee->pmgp->nx;
01194     ny = thee->pmgp->ny;
01195     nz = thee->pmgp->nz;
01196     pbe = thee->pbe;
01197     epsp = Vpbe_getSoluteDiel(pbe);
01198     eps_w = Vpbe_getSolventDiel(pbe);
01199     alist = pbe->alist;
01200     charge = thee->charge;
01201
01202     /* Calculate the prefactor for Coulombic calculations */
01203     T = Vpbe_getTemperature(pbe);
01204     pre = (Vunit_ec*Vunit_ec)/(4*VPI*Vunit_eps0*eps_w*Vunit_kb*T);
01205     pre = pre*(1.0e10);
01206
01207     /* Set up Vgrid object with solution */
01208     potgrid = Vgrid_ctor(nx, ny, nz, hx, hy, hzed, xmin, ymin, zmin, thee->u);
01209
01210     /* Calculate polarization charge */
01211     energy = 0.0;
01212     for (i=1; i<(nx-1); i++) {
01213         pt[0] = xmin + hx*i;
01214         for (j=1; j<(ny-1); j++) {
01215             pt[1] = ymin + hy*j;
01216             for (k=1; k<(nz-1); k++) {
01217                 pt[2] = zmin + hzed*k;
01218
01219                 /* Calculate polarization charge */
01220                 VASSERT(Vgrid_curvature(potgrid, pt, 1, &lap));
01221                 ijk = IJK(i,j,k);
01222                 polq = charge[ijk] + epsp*lap*3.0;
01223
01224                 /* Calculate interaction energy with atoms */
01225                 if (VABS(polq) > VSMALL) {

```

```

01226         for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
01227             atom = Valist_getAtom(alist, iatom);
01228             q = Vatom_getCharge(atom);
01229             pos = Vatom_getPosition(atom);
01230             dist2 = VSQR(pos[0]-pt[0]) + VSQR(pos[1]-pt[1]) \
01231                 + VSQR(pos[2]-pt[2]);
01232             dist = VSQRT(dist2);
01233
01234             if (dist < VSMALL) {
01235                 Vnm_print(2, "Vpmg_polarizEnergy: atom on grid point; ignoring!\n");
01236             } else {
01237                 energy = energy + polq*q/dist;
01238             }
01239         }
01240     }
01241 }
01242 }
01243 }
01244
01245     return pre*energy;
01246 }
01247
01248 VPUBLIC double Vpmg_energy(Vpmg *thee,
01249                             int extFlag
01250                         ) {
01251
01252     double totEnergy = 0.0,
01253            dielEnergy = 0.0,
01254            qmEnergy = 0.0,
01255            qfEnergy = 0.0;
01256
01257     VASSERT(thee != VNULL);
01258
01259     if ((thee->pmgp->nonlin) && (Vpbe_getBulkIonicStrength(thee->pbe) > 0.)) {
01260         Vnm_print(0, "Vpmg_energy: calculating full PBE energy\n");
01261         qmEnergy = Vpmg_qmEnergy(thee, extFlag);
01262         Vnm_print(0, "Vpmg_energy: qmEnergy = %1.12E kT\n", qmEnergy);
01263         qfEnergy = Vpmg_qfEnergy(thee, extFlag);
01264         Vnm_print(0, "Vpmg_energy: qfEnergy = %1.12E kT\n", qfEnergy);
01265         dielEnergy = Vpmg_dielEnergy(thee, extFlag);
01266         Vnm_print(0, "Vpmg_energy: dielEnergy = %1.12E kT\n", dielEnergy);
01267         totEnergy = qfEnergy - dielEnergy - qmEnergy;
01268     } else {
01269         Vnm_print(0, "Vpmg_energy: calculating only q-phi energy\n");
01270         qfEnergy = Vpmg_qfEnergy(thee, extFlag);
01271         Vnm_print(0, "Vpmg_energy: qfEnergy = %1.12E kT\n", qfEnergy);
01272         totEnergy = 0.5*qfEnergy;
01273     }
01274
01275     return totEnergy;
01276 }
01277 }
01278
01279 VPUBLIC double Vpmg_dielEnergy(Vpmg *thee,
01280                                 int extFlag
01281                             ) {
01282
01283     double hx,
01284            hy,
01285            hzed,
01286            energy,
01287            nrgx,
01288            nrgy,
01289            nrgz,
01290            pvecx,
01291            pvecy,
01292            pvecz;
01293
01294     int i,
01295         j,
01296         k,
01297         nx,
01298         ny,
01299         nz;
01300
01301     VASSERT(thee != VNULL);
01302
01303     /* Get the mesh information */
01304     nx = thee->pmgp->nx;
01305     ny = thee->pmgp->ny;
01306     nz = thee->pmgp->nz;
01307     hx = thee->pmgp->hx;

```

```

01307     hy = thee->pmgp->hy;
01308     hzed = thee->pmgp->hzed;
01309
01310     energy = 0.0;
01311
01312     if (!thee->filled) {
01313         Vnm_print(2, "Vpmg_dielEnergy: Need to call Vpmg_fillco!\n");
01314         VASSERT(0);
01315     }
01316
01317     for (k=0; k<(nz-1); k++) {
01318         for (j=0; j<(ny-1); j++) {
01319             for (i=0; i<(nx-1); i++) {
01320                 pvecx = 0.5*(thee->pvec[IJK(i,j,k)]+thee->pvec[IJK(i+1,j,k)]);
01321                 pvecy = 0.5*(thee->pvec[IJK(i,j,k)]+thee->pvec[IJK(i,j+1,k)]);
01322                 pvecz = 0.5*(thee->pvec[IJK(i,j,k)]+thee->pvec[IJK(i,j,k+1)]);
01323                 nrgx = thee->epsx[IJK(i,j,k)]*pvecx
01324                     * VSQR((thee->u[IJK(i,j,k)]-thee->u[IJK(i+1,j,k)]) /hx);
01325                 nrgy = thee->epsy[IJK(i,j,k)]*pvecy
01326                     * VSQR((thee->u[IJK(i,j,k)]-thee->u[IJK(i,j+1,k)]) /hy);
01327                 nrgz = thee->epsz[IJK(i,j,k)]*pvecz
01328                     * VSQR((thee->u[IJK(i,j,k)]-thee->u[IJK(i,j,k+1)]) /hzed);
01329                 energy += (nrgx + nrgy + nrgz);
01330             }
01331         }
01332     }
01333
01334     energy = 0.5*energy*hx*hy*hzed;
01335     energy = energy/Vpbe_getZmagic(thee->pbe);
01336
01337     if (extFlag == 1) energy += (thee->extDiEnergy);
01338
01339     return energy;
01340 }
01341
01342 VPUBLIC double Vpmg_dielGradNorm(Vpmg *thee) {
01343
01344     double hx, hy, hzed, energy, nrgx, nrgy, nrgz, pvecx, pvecy, pvecz;
01345     int i, j, k, nx, ny, nz;
01346
01347     VASSERT(thee != VNULL);
01348
01349     /* Get the mesh information */
01350     nx = thee->pmgp->nx;
01351     ny = thee->pmgp->ny;
01352     nz = thee->pmgp->nz;
01353     hx = thee->pmgp->hx;
01354     hy = thee->pmgp->hy;
01355     hzed = thee->pmgp->hzed;
01356
01357     energy = 0.0;
01358
01359     if (!thee->filled) {
01360         Vnm_print(2, "Vpmg_dielGradNorm: Need to call Vpmg_fillco!\n");
01361         VASSERT(0);
01362     }
01363
01364     for (k=1; k<nz; k++) {
01365         for (j=1; j<ny; j++) {
01366             for (i=1; i<nx; i++) {
01367                 pvecx = 0.5*(thee->pvec[IJK(i,j,k)]+thee->pvec[IJK(i-1,j,k)]);
01368                 pvecy = 0.5*(thee->pvec[IJK(i,j,k)]+thee->pvec[IJK(i,j-1,k)]);
01369                 pvecz = 0.5*(thee->pvec[IJK(i,j,k)]+thee->pvec[IJK(i,j,k-1)]);
01370                 nrgx = pvecx
01371                     * VSQR((thee->epsx[IJK(i,j,k)]-thee->epsx[IJK(i-1,j,k)]) /hx);
01372                 nrgy = pvecy
01373                     * VSQR((thee->epsy[IJK(i,j,k)]-thee->epsy[IJK(i,j-1,k)]) /hy);
01374                 nrgz = pvecz
01375                     * VSQR((thee->epsz[IJK(i,j,k)]-thee->epsz[IJK(i,j,k-1)]) /hzed);
01376                 energy += VSQRT(nrgx + nrgy + nrgz);
01377             }
01378         }
01379     }
01380
01381     energy = energy*hx*hy*hzed;
01382
01383     return energy;
01384 }
01385
01386 VPUBLIC double Vpmg_qmEnergy(Vpmg *thee,
01387                             int extFlag

```



```

01388         ) {
01389
01390     double energy;
01391
01392     if (thee->pbe->ipkey == IPKEY_SMPBE) {
01393         energy = Vpmg_qmEnergySMPBE(thee, extFlag);
01394     } else {
01395         energy = Vpmg_qmEnergyNONLIN(thee, extFlag);
01396     }
01397
01398     return energy;
01399 }
01400
01401 VPRIVATE double Vpmg_qmEnergyNONLIN(Vpmg *thee,
01402                                     int extFlag
01403                                     ) {
01404
01405     double hx,
01406           hy,
01407           hzed,
01408           energy,
01409           ionConc[MAXION],
01410           ionRadii[MAXION],
01411           ionQ[MAXION],
01412           zkappa2,
01413           ionstr,
01414           zks2;
01415     int i, /* Loop variable */
01416         j,
01417         nx,
01418         ny,
01419         nz,
01420         nion,
01421         ichop,
01422         nchop,
01423         len; /* Stores number of iterations for loops to avoid multiple recalculations */
01424
01425     VASSERT(thee != VNULL);
01426
01427     /* Get the mesh information */
01428     nx = thee->pmgp->nx;
01429     ny = thee->pmgp->ny;
01430     nz = thee->pmgp->nz;
01431     hx = thee->pmgp->hx;
01432     hy = thee->pmgp->hy;
01433     hzed = thee->pmgp->hzed;
01434     zkappa2 = Vpbe_getZkappa2(thee->pbe);
01435     ionstr = Vpbe_getBulkIonicStrength(thee->pbe);
01436
01437     /* Bail if we're at zero ionic strength */
01438     if (zkappa2 < VSMALL) {
01439
01440 #ifndef VAPBSQUIET
01441         Vnm_print(0, "Vpmg_qmEnergy: Zero energy for zero ionic strength!\n");
01442 #endif
01443
01444         return 0.0;
01445     }
01446     zks2 = 0.5*zkappa2/ionstr;
01447
01448     if (!thee->filled) {
01449         Vnm_print(2, "Vpmg_qmEnergy: Need to call Vpmg_fillco()!\n");
01450         VASSERT(0);
01451     }
01452
01453     energy = 0.0;
01454     nchop = 0;
01455     Vpbe_getIons(thee->pbe, &nion, ionConc, ionRadii, ionQ);
01456     if (thee->pmgp->nonlin) {
01457         Vnm_print(0, "Vpmg_qmEnergy: Calculating nonlinear energy\n");
01458         for (i=0, len=nx*ny*nz; i<len; i++) {
01459             if (thee->pvec[i]*thee->kappa[i] > VSMALL) {
01460                 for (j=0; j<nion; j++) {
01461                     energy += (thee->pvec[i]*thee->kappa[i]*zks2
01462                               * ionConc[j]
01463                               * (Vcap_exp(-ionQ[j]*thee->u[i], &ichop)-1.0));
01464                     nchop += ichop;
01465                 }
01466             }
01467         }
01468         if (nchop > 0) {

```

```

01469         Vnm_print(2, "Vpmg_qmEnergy: Chopped EXP %d times!\n",nchop);
01470         Vnm_print(2, "\nERROR! Detected large potential values in energy evaluation! \nERROR! This
calculation failed -- please report to the APBS developers!\n\n");
01471         VASSERT(0);
01472     }
01473 } else {
01474     /* Zkappa2 OK here b/c LPBE approx */
01475     Vnm_print(0, "Vpmg_qmEnergy: Calculating linear energy\n");
01476     for (i=0, len=nx*ny*nz; i<len; i++) {
01477         if (thee->pvec[i]*thee->kappa[i] > VSMALL)
01478             energy += (thee->pvec[i]*zkappa2*thee->kappa[i]*VSQR(thee->u[i]));
01479     }
01480     energy = 0.5*energy;
01481 }
01482 energy = energy*hx*hy*hzed;
01483 energy = energy/Vpbe_getZmagic(thee->pbe);
01484
01485 if (extFlag == 1) energy += thee->extQmEnergy;
01486
01487 return energy;
01488 }
01489
01490 VPUBLIC double Vpmg_qmEnergySMPBE(Vpmg *thee,
01491                                   int extFlag
01492                                   ) {
01493
01494     double hx,
01495           hy,
01496           hzed,
01497           energy,
01498           ionConc[MAXION],
01499           ionRadii[MAXION],
01500           ionQ[MAXION],
01501           zkappa2,
01502           ionstr,
01503           zks2;
01504
01505     int i,
01506         //j, // gcc: not used
01507         nx,
01508         ny,
01509         nz,
01510         nion,
01511         //ichop, // gcc: not used
01512         nchop,
01513         len; /* Loop variable */
01514
01515     /* SMPB Modification (vchu, 09/21/06)*/
01516     /* variable declarations for SMPB energy terms */
01517     double a,
01518           k,
01519           z1,
01520           z2,
01521           z3,
01522           cb1,
01523           cb2,
01524           cb3,
01525           a1,
01526           a2,
01527           a3,
01528           c1,
01529           c2,
01530           c3,
01531           currEnergy,
01532           fracOccA,
01533           fracOccB,
01534           fracOccC,
01535           phi,
01536           gpark,
01537           denom;
01538     // Na; /**< @todo remove if no conflicts are caused - This constant is already defined in
vpde.h. no need to redefine. */
01539     int ichop1,
01540         ichop2,
01541         ichop3;
01542
01543     VASSERT(thee != VNULL);
01544
01545     /* Get the mesh information */
01546     nx = thee->pmgp->nx;
01547     ny = thee->pmgp->ny;
01548     nz = thee->pmgp->nz;

```

```

01548     hx = thee->pmgp->hx;
01549     hy = thee->pmgp->hy;
01550     hzed = thee->pmgp->hzed;
01551     zkappa2 = Vpbe_getZkappa2(thee->pbe);
01552     ionstr = Vpbe_getBulkIonicStrength(thee->pbe);
01553
01554     /* Bail if we're at zero ionic strength */
01555     if (zkappa2 < VSMALL) {
01556
01557 #ifndef VAPBSQUIET
01558         Vnm_print(0, "Vpmg_qmEnergySMPBE: Zero energy for zero ionic strength!\n");
01559 #endif
01560
01561         return 0.0;
01562     }
01563     zks2 = 0.5*zkappa2/ionstr;
01564
01565     if (!thee->filled) {
01566         Vnm_print(2, "Vpmg_qmEnergySMPBE: Need to call Vpmg_fillco()!\n");
01567         VASSERT(0);
01568     }
01569
01570     energy = 0.0;
01571     nchop = 0;
01572     Vpbe_getIons(thee->pbe, &nion, ionConc, ionRadii, ionQ);
01573
01574     /* SMPB Modification (vchu, 09/21/06) */
01575     /* Extensive modification to the first part of the if statement
01576        where that handles the thee->pmgp->nonlin part. Basically, I've
01577        deleted all of the original code and written my own code that computes
01578        the electrostatic free energy in the SMPB framework. Definitely really hacky
01579        at this stage of the game, but gets the job done. The second part of the
01580        if statement (the part that handles linear poisson-boltzmann) has been deleted
01581        because there will be no linearized SMPB energy.. */
01582
01583     z1 = ionQ[0];
01584     z2 = ionQ[1];
01585     z3 = ionQ[2];
01586     cb1 = ionConc[0];
01587     cb2 = ionConc[1];
01588     cb3 = ionConc[2];
01589     a = thee->pbe->smvolume;
01590     k = thee->pbe->smsize;
01591
01592     // This constant is defined in vpde.h Do not need to redefine
01593     //Na = 6.022045000e-04; /* Converts from Molar to N/A^3 */
01594
01595     fracOccA = Na*cb1*VCUB(a);
01596     fracOccB = Na*cb2*VCUB(a);
01597     fracOccC = Na*cb3*VCUB(a);
01598
01599     phi = (fracOccA/k) + fracOccB + fracOccC;
01600
01601     if (thee->pmgp->nonlin) {
01602         Vnm_print(0, "Vpmg_qmEnergySMPBE: Calculating nonlinear energy using SMPB functional!\n");
01603         for (i=0, len=nx*ny*nz; i<len; i++) {
01604             if (((k-1) > VSMALL) && (thee->pvec[i]*thee->kappa[i] > VSMALL)) {
01605
01606                 a1 = Vcap_exp(-1.0*z1*thee->u[i], &ichop1);
01607                 a2 = Vcap_exp(-1.0*z2*thee->u[i], &ichop2);
01608                 a3 = Vcap_exp(-1.0*z3*thee->u[i], &ichop3);
01609
01610                 nchop += ichop1 + ichop2 + ichop3;
01611
01612                 gpark = (1 - phi + (fracOccA/k)*a1);
01613                 denom = VPOW(gpark, k) + VPOW(1-fracOccB-fracOccC, k-1)*(fracOccB*a2+fracOccC*a3);
01614
01615                 if (cb1 > VSMALL) {
01616                     c1 = Na*cb1*VPOW(gpark, k-1)*a1/denom;
01617                     if (c1 != c1) c1 = 0.;
01618                 } else c1 = 0.;
01619
01620                 if (cb2 > VSMALL) {
01621                     c2 = Na*cb2*VPOW(1-fracOccB-fracOccC, k-1)*a2/denom;
01622                     if (c2 != c2) c2 = 0.;
01623                 } else c2 = 0.;
01624
01625                 if (cb3 > VSMALL) {
01626                     c3 = Na*cb3*VPOW(1-fracOccB-fracOccC, k-1)*a3/denom;
01627                     if (c3 != c3) c3 = 0.;
01628                 } else c3 = 0.;
01629

```

```

01630
01631         currEnergy = k*VLOG((1-(c1*VCUB(a)/k)-c2*VCUB(a)-c3*VCUB(a))/(1-phi))
01632             -(k-1)*VLOG((1-c2*VCUB(a)-c3*VCUB(a))/(1-phi+(fracOccA/k)));
01633
01634         energy += thee->pvec[i]*thee->kappa[i]*currEnergy;
01635
01636     } else if (thee->pvec[i]*thee->kappa[i] > VSMALL){
01637
01638         a1 = Vcap_exp(-1.0*z1*thee->u[i], &ichop1);
01639         a2 = Vcap_exp(-1.0*z2*thee->u[i], &ichop2);
01640         a3 = Vcap_exp(-1.0*z3*thee->u[i], &ichop3);
01641
01642         nchop += ichop1 + ichop2 + ichop3;
01643
01644         gpark = (1 - phi + (fracOccA)*a1);
01645         denom = gpark + (fracOccB*a2+fracOccC*a3);
01646
01647         if (cb1 > VSMALL) {
01648             c1 = Na*cb1*a1/denom;
01649             if(c1 != c1) c1 = 0.;
01650         } else c1 = 0.;
01651
01652         if (cb2 > VSMALL) {
01653             c2 = Na*cb2*a2/denom;
01654             if(c2 != c2) c2 = 0.;
01655         } else c2 = 0.;
01656
01657         if (cb3 > VSMALL) {
01658             c3 = Na*cb3*a3/denom;
01659             if(c3 != c3) c3 = 0.;
01660         } else c3 = 0.;
01661
01662         currEnergy = VLOG((1-c1*VCUB(a)-c2*VCUB(a)-c3*VCUB(a))/(1-fracOccA-fracOccB-fracOccC));
01663
01664         energy += thee->pvec[i]*thee->kappa[i]*currEnergy;
01665     }
01666 }
01667
01668 energy = -energy/VCUB(a);
01669
01670 if (nchop > 0) Vnm_print(2, "Vpmg_qmEnergySMPBE: Chopped EXP %d times!\n",
01671                         nchop);
01672
01673 } else {
01674     /* Zkappa2 OK here b/c LPBE approx */
01675     Vnm_print(0, "Vpmg_qmEnergySMPBE: ERROR: NO LINEAR ENERGY!! Returning 0!\n");
01676
01677     energy = 0.0;
01678 }
01679 }
01680 energy = energy*hx*hy*hzed;
01681
01682 if (extFlag == 1) energy += thee->extQmEnergy;
01683
01684 return energy;
01685 }
01686
01687 VPUBLIC double Vpmg_qfEnergy(Vpmg *thee,
01688                             int extFlag
01689                             ) {
01690
01691     double energy = 0.0;
01692
01693     VASSERT(thee != VNULL);
01694
01695     if ((thee->useChargeMap) || (thee->chargeMeth == VCM_BSPL2)) {
01696         energy = Vpmg_qfEnergyVolume(thee, extFlag);
01697     } else {
01698         energy = Vpmg_qfEnergyPoint(thee, extFlag);
01699     }
01700
01701     return energy;
01702 }
01703
01704 VPRIVATE double Vpmg_qfEnergyPoint(Vpmg *thee,
01705                                    int extFlag
01706                                    ) {
01707
01708     int iatom, nx, ny, nz, ihi, ilo, jhi, jlo, khi, klo;
01709     double xmax, ymax, zmax, xmin, ymin, zmin, hx, hy, hzed, ifloat, jfloat;
01710     double charge, kfloat, dx, dy, dz, energy, uval, *position;

```

```

01711     double *u;
01712     double *pvec;
01713     Valist *alist;
01714     Vatom *atom;
01715     Vpbe *pbe;
01716
01717     pbe = thee->pbe;
01718     alist = pbe->alist;
01719     VASSERT(alist != VNULL);
01720
01721     /* Get the mesh information */
01722     nx = thee->pmgp->nx;
01723     ny = thee->pmgp->ny;
01724     nz = thee->pmgp->nz;
01725     hx = thee->pmgp->hx;
01726     hy = thee->pmgp->hy;
01727     hzed = thee->pmgp->hzd;
01728     xmax = thee->pmgp->xmax;
01729     ymax = thee->pmgp->ymax;
01730     zmax = thee->pmgp->zmax;
01731     xmin = thee->pmgp->xmin;
01732     ymin = thee->pmgp->ymin;
01733     zmin = thee->pmgp->zmin;
01734
01735     u = thee->u;
01736     pvec = thee->pvec;
01737
01738     energy = 0.0;
01739
01740     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
01741
01742         /* Get atomic information */
01743         atom = Valist_getAtom(alist, iatom);
01744
01745         position = Vatom_getPosition(atom);
01746         charge = Vatom_getCharge(atom);
01747
01748         /* Figure out which vertices we're next to */
01749         ifloat = (position[0] - xmin)/hx;
01750         jfloat = (position[1] - ymin)/hy;
01751         kfloat = (position[2] - zmin)/hzd;
01752         ihi = (int)ceil(ifloat);
01753         ilo = (int)floor(ifloat);
01754         jhi = (int)ceil(jfloat);
01755         jlo = (int)floor(jfloat);
01756         khi = (int)ceil(kfloat);
01757         klo = (int)floor(kfloat);
01758
01759         if (atom->partID > 0) {
01760
01761             if ((ihi<nx) && (jhi<ny) && (khi<nz) &&
01762                 (ilo>=0) && (jlo>=0) && (klo>=0)) {
01763
01764                 /* Now get trilinear interpolation constants */
01765                 dx = ifloat - (double)(ilo);
01766                 dy = jfloat - (double)(jlo);
01767                 dz = kfloat - (double)(klo);
01768                 uval =
01769                     dx*dy*dz*u[IJK(ihi,jhi,khi)]
01770                     + dx*(1.0-dy)*dz*u[IJK(ihi,jlo,khi)]
01771                     + dx*dy*(1.0-dz)*u[IJK(ihi,jhi,klo)]
01772                     + dx*(1.0-dy)*(1.0-dz)*u[IJK(ihi,jlo,klo)]
01773                     + (1.0-dx)*dy*dz*u[IJK(ilo,jhi,khi)]
01774                     + (1.0-dx)*(1.0-dy)*dz*u[IJK(ilo,jlo,khi)]
01775                     + (1.0-dx)*dy*(1.0-dz)*u[IJK(ilo,jhi,klo)]
01776                     + (1.0-dx)*(1.0-dy)*(1.0-dz)*u[IJK(ilo,jlo,klo)];
01777                 energy += (uval*charge*atom->partID);
01778             } else if (thee->pmgp->bcfl != BCFL_FOCUS) {
01779                 Vnm_print(2, "Vpmg_qfEnergy: Atom #d at (%4.3f, %4.3f, \
01780 %4.3f) is off the mesh (ignoring)!\n",
01781                     iatom, position[0], position[1], position[2]);
01782             }
01783         }
01784     }
01785
01786     if (extFlag) energy += thee->extQfEnergy;
01787
01788     return energy;
01789 }
01790
01791 VPUBLIC double Vpmg_qfAtomEnergy(Vpmg *thee, Vatom *atom) {

```

```

01792
01793     int nx, ny, nz, ihi, ilo, jhi, jlo, khi, klo;
01794     double xmax, xmin, ymax, ymin, zmax, zmin, hx, hy, hzed, ifloat, jfloat;
01795     double charge, kfloat, dx, dy, dz, energy, uval, *position;
01796     double *u;
01797
01798
01799     /* Get the mesh information */
01800     nx = thee->pmg->nx;
01801     ny = thee->pmg->ny;
01802     nz = thee->pmg->nz;
01803     hx = thee->pmg->hx;
01804     hy = thee->pmg->hy;
01805     hzed = thee->pmg->hzed;
01806     xmax = thee->xf[nx-1];
01807     ymax = thee->yf[ny-1];
01808     zmax = thee->zf[nz-1];
01809     xmin = thee->xf[0];
01810     ymin = thee->yf[0];
01811     zmin = thee->zf[0];
01812
01813     u = thee->u;
01814
01815     energy = 0.0;
01816
01817
01818     position = Vatom_getPosition(atom);
01819     charge = Vatom_getCharge(atom);
01820
01821     /* Figure out which vertices we're next to */
01822     ifloat = (position[0] - xmin)/hx;
01823     jfloat = (position[1] - ymin)/hy;
01824     kfloat = (position[2] - zmin)/hzed;
01825     ihi = (int)ceil(ifloat);
01826     ilo = (int)floor(ifloat);
01827     jhi = (int)ceil(jfloat);
01828     jlo = (int)floor(jfloat);
01829     khi = (int)ceil(kfloat);
01830     klo = (int)floor(kfloat);
01831
01832     if (atom->partID > 0) {
01833
01834         if ((ihi<nx) && (jhi<ny) && (khi<nz) &&
01835             (ilo>=0) && (jlo>=0) && (klo>=0)) {
01836
01837             /* Now get trilinear interpolation constants */
01838             dx = ifloat - (double)(ilo);
01839             dy = jfloat - (double)(jlo);
01840             dz = kfloat - (double)(klo);
01841             uval =
01842                 dx*dy*dz*u[IJK(ihi,jhi,khi)]
01843                 + dx*(1.0-dy)*dz*u[IJK(ihi,jlo,khi)]
01844                 + dx*dy*(1.0-dz)*u[IJK(ihi,jhi,klo)]
01845                 + dx*(1.0-dy)*(1.0-dz)*u[IJK(ihi,jlo,klo)]
01846                 + (1.0-dx)*dy*dz*u[IJK(ilo,jhi,khi)]
01847                 + (1.0-dx)*(1.0-dy)*dz*u[IJK(ilo,jlo,khi)]
01848                 + (1.0-dx)*dy*(1.0-dz)*u[IJK(ilo,jhi,klo)]
01849                 + (1.0-dx)*(1.0-dy)*(1.0-dz)*u[IJK(ilo,jlo,klo)];
01850             energy += (uval*charge*atom->partID);
01851         } else if (thee->pmg->bcfl != BCFL_FOCUS) {
01852             Vnm_print(2, "Vpmg_qfAtomEnergy: Atom at (%4.3f, %4.3f, \
01853 %4.3f) is off the mesh (ignoring)!\n",
01854                 position[0], position[1], position[2]);
01855         }
01856     }
01857
01858     return energy;
01859 }
01860
01861 VPRIVATE double Vpmg_qfEnergyVolume(Vpmg *thee, int extFlag) {
01862
01863     double hx, hy, hzed, energy;
01864     int i, nx, ny, nz;
01865
01866     VASSERT(thee != VNULL);
01867
01868     /* Get the mesh information */
01869     nx = thee->pmg->nx;
01870     ny = thee->pmg->ny;
01871     nz = thee->pmg->nz;
01872     hx = thee->pmg->hx;

```

```

01873     hy = thee->pmgp->hy;
01874     hzed = thee->pmgp->hzed;
01875
01876     if (!thee->filled) {
01877         Vnm_print(2, "Vpmg_qfEnergyVolume: need to call Vpmg_fillco!\n");
01878         VASSERT(0);
01879     }
01880
01881     energy = 0.0;
01882     Vnm_print(0, "Vpmg_qfEnergyVolume: Calculating energy\n");
01883     for (i=0; i<(nx*ny*nz); i++) {
01884         energy += (thee->pvec[i]*thee->u[i]*thee->charge[i]);
01885     }
01886     energy = energy*hx*hy*hzed/Vpbe_getZmagic(thee->pbe);
01887
01888     if (extFlag == 1) energy += thee->extQfEnergy;
01889
01890     return energy;
01891 }
01892
01893 VPRIVATE void Vpmg_splineSelect(int srfm,Vacc *acc,double *gpos,double win,
01894                                 double infrad,Vatom *atom,double *force){
01895
01896     switch (srfm) {
01897         case VSM_SPLINE :
01898             Vacc_splineAccGradAtomNorm(acc, gpos, win, infrad, atom, force);
01899             break;
01900         case VSM_SPLINE3:
01901             Vacc_splineAccGradAtomNorm3(acc, gpos, win, infrad, atom, force);
01902             break;
01903         case VSM_SPLINE4 :
01904             Vacc_splineAccGradAtomNorm4(acc, gpos, win, infrad, atom, force);
01905             break;
01906         default:
01907             Vnm_print(2, "Vpmg_dbnbForce: Unknown surface method.\n");
01908             return;
01909     }
01910
01911     return;
01912 }
01913
01914 VPRIVATE void focusFillBound(Vpmg *thee,
01915                             Vpmg *pmgOLD
01916 ) {
01917
01918     Vpbe *pbe;
01919     double hxOLD,
01920            hyOLD,
01921            hzOLD,
01922            xminOLD,
01923            yminOLD,
01924            zminOLD,
01925            xmaxOLD,
01926            ymaxOLD,
01927            zmaxOLD,
01928            hxNEW,
01929            hyNEW,
01930            hzNEW,
01931            xminNEW,
01932            yminNEW,
01933            zminNEW,
01934            xmaxNEW,
01935            ymaxNEW,
01936            zmaxNEW,
01937            x,
01938            y,
01939            z,
01940            dx,
01941            dy,
01942            dz,
01943            ifloat,
01944            jfloat,
01945            kfloat,
01946            uval,
01947            eps_w,
01948            T,
01949            prel,
01950            xkappa,
01951            size,
01952            *apos,
01953            charge,

```

```

01954         //pos[3], // gcc: not used
01955         uvalMin,
01956         uvalMax,
01957         *data;
01958     int nxOLD,
01959         nyOLD,
01960         nzOLD,
01961         nxNEW,
01962         nyNEW,
01963         nzNEW,
01964         i,
01965         j,
01966         k,
01967         ihi,
01968         ilo,
01969         jhi,
01970         jlo,
01971         khi,
01972         klo,
01973         nx,
01974         ny,
01975         nz;
01976
01977     /* Calculate new problem dimensions */
01978     hxNEW = thee->pmgp->hx;
01979     hyNEW = thee->pmgp->hy;
01980     hzNEW = thee->pmgp->hz;
01981     nx = thee->pmgp->nx;
01982     ny = thee->pmgp->ny;
01983     nz = thee->pmgp->nz;
01984     nxNEW = thee->pmgp->nx;
01985     nyNEW = thee->pmgp->ny;
01986     nzNEW = thee->pmgp->nz;
01987     xminNEW = thee->pmgp->xcent - ((double) (nxNEW-1) * hxNEW) / 2.0;
01988     xmaxNEW = thee->pmgp->xcent + ((double) (nxNEW-1) * hxNEW) / 2.0;
01989     yminNEW = thee->pmgp->ycent - ((double) (nyNEW-1) * hyNEW) / 2.0;
01990     ymaxNEW = thee->pmgp->ycent + ((double) (nyNEW-1) * hyNEW) / 2.0;
01991     zminNEW = thee->pmgp->zcent - ((double) (nzNEW-1) * hzNEW) / 2.0;
01992     zmaxNEW = thee->pmgp->zcent + ((double) (nzNEW-1) * hzNEW) / 2.0;
01993
01994     if (pmgOLD != VNULL) {
01995         /* Relevant old problem parameters */
01996         hxOLD = pmgOLD->pmgp->hx;
01997         hyOLD = pmgOLD->pmgp->hy;
01998         hzOLD = pmgOLD->pmgp->hz;
01999         nxOLD = pmgOLD->pmgp->nx;
02000         nyOLD = pmgOLD->pmgp->ny;
02001         nzOLD = pmgOLD->pmgp->nz;
02002         xminOLD = pmgOLD->pmgp->xcent - ((double) (nxOLD-1) * hxOLD) / 2.0;
02003         xmaxOLD = pmgOLD->pmgp->xcent + ((double) (nxOLD-1) * hxOLD) / 2.0;
02004         yminOLD = pmgOLD->pmgp->ycent - ((double) (nyOLD-1) * hyOLD) / 2.0;
02005         ymaxOLD = pmgOLD->pmgp->ycent + ((double) (nyOLD-1) * hyOLD) / 2.0;
02006         zminOLD = pmgOLD->pmgp->zcent - ((double) (nzOLD-1) * hzOLD) / 2.0;
02007         zmaxOLD = pmgOLD->pmgp->zcent + ((double) (nzOLD-1) * hzOLD) / 2.0;
02008
02009         data = pmgOLD->u;
02010     } else {
02011         /* Relevant old problem parameters */
02012         hxOLD = thee->potMap->hx;
02013         hyOLD = thee->potMap->hy;
02014         hzOLD = thee->potMap->hz;
02015         nxOLD = thee->potMap->nx;
02016         nyOLD = thee->potMap->ny;
02017         nzOLD = thee->potMap->nz;
02018         xminOLD = thee->potMap->xmin;
02019         xmaxOLD = thee->potMap->xmax;
02020         yminOLD = thee->potMap->ymin;
02021         ymaxOLD = thee->potMap->ymax;
02022         zminOLD = thee->potMap->zmin;
02023         zmaxOLD = thee->potMap->zmax;
02024
02025         data = thee->potMap->data;
02026     }
02027     /* BOUNDARY CONDITION SETUP FOR POINTS OFF OLD MESH:
02028     * For each "atom" (only one for bcfl=1), we use the following formula to
02029     * calculate the boundary conditions:
02030     * 
$$g(x) = \frac{q e_c}{4\pi\epsilon_0\epsilon_w k_B T} \left( \frac{\exp(-\kappa(d-a))}{1+\kappa a} \right)$$

02031     * 
$$+ \frac{1}{d}$$

02032     * where  $d = ||x - x_0||$  (in m) and  $a$  is the size of the atom (in m).
02033     * We only need to evaluate some of these prefactors once:

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02035      *   prel = \frac{e_c}{4*\pi*\epsilon_0*\epsilon_w*k_b*T}
02036      *   which gives the potential as
02037      *   g(x) = prel * q/d * \frac{\exp(-xkappa*(d - a))}{1+xkappa*a}
02038      */
02039     pbe = three->pbe;
02040     eps_w = Vpbe_getSolventDiel(pbe);           /* Dimensionless */
02041     T = Vpbe_getTemperature(pbe);              /* K */
02042     prel = (Vunit_ec)/(4*VPI*Vunit_eps0*eps_w*Vunit_kb*T);
02043
02044     /* Finally, if we convert keep xkappa in A^{-1} and scale prel by
02045      * m/A, then we will only need to deal with distances and sizes in
02046      * Angstroms rather than meters. */
02047     xkappa = Vpbe_getXkappa(pbe);              /* A^{-1} */
02048     prel = prel*(1.0e10);
02049     size = Vpbe_getSoluteRadius(pbe);
02050     apos = Vpbe_getSoluteCenter(pbe);
02051     charge = Vunit_ec*Vpbe_getSoluteCharge(pbe);
02052
02053     /* Check for rounding error */
02054     if (VABS(xminOLD-xminNEW) < VSMALL) xminNEW = xminOLD;
02055     if (VABS(xmaxOLD-xmaxNEW) < VSMALL) xmaxNEW = xmaxOLD;
02056     if (VABS(yminOLD-yminNEW) < VSMALL) yminNEW = yminOLD;
02057     if (VABS(ymaxOLD-ymaxNEW) < VSMALL) ymaxNEW = ymaxOLD;
02058     if (VABS(zminOLD-zminNEW) < VSMALL) zminNEW = zminOLD;
02059     if (VABS(zmaxOLD-zmaxNEW) < VSMALL) zmaxNEW = zmaxOLD;
02060
02061
02062     /* Sanity check: make sure we're within the old mesh */
02063     Vnm_print(0, "VPMG::focusFillBound -- New mesh mins = %g, %g, %g\n",
02064              xminNEW, yminNEW, zminNEW);
02065     Vnm_print(0, "VPMG::focusFillBound -- New mesh maxs = %g, %g, %g\n",
02066              xmaxNEW, ymaxNEW, zmaxNEW);
02067     Vnm_print(0, "VPMG::focusFillBound -- Old mesh mins = %g, %g, %g\n",
02068              xminOLD, yminOLD, zminOLD);
02069     Vnm_print(0, "VPMG::focusFillBound -- Old mesh maxs = %g, %g, %g\n",
02070              xmaxOLD, ymaxOLD, zmaxOLD);
02071
02072     /* The following is obsolete; we'll substitute analytical boundary
02073      * condition values when the new mesh falls outside the old */
02074     if ((xmaxNEW>xmaxOLD) || (ymaxNEW>ymaxOLD) || (zmaxNEW>zmaxOLD) ||
02075         (xminOLD>xminNEW) || (yminOLD>yminNEW) || (zminOLD>zminNEW)) {
02076
02077         Vnm_print(2, "Vpmg::focusFillBound -- new mesh not contained in old!\n");
02078         Vnm_print(2, "Vpmg::focusFillBound -- old mesh min = (%g, %g, %g)\n",
02079                  xminOLD, yminOLD, zminOLD);
02080         Vnm_print(2, "Vpmg::focusFillBound -- old mesh max = (%g, %g, %g)\n",
02081                  xmaxOLD, ymaxOLD, zmaxOLD);
02082         Vnm_print(2, "Vpmg::focusFillBound -- new mesh min = (%g, %g, %g)\n",
02083                  xminNEW, yminNEW, zminNEW);
02084         Vnm_print(2, "Vpmg::focusFillBound -- new mesh max = (%g, %g, %g)\n",
02085                  xmaxNEW, ymaxNEW, zmaxNEW);
02086         fflush(stderr);
02087         VASSERT(0);
02088     }
02089
02090     uvalMin = VPMGSMALL;
02091     uvalMax = -VPMGSMALL;
02092
02093     /* Fill the "i" boundaries (dirichlet) */
02094     for (k=0; k<nzNEW; k++) {
02095         for (j=0; j<nyNEW; j++) {
02096             /* Low X face */
02097             x = xminNEW;
02098             y = yminNEW + j*hyNEW;
02099             z = zminNEW + k*hzNEW;
02100             if ((x >= (xminOLD-VSMALL)) && (y >= (yminOLD-VSMALL)) && (z >= (zminOLD-VSMALL)) &&
02101                 (x <= (xmaxOLD+VSMALL)) && (y <= (ymaxOLD+VSMALL)) && (z <= (zmaxOLD+VSMALL))) {
02102                 ifloat = (x - xminOLD)/hxOLD;
02103                 jfloat = (y - yminOLD)/hyOLD;
02104                 kfloat = (z - zminOLD)/hzOLD;
02105                 ihi = (int)ceil(ifloat);
02106                 if (ihi > (nxOLD-1)) ihi = nxOLD-1;
02107                 ilo = (int)floor(ifloat);
02108                 if (ilo < 0) ilo = 0;
02109                 jhi = (int)ceil(jfloat);
02110                 if (jhi > (nyOLD-1)) jhi = nyOLD-1;
02111                 jlo = (int)floor(jfloat);
02112                 if (jlo < 0) jlo = 0;
02113                 khi = (int)ceil(kfloat);
02114                 if (khi > (nzOLD-1)) khi = nzOLD-1;
02115                 klo = (int)floor(kfloat);

```

```

02116         if (klo < 0) klo = 0;
02117         dx = ifloat - (double)(ilo);
02118         dy = jfloat - (double)(jlo);
02119         dz = kfloat - (double)(klo);
02120         nx = nxOLD; ny = nyOLD; nz = nzOLD;
02121         uval = dx*dy*dz*(data[IJK(ihi,jhi,khi)])
02122         + dx*(1.0-dy)*dz*(data[IJK(ihi,jlo,khi)])
02123         + dx*dy*(1.0-dz)*(data[IJK(ihi,jhi,klo)])
02124         + dx*(1.0-dy)*(1.0-dz)*(data[IJK(ihi,jlo,klo)])
02125         + (1.0-dx)*dy*dz*(data[IJK(ilo,jhi,khi)])
02126         + (1.0-dx)*(1.0-dy)*dz*(data[IJK(ilo,jlo,khi)])
02127         + (1.0-dx)*dy*(1.0-dz)*(data[IJK(ilo,jhi,klo)])
02128         + (1.0-dx)*(1.0-dy)*(1.0-dz)*(data[IJK(ilo,jlo,klo)]);
02129         nx = nxNEW; ny = nyNEW; nz = nzNEW;
02130     } else {
02131         Vnm_print(2, "focusFillBound (%s, %d): Off old mesh at %g, %g \
02132             %g!\n", __FILE__, __LINE__, x, y, z);
02133         Vnm_print(2, "focusFillBound (%s, %d): old mesh lower corner at \
02134             %g %g %g.\n", __FILE__, __LINE__, xminOLD, yminOLD, zminOLD);
02135         Vnm_print(2, "focusFillBound (%s, %d): old mesh upper corner at \
02136             %g %g %g.\n", __FILE__, __LINE__, xmaxOLD, ymaxOLD, zmaxOLD);
02137         VASSERT(0);
02138     }
02139     nx = nxNEW; ny = nyNEW; nz = nzNEW;
02140     thee->gxpcf[IJKx(j,k,0)] = uval;
02141     if(uval < uvalMin) uvalMin = uval;
02142     if(uval > uvalMax) uvalMax = uval;
02143
02144     /* High X face */
02145     x = xmaxNEW;
02146     if ((x >= (xminOLD-VSMALL)) && (y >= (yminOLD-VSMALL)) && (z >= (zminOLD-VSMALL)) &&
02147         (x <= (xmaxOLD+VSMALL)) && (y <= (ymaxOLD+VSMALL)) && (z <= (zmaxOLD+VSMALL))) {
02148         ifloat = (x - xminOLD)/hxOLD;
02149         jfloat = (y - yminOLD)/hyOLD;
02150         kfloat = (z - zminOLD)/hzOLD;
02151         ihi = (int)ceil(ifloat);
02152         if (ihi > (nxOLD-1)) ihi = nxOLD-1;
02153         ilo = (int)floor(ifloat);
02154         if (ilo < 0) ilo = 0;
02155         jhi = (int)ceil(jfloat);
02156         if (jhi > (nyOLD-1)) jhi = nyOLD-1;
02157         jlo = (int)floor(jfloat);
02158         if (jlo < 0) jlo = 0;
02159         khi = (int)ceil(kfloat);
02160         if (khi > (nzOLD-1)) khi = nzOLD-1;
02161         klo = (int)floor(kfloat);
02162         if (klo < 0) klo = 0;
02163         dx = ifloat - (double)(ilo);
02164         dy = jfloat - (double)(jlo);
02165         dz = kfloat - (double)(klo);
02166         nx = nxOLD; ny = nyOLD; nz = nzOLD;
02167         uval = dx*dy*dz*(data[IJK(ihi,jhi,khi)])
02168         + dx*(1.0-dy)*dz*(data[IJK(ihi,jlo,khi)])
02169         + dx*dy*(1.0-dz)*(data[IJK(ihi,jhi,klo)])
02170         + dx*(1.0-dy)*(1.0-dz)*(data[IJK(ihi,jlo,klo)])
02171         + (1.0-dx)*dy*dz*(data[IJK(ilo,jhi,khi)])
02172         + (1.0-dx)*(1.0-dy)*dz*(data[IJK(ilo,jlo,khi)])
02173         + (1.0-dx)*dy*(1.0-dz)*(data[IJK(ilo,jhi,klo)])
02174         + (1.0-dx)*(1.0-dy)*(1.0-dz)*(data[IJK(ilo,jlo,klo)]);
02175         nx = nxNEW; ny = nyNEW; nz = nzNEW;
02176     } else {
02177         Vnm_print(2, "focusFillBound (%s, %d): Off old mesh at %g, %g \
02178             %g!\n", __FILE__, __LINE__, x, y, z);
02179         Vnm_print(2, "focusFillBound (%s, %d): old mesh lower corner at \
02180             %g %g %g.\n", __FILE__, __LINE__, xminOLD, yminOLD, zminOLD);
02181         Vnm_print(2, "focusFillBound (%s, %d): old mesh upper corner at \
02182             %g %g %g.\n", __FILE__, __LINE__, xmaxOLD, ymaxOLD, zmaxOLD);
02183         VASSERT(0);
02184     }
02185     nx = nxNEW; ny = nyNEW; nz = nzNEW;
02186     thee->gxpcf[IJKx(j,k,1)] = uval;
02187     if(uval < uvalMin) uvalMin = uval;
02188     if(uval > uvalMax) uvalMax = uval;
02189
02190     /* Zero Neumann conditions */
02191     nx = nxNEW; ny = nyNEW; nz = nzNEW;
02192     thee->gxpcf[IJKx(j,k,2)] = 0.0;
02193     nx = nxNEW; ny = nyNEW; nz = nzNEW;
02194     thee->gxpcf[IJKx(j,k,3)] = 0.0;
02195 }
02196 }

```

```

02197
02198 /* Fill the "j" boundaries (dirichlet) */
02199 for (k=0; k<nzNEW; k++) {
02200     for (i=0; i<nxNEW; i++) {
02201         /* Low Y face */
02202         x = xminNEW + i*hxNEW;
02203         y = yminNEW;
02204         z = zminNEW + k*hzNEW;
02205         if ((x >= (xminOLD-VSMALL)) && (y >= (yminOLD-VSMALL)) && (z >= (zminOLD-VSMALL)) &&
02206             (x <= (xmaxOLD+VSMALL)) && (y <= (ymaxOLD+VSMALL)) && (z <= (zmaxOLD+VSMALL))) {
02207             ifloat = (x - xminOLD)/hxOLD;
02208             jfloat = (y - yminOLD)/hyOLD;
02209             kfloat = (z - zminOLD)/hzOLD;
02210             ihi = (int)ceil(ifloat);
02211             if (ihi > (nxOLD-1)) ihi = nxOLD-1;
02212             ilo = (int)floor(ifloat);
02213             if (ilo < 0) ilo = 0;
02214             jhi = (int)ceil(jfloat);
02215             if (jhi > (nyOLD-1)) jhi = nyOLD-1;
02216             jlo = (int)floor(jfloat);
02217             if (jlo < 0) jlo = 0;
02218             khi = (int)ceil(kfloat);
02219             if (khi > (nzOLD-1)) khi = nzOLD-1;
02220             klo = (int)floor(kfloat);
02221             if (klo < 0) klo = 0;
02222             dx = ifloat - (double)(ilo);
02223             dy = jfloat - (double)(jlo);
02224             dz = kfloat - (double)(klo);
02225             nx = nxOLD; ny = nyOLD; nz = nzOLD;
02226             uval = dx*dy*dz*(data[IJK(ihi,jhi,khi)])
02227                 + dx*(1.0-dy)*dz*(data[IJK(ihi,jlo,khi)])
02228                 + dx*dy*(1.0-dz)*(data[IJK(ihi,jhi,klo)])
02229                 + dx*(1.0-dy)*(1.0-dz)*(data[IJK(ihi,jlo,klo)])
02230                 + (1.0-dx)*dy*dz*(data[IJK(ilo,jhi,khi)])
02231                 + (1.0-dx)*(1.0-dy)*dz*(data[IJK(ilo,jlo,khi)])
02232                 + (1.0-dx)*dy*(1.0-dz)*(data[IJK(ilo,jhi,klo)])
02233                 + (1.0-dx)*(1.0-dy)*(1.0-dz)*(data[IJK(ilo,jlo,klo)]);
02234             nx = nxNEW; ny = nyNEW; nz = nzNEW;
02235         } else {
02236             Vnm_print(2, "focusFillBound (%s, %d): Off old mesh at %g, %g \
02237                 %g!\n", __FILE__, __LINE__, x, y, z);
02238             Vnm_print(2, "focusFillBound (%s, %d): old mesh lower corner at \
02239                 %g %g %g.\n", __FILE__, __LINE__, xminOLD, yminOLD, zminOLD);
02240             Vnm_print(2, "focusFillBound (%s, %d): old mesh upper corner at \
02241                 %g %g %g.\n", __FILE__, __LINE__, xmaxOLD, ymaxOLD, zmaxOLD);
02242             VASSERT(0);
02243         }
02244         nx = nxNEW; ny = nyNEW; nz = nzNEW;
02245         thee->gycf[IJKy(i,k,0)] = uval;
02246         if(uval < uvalMin) uvalMin = uval;
02247         if(uval > uvalMax) uvalMax = uval;
02248
02249         /* High Y face */
02250         y = ymaxNEW;
02251         if ((x >= (xminOLD-VSMALL)) && (y >= (yminOLD-VSMALL)) && (z >= (zminOLD-VSMALL)) &&
02252             (x <= (xmaxOLD+VSMALL)) && (y <= (ymaxOLD+VSMALL)) && (z <= (zmaxOLD+VSMALL))) {
02253             ifloat = (x - xminOLD)/hxOLD;
02254             jfloat = (y - yminOLD)/hyOLD;
02255             kfloat = (z - zminOLD)/hzOLD;
02256             ihi = (int)ceil(ifloat);
02257             if (ihi > (nxOLD-1)) ihi = nxOLD-1;
02258             ilo = (int)floor(ifloat);
02259             if (ilo < 0) ilo = 0;
02260             jhi = (int)ceil(jfloat);
02261             if (jhi > (nyOLD-1)) jhi = nyOLD-1;
02262             jlo = (int)floor(jfloat);
02263             if (jlo < 0) jlo = 0;
02264             khi = (int)ceil(kfloat);
02265             if (khi > (nzOLD-1)) khi = nzOLD-1;
02266             klo = (int)floor(kfloat);
02267             if (klo < 0) klo = 0;
02268             dx = ifloat - (double)(ilo);
02269             dy = jfloat - (double)(jlo);
02270             dz = kfloat - (double)(klo);
02271             nx = nxOLD; ny = nyOLD; nz = nzOLD;
02272             uval = dx*dy*dz*(data[IJK(ihi,jhi,khi)])
02273                 + dx*(1.0-dy)*dz*(data[IJK(ihi,jlo,khi)])
02274                 + dx*dy*(1.0-dz)*(data[IJK(ihi,jhi,klo)])
02275                 + dx*(1.0-dy)*(1.0-dz)*(data[IJK(ihi,jlo,klo)])
02276                 + (1.0-dx)*dy*dz*(data[IJK(ilo,jhi,khi)])
02277                 + (1.0-dx)*(1.0-dy)*dz*(data[IJK(ilo,jlo,khi)])

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```

02278         + (1.0-dx)*dy*(1.0-dz)*(data[IJK(ilo,jhi,klo)])
02279         + (1.0-dx)*(1.0-dy)*(1.0-dz)*(data[IJK(ilo,jlo,klo)]);
02280         nx = nxNEW; ny = nyNEW; nz = nzNEW;
02281     } else {
02282         Vnm_print(2, "focusFillBound (%s, %d): Off old mesh at %g, %g \
02283             %g!\n", __FILE__, __LINE__, x, y, z);
02284         Vnm_print(2, "focusFillBound (%s, %d): old mesh lower corner at \
02285             %g %g %g.\n", __FILE__, __LINE__, xminOLD, yminOLD, zminOLD);
02286         Vnm_print(2, "focusFillBound (%s, %d): old mesh upper corner at \
02287             %g %g %g.\n", __FILE__, __LINE__, xmaxOLD, ymaxOLD, zmaxOLD);
02288         VASSERT(0);
02289     }
02290     nx = nxNEW; ny = nyNEW; nz = nzNEW;
02291     thee->gycf[IJKy(i,k,1)] = uval;
02292     if(uval < uvalMin) uvalMin = uval;
02293     if(uval > uvalMax) uvalMax = uval;
02294
02295     /* Zero Neumann conditions */
02296     nx = nxNEW; ny = nyNEW; nz = nzNEW;
02297     thee->gycf[IJKy(i,k,2)] = 0.0;
02298     nx = nxNEW; ny = nyNEW; nz = nzNEW;
02299     thee->gycf[IJKy(i,k,3)] = 0.0;
02300 }
02301 }
02302
02303 /* Fill the "k" boundaries (dirichlet) */
02304 for (j=0; j<nyNEW; j++) {
02305     for (i=0; i<nxNEW; i++) {
02306         /* Low Z face */
02307         x = xminNEW + i*hxNEW;
02308         y = yminNEW + j*hyNEW;
02309         z = zminNEW;
02310         if ((x >= (xminOLD-VSMALL)) && (y >= (yminOLD-VSMALL)) && (z >= (zminOLD-VSMALL)) &&
02311             (x <= (xmaxOLD+VSMALL)) && (y <= (ymaxOLD+VSMALL)) && (z <= (zmaxOLD+VSMALL))) {
02312             ifloat = (x - xminOLD)/hxOLD;
02313             jfloat = (y - yminOLD)/hyOLD;
02314             kfloat = (z - zminOLD)/hzOLD;
02315             ihi = (int)ceil(ifloat);
02316             if (ihi > (nxOLD-1)) ihi = nxOLD-1;
02317             ilo = (int)floor(ifloat);
02318             if (ilo < 0) ilo = 0;
02319             jhi = (int)ceil(jfloat);
02320             if (jhi > (nyOLD-1)) jhi = nyOLD-1;
02321             jlo = (int)floor(jfloat);
02322             if (jlo < 0) jlo = 0;
02323             khi = (int)ceil(kfloat);
02324             if (khi > (nzOLD-1)) khi = nzOLD-1;
02325             klo = (int)floor(kfloat);
02326             if (klo < 0) klo = 0;
02327             dx = ifloat - (double)(ilo);
02328             dy = jfloat - (double)(jlo);
02329             dz = kfloat - (double)(klo);
02330             nx = nxOLD; ny = nyOLD; nz = nzOLD;
02331             uval = dx*dy*dz*(data[IJK(ihi,jhi,khi)])
02332             + dx*(1.0-dy)*dz*(data[IJK(ihi,jlo,khi)])
02333             + dx*dy*(1.0-dz)*(data[IJK(ihi,jhi,klo)])
02334             + dx*(1.0-dy)*(1.0-dz)*(data[IJK(ihi,jlo,klo)])
02335             + (1.0-dx)*dy*dz*(data[IJK(ilo,jhi,khi)])
02336             + (1.0-dx)*(1.0-dy)*dz*(data[IJK(ilo,jlo,khi)])
02337             + (1.0-dx)*dy*(1.0-dz)*(data[IJK(ilo,jhi,klo)])
02338             + (1.0-dx)*(1.0-dy)*(1.0-dz)*(data[IJK(ilo,jlo,klo)]);
02339             nx = nxNEW; ny = nyNEW; nz = nzNEW;
02340         } else {
02341             Vnm_print(2, "focusFillBound (%s, %d): Off old mesh at %g, %g \
02342                 %g!\n", __FILE__, __LINE__, x, y, z);
02343             Vnm_print(2, "focusFillBound (%s, %d): old mesh lower corner at \
02344                 %g %g %g.\n", __FILE__, __LINE__, xminOLD, yminOLD, zminOLD);
02345             Vnm_print(2, "focusFillBound (%s, %d): old mesh upper corner at \
02346                 %g %g %g.\n", __FILE__, __LINE__, xmaxOLD, ymaxOLD, zmaxOLD);
02347             VASSERT(0);
02348         }
02349         nx = nxNEW; ny = nyNEW; nz = nzNEW;
02350         thee->gzcf[IJKz(i,j,0)] = uval;
02351         if(uval < uvalMin) uvalMin = uval;
02352         if(uval > uvalMax) uvalMax = uval;
02353
02354         /* High Z face */
02355         z = zmaxNEW;
02356         if ((x >= (xminOLD-VSMALL)) && (y >= (yminOLD-VSMALL)) && (z >= (zminOLD-VSMALL)) &&
02357             (x <= (xmaxOLD+VSMALL)) && (y <= (ymaxOLD+VSMALL)) && (z <= (zmaxOLD+VSMALL))) {
02358             ifloat = (x - xminOLD)/hxOLD;

```

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02359         jfloat = (y - yminOLD)/hyOLD;
02360         kfloat = (z - zminOLD)/hzOLD;
02361         ihi = (int)ceil(ifloat);
02362         if (ihi > (nxOLD-1)) ihi = nxOLD-1;
02363         ilo = (int)floor(ifloat);
02364         if (ilo < 0) ilo = 0;
02365         jhi = (int)ceil(jfloat);
02366         if (jhi > (nyOLD-1)) jhi = nyOLD-1;
02367         jlo = (int)floor(jfloat);
02368         if (jlo < 0) jlo = 0;
02369         khi = (int)ceil(kfloat);
02370         if (khi > (nzOLD-1)) khi = nzOLD-1;
02371         klo = (int)floor(kfloat);
02372         if (klo < 0) klo = 0;
02373         dx = ifloat - (double)(ilo);
02374         dy = jfloat - (double)(jlo);
02375         dz = kfloat - (double)(klo);
02376         nx = nxOLD; ny = nyOLD; nz = nzOLD;
02377         uval = dx*dy*dz*(data[IJK(ihi,jhi,khi)])
02378         + dx*(1.0-dy)*dz*(data[IJK(ihi,jlo,khi)])
02379         + dx*dy*(1.0-dz)*(data[IJK(ihi,jhi,klo)])
02380         + dx*(1.0-dy)*(1.0-dz)*(data[IJK(ihi,jlo,klo)])
02381         + (1.0-dx)*dy*dz*(data[IJK(ilo,jhi,khi)])
02382         + (1.0-dx)*(1.0-dy)*dz*(data[IJK(ilo,jlo,khi)])
02383         + (1.0-dx)*dy*(1.0-dz)*(data[IJK(ilo,jhi,klo)])
02384         + (1.0-dx)*(1.0-dy)*(1.0-dz)*(data[IJK(ilo,jlo,klo)]);
02385         nx = nxNEW; ny = nyNEW; nz = nzNEW;
02386     } else {
02387         Vnm_print(2, "focusFillBound (%s, %d): Off old mesh at %g, %g \
02388             %g!\n", __FILE__, __LINE__, x, y, z);
02389         Vnm_print(2, "focusFillBound (%s, %d): old mesh lower corner at \
02390             %g %g %g.\n", __FILE__, __LINE__, xminOLD, yminOLD, zminOLD);
02391         Vnm_print(2, "focusFillBound (%s, %d): old mesh upper corner at \
02392             %g %g %g.\n", __FILE__, __LINE__, xmaxOLD, ymaxOLD, zmaxOLD);
02393         VASSERT(0);
02394     }
02395     nx = nxNEW; ny = nyNEW; nz = nzNEW;
02396     thee->gzcf[IJKz(i,j,1)] = uval;
02397     if(uval < uvalMin) uvalMin = uval;
02398     if(uval > uvalMax) uvalMax = uval;
02399
02400     /* Zero Neumann conditions */
02401     nx = nxNEW; ny = nyNEW; nz = nzNEW;
02402     thee->gzcf[IJKz(i,j,2)] = 0.0;
02403     nx = nxNEW; ny = nyNEW; nz = nzNEW;
02404     thee->gzcf[IJKz(i,j,3)] = 0.0;
02405 }
02406 }
02407
02408 VWARN_MSG0 (
02409     uvalMin >= SINH_MIN && uvalMax <= SINH_MAX,
02410     "Unusually large potential values\n"
02411     "    detected on the focusing boundary!\n"
02412     "    Convergence not guaranteed for NPBE/NRPBE calculations!"
02413 );
02414 }
02415
02416 VPRIVATE void extEnergy(Vpmg *thee, Vpmg *pmgOLD, PBEparm_calcEnergy extFlag,
02417     double partMin[3], double partMax[3], int bflags[6]) {
02418
02419     Vatom *atom;
02420     double hxNEW, hyNEW, hzNEW;
02421     double lowerCorner[3], upperCorner[3];
02422     int nxNEW, nyNEW, nzNEW;
02423     int nxOLD, nyOLD, nzOLD;
02424     int i,j,k;
02425     double xmin, xmax, ymin, ymax, zmin, zmax;
02426     double hxOLD, hyOLD, hzOLD;
02427     double xval, yval, zval;
02428     double x,y,z;
02429     int nx, ny, nz;
02430
02431     /* Set the new external energy contribution to zero. Any external
02432      * contributions from higher levels will be included in the appropriate
02433      * energy function call. */
02434     thee->extQmEnergy = 0;
02435     thee->extQfEnergy = 0;
02436     thee->extDiEnergy = 0;
02437
02438     /* New problem dimensions */
02439     hxNEW = thee->pmgp->hx;

```

```

02440     hyNEW = thee->pmgp->hy;
02441     hzNEW = thee->pmgp->hz;
02442     nxNEW = thee->pmgp->nx;
02443     nyNEW = thee->pmgp->ny;
02444     nzNEW = thee->pmgp->nz;
02445     lowerCorner[0] = thee->pmgp->xcent - ((double) (nxNEW-1)*hxNEW)/2.0;
02446     upperCorner[0] = thee->pmgp->xcent + ((double) (nxNEW-1)*hxNEW)/2.0;
02447     lowerCorner[1] = thee->pmgp->ycent - ((double) (nyNEW-1)*hyNEW)/2.0;
02448     upperCorner[1] = thee->pmgp->ycent + ((double) (nyNEW-1)*hyNEW)/2.0;
02449     lowerCorner[2] = thee->pmgp->zcent - ((double) (nzNEW-1)*hzNEW)/2.0;
02450     upperCorner[2] = thee->pmgp->zcent + ((double) (nzNEW-1)*hzNEW)/2.0;
02451
02452     Vnm_print(0, "VPMG::extEnergy:  energy flag = %d\n", extFlag);
02453
02454     /* Old problem dimensions */
02455     nxOLD = pmgOLD->pmgp->nx;
02456     nyOLD = pmgOLD->pmgp->ny;
02457     nzOLD = pmgOLD->pmgp->nz;
02458
02459     /* Create a partition based on the new problem dimensions */
02460     /* Vnm_print(1, "DEBUG (%s, %d):  extEnergy calling Vpmg_setPart for old PMG.\n",
02461        __FILE__, __LINE__); */
02462     Vpmg_setPart(pmgOLD, lowerCorner, upperCorner, bflags);
02463
02464
02465     Vnm_print(0, "VPMG::extEnergy:  Finding extEnergy dimensions...\n");
02466     Vnm_print(0, "VPMG::extEnergy  Disj part lower corner = (%g, %g, %g)\n",
02467        partMin[0], partMin[1], partMin[2]);
02468     Vnm_print(0, "VPMG::extEnergy  Disj part upper corner = (%g, %g, %g)\n",
02469        partMax[0], partMax[1], partMax[2]);
02470
02471     /* Find the old dimensions */
02472
02473     hxOLD = pmgOLD->pmgp->hx;
02474     hyOLD = pmgOLD->pmgp->hy;
02475     hzOLD = pmgOLD->pmgp->hz;
02476     xmin = pmgOLD->pmgp->xcent - 0.5*hxOLD*(nxOLD-1);
02477     ymin = pmgOLD->pmgp->ycent - 0.5*hyOLD*(nyOLD-1);
02478     zmin = pmgOLD->pmgp->zcent - 0.5*hzOLD*(nzOLD-1);
02479     xmax = xmin+hxOLD*(nxOLD-1);
02480     ymax = ymin+hyOLD*(nyOLD-1);
02481     zmax = zmin+hzOLD*(nzOLD-1);
02482
02483     Vnm_print(0, "VPMG::extEnergy  Old lower corner = (%g, %g, %g)\n",
02484        xmin, ymin, zmin);
02485     Vnm_print(0, "VPMG::extEnergy  Old upper corner = (%g, %g, %g)\n",
02486        xmax, ymax, zmax);
02487
02488     /* Flip the partition, but do not include any points that will
02489        be included by another processor */
02490
02491     nx = nxOLD;
02492     ny = nyOLD;
02493     nz = nzOLD;
02494
02495     for(i=0; i<nx; i++) {
02496         xval = 1;
02497         x = i*hxOLD + xmin;
02498         if (x < partMin[0] && bflags[VAPBS_LEFT] == 1) xval = 0;
02499         else if (x > partMax[0] && bflags[VAPBS_RIGHT] == 1) xval = 0;
02500
02501         for(j=0; j<ny; j++) {
02502             yval = 1;
02503             y = j*hyOLD + ymin;
02504             if (y < partMin[1] && bflags[VAPBS_BACK] == 1) yval = 0;
02505             else if (y > partMax[1] && bflags[VAPBS_FRONT] == 1) yval = 0;
02506
02507             for(k=0; k<nz; k++) {
02508                 zval = 1;
02509                 z = k*hzOLD + zmin;
02510                 if (z < partMin[2] && bflags[VAPBS_DOWN] == 1) zval = 0;
02511                 else if (z > partMax[2] && bflags[VAPBS_UP] == 1) zval = 0;
02512
02513                 if (pmgOLD->pvec[IJK(i, j, k)] > VSMALL) pmgOLD->pvec[IJK(i, j, k)] = 1.0;
02514                 pmgOLD->pvec[IJK(i, j, k)] = (1 - (pmgOLD->pvec[IJK(i, j, k)])) * (xval*yval*zval);
02515             }
02516         }
02517     }
02518
02519     for (i=0; i<Valist_getNumberAtoms(thee->pbe->alist); i++) {
02520         xval=1;

```

```

02521     yval=1;
02522     zval=1;
02523     atom = Valist_getAtom(thee->pbe->alist, i);
02524     x = atom->position[0];
02525     y = atom->position[1];
02526     z = atom->position[2];
02527     if (x < partMin[0] && bflags[VAPBS_LEFT] == 1) xval = 0;
02528     else if (x > partMax[0] && bflags[VAPBS_RIGHT] == 1) xval = 0;
02529     if (y < partMin[1] && bflags[VAPBS_BACK] == 1) yval = 0;
02530     else if (y > partMax[1] && bflags[VAPBS_FRONT] == 1) yval = 0;
02531     if (z < partMin[2] && bflags[VAPBS_DOWN] == 1) zval = 0;
02532     else if (z > partMax[2] && bflags[VAPBS_UP] == 1) zval = 0;
02533     if (atom->partID > VSMALL) atom->partID = 1.0;
02534     atom->partID = (1 - atom->partID) * (xval*yval*zval);
02535 }
02536
02537 /* Now calculate the energy on inverted subset of the domain */
02538 thee->extQmEnergy = Vpmg_qmEnergy(pmgOLD, 1);
02539 Vnm_print(0, "VPMG::extEnergy: extQmEnergy = %g kT\n", thee->extQmEnergy);
02540 thee->extQfEnergy = Vpmg_qfEnergy(pmgOLD, 1);
02541 Vnm_print(0, "VPMG::extEnergy: extQfEnergy = %g kT\n", thee->extQfEnergy);
02542 thee->extDiEnergy = Vpmg_dielEnergy(pmgOLD, 1);
02543 Vnm_print(0, "VPMG::extEnergy: extDiEnergy = %g kT\n", thee->extDiEnergy);
02544 Vpmg_unsetPart(pmgOLD);
02545 }
02546
02547 VPRIVATE double bcfllsp(double size, double *apos, double charge,
02548     double xkappa, double prel, double *pos) {
02549
02550     double dist, val;
02551
02552     dist = VSQRT(VSQR(pos[0]-apos[0]) + VSQR(pos[1]-apos[1])
02553         + VSQR(pos[2]-apos[2]));
02554     if (xkappa > VSMALL) {
02555         val = prel*(charge/dist)*VEXP(-xkappa*(dist-size))
02556             / (1+xkappa*size);
02557     } else {
02558         val = prel*(charge/dist);
02559     }
02560
02561     return val;
02562 }
02563
02564 VPRIVATE void bcfll(double size, double *apos, double charge,
02565     double xkappa, double prel, double *gxcf, double *gycf, double *gzcf,
02566     double *xf, double *yf, double *zf, int nx, int ny, int nz) {
02567
02568     int i, j, k;
02569     double dist, val;
02570     double gpos[3];
02571
02572     /* the "i" boundaries (dirichlet) */
02573     for (k=0; k<nz; k++) {
02574         gpos[2] = zf[k];
02575         for (j=0; j<ny; j++) {
02576             gpos[1] = yf[j];
02577             gpos[0] = xf[0];
02578             dist = VSQRT(VSQR(gpos[0]-apos[0]) + VSQR(gpos[1]-apos[1])
02579                 + VSQR(gpos[2]-apos[2]));
02580             if (xkappa > VSMALL) {
02581                 val = prel*(charge/dist)*VEXP(-xkappa*(dist-size))
02582                     / (1+xkappa*size);
02583             } else {
02584                 val = prel*(charge/dist);
02585             }
02586             gxcf[IJKx(j,k,0)] += val;
02587             gpos[0] = xf[nx-1];
02588             dist = VSQRT(VSQR(gpos[0]-apos[0]) + VSQR(gpos[1]-apos[1])
02589                 + VSQR(gpos[2]-apos[2]));
02590             if (xkappa > VSMALL) {
02591                 val = prel*(charge/dist)*VEXP(-xkappa*(dist-size))
02592                     / (1+xkappa*size);
02593             } else {
02594                 val = prel*(charge/dist);
02595             }
02596             gxcf[IJKx(j,k,1)] += val;
02597         }
02598     }
02599
02600     /* the "j" boundaries (dirichlet) */
02601     for (k=0; k<nz; k++) {

```

```

02602     gpos[2] = zf[k];
02603     for (i=0; i<nx; i++) {
02604         gpos[0] = xf[i];
02605         gpos[1] = yf[0];
02606         dist = VSQRT(VSQR(gpos[0]-apos[0]) + VSQR(gpos[1]-apos[1])
02607                     + VSQR(gpos[2]-apos[2]));
02608         if (xkappa > VSMALL) {
02609             val = pre1*(charge/dist)*VEXP(-xkappa*(dist-size))
02610                 / (1+xkappa*size);
02611         } else {
02612             val = pre1*(charge/dist);
02613         }
02614         gycf[IJKy(i,k,0)] += val;
02615         gpos[1] = yf[ny-1];
02616         dist = VSQRT(VSQR(gpos[0]-apos[0]) + VSQR(gpos[1]-apos[1])
02617                     + VSQR(gpos[2]-apos[2]));
02618         if (xkappa > VSMALL) {
02619             val = pre1*(charge/dist)*VEXP(-xkappa*(dist-size))
02620                 / (1+xkappa*size);
02621         } else {
02622             val = pre1*(charge/dist);
02623         }
02624         gycf[IJKy(i,k,1)] += val;
02625     }
02626 }
02627
02628 /* the "k" boundaries (dirichlet) */
02629 for (j=0; j<ny; j++) {
02630     gpos[1] = yf[j];
02631     for (i=0; i<nx; i++) {
02632         gpos[0] = xf[i];
02633         gpos[2] = zf[0];
02634         dist = VSQRT(VSQR(gpos[0]-apos[0]) + VSQR(gpos[1]-apos[1])
02635                     + VSQR(gpos[2]-apos[2]));
02636         if (xkappa > VSMALL) {
02637             val = pre1*(charge/dist)*VEXP(-xkappa*(dist-size))
02638                 / (1+xkappa*size);
02639         } else {
02640             val = pre1*(charge/dist);
02641         }
02642         gzcfc[IJKz(i,j,0)] += val;
02643         gpos[2] = zf[nz-1];
02644         dist = VSQRT(VSQR(gpos[0]-apos[0]) + VSQR(gpos[1]-apos[1])
02645                     + VSQR(gpos[2]-apos[2]));
02646         if (xkappa > VSMALL) {
02647             val = pre1*(charge/dist)*VEXP(-xkappa*(dist-size))
02648                 / (1+xkappa*size);
02649         } else {
02650             val = pre1*(charge/dist);
02651         }
02652         gzcfc[IJKz(i,j,1)] += val;
02653     }
02654 }
02655 }
02656
02657 VPRIVATE void bcf12(double size, double *apos,
02658                   double charge, double *dipole, double *quad,
02659                   double xkappa, double eps_p, double eps_w, double T,
02660                   double *gxcf, double *gycf, double *gzcfc,
02661                   double *xf, double *yf, double *zf,
02662                   int nx, int ny, int nz) {
02663
02664     int i, j, k;
02665     double val;
02666     double gpos[3], tensor[3];
02667     double ux, uy, uz, xr, yr, zr;
02668     double qxx, qxy, qxz, qyx, qyy, qyz, qzx, qzy, qzz;
02669     double dist, pre;
02670
02671     VASSERT(dipole != VNULL);
02672     ux = dipole[0];
02673     uy = dipole[1];
02674     uz = dipole[2];
02675     if (quad != VNULL) {
02676         /* The factor of 1/3 results from using a
02677          traceless quadrupole definition. See, for example,
02678          "The Theory of Intermolecular Forces" by A.J. Stone,
02679          Chapter 3. */
02680         qxx = quad[0] / 3.0;
02681         qxy = quad[1] / 3.0;
02682         qxz = quad[2] / 3.0;

```



```

02683     qyx = quad[3] / 3.0;
02684     qyy = quad[4] / 3.0;
02685     qyz = quad[5] / 3.0;
02686     qzx = quad[6] / 3.0;
02687     qzy = quad[7] / 3.0;
02688     qzz = quad[8] / 3.0;
02689 } else {
02690     qxx = 0.0;
02691     qxy = 0.0;
02692     qxz = 0.0;
02693     qyx = 0.0;
02694     qyy = 0.0;
02695     qyz = 0.0;
02696     qzx = 0.0;
02697     qzy = 0.0;
02698     qzz = 0.0;
02699 }
02700
02701 pre = (Vunit_ec*Vunit_ec)/(4*VPI*Vunit_eps0*Vunit_kb*T);
02702 pre = pre*(1.0e10);
02703
02704 /* the "i" boundaries (dirichlet) */
02705 for (k=0; k<nz; k++) {
02706     gpos[2] = zf[k];
02707     for (j=0; j<ny; j++) {
02708         gpos[1] = yf[j];
02709         gpos[0] = xf[0];
02710         xr = gpos[0] - apos[0];
02711         yr = gpos[1] - apos[1];
02712         zr = gpos[2] - apos[2];
02713         dist = VSQRT(VSQR(xr) + VSQR(yr) + VSQR(zr));
02714         multipolebc(dist, xkappa, eps_p, eps_w, size, tensor);
02715         val = pre*charge*tensor[0];
02716         val -= pre*ux*xr*tensor[1];
02717         val -= pre*uy*yr*tensor[1];
02718         val -= pre*uz*zr*tensor[1];
02719         val += pre*qxx*xr*xr*tensor[2];
02720         val += pre*qyy*yr*yr*tensor[2];
02721         val += pre*qzz*zr*zr*tensor[2];
02722         val += pre*2.0*qxy*xr*yr*tensor[2];
02723         val += pre*2.0*qxz*xr*zr*tensor[2];
02724         val += pre*2.0*qyz*yr*zr*tensor[2];
02725         gxcf[IJKx(j,k,0)] += val;
02726
02727         gpos[0] = xf[nx-1];
02728         xr = gpos[0] - apos[0];
02729         dist = VSQRT(VSQR(xr) + VSQR(yr) + VSQR(zr));
02730         multipolebc(dist, xkappa, eps_p, eps_w, size, tensor);
02731         val = pre*charge*tensor[0];
02732         val -= pre*ux*xr*tensor[1];
02733         val -= pre*uy*yr*tensor[1];
02734         val -= pre*uz*zr*tensor[1];
02735         val += pre*qxx*xr*xr*tensor[2];
02736         val += pre*qyy*yr*yr*tensor[2];
02737         val += pre*qzz*zr*zr*tensor[2];
02738         val += pre*2.0*qxy*xr*yr*tensor[2];
02739         val += pre*2.0*qxz*xr*zr*tensor[2];
02740         val += pre*2.0*qyz*yr*zr*tensor[2];
02741         gxcf[IJKx(j,k,1)] += val;
02742     }
02743 }
02744
02745 /* the "j" boundaries (dirichlet) */
02746 for (k=0; k<nz; k++) {
02747     gpos[2] = zf[k];
02748     for (i=0; i<nx; i++) {
02749         gpos[0] = xf[i];
02750         gpos[1] = yf[0];
02751         xr = gpos[0] - apos[0];
02752         yr = gpos[1] - apos[1];
02753         zr = gpos[2] - apos[2];
02754         dist = VSQRT(VSQR(xr) + VSQR(yr) + VSQR(zr));
02755         multipolebc(dist, xkappa, eps_p, eps_w, size, tensor);
02756         val = pre*charge*tensor[0];
02757         val -= pre*ux*xr*tensor[1];
02758         val -= pre*uy*yr*tensor[1];
02759         val -= pre*uz*zr*tensor[1];
02760         val += pre*qxx*xr*xr*tensor[2];
02761         val += pre*qyy*yr*yr*tensor[2];
02762         val += pre*qzz*zr*zr*tensor[2];
02763         val += pre*2.0*qxy*xr*yr*tensor[2];

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02764         val += pre*2.0*qxz*xr*zr*tensor[2];
02765         val += pre*2.0*qyz*yr*zr*tensor[2];
02766         gycf[IJKy(i,k,0)] += val;
02767
02768         gpos[1] = yf[ny-1];
02769         yr = gpos[1] - apos[1];
02770         dist = VSQRT(VSQR(xr) + VSQR(yr) + VSQR(zr));
02771         multipolebc(dist, xkappa, eps_p, eps_w, size, tensor);
02772         val = pre*charge*tensor[0];
02773         val -= pre*ux*xr*tensor[1];
02774         val -= pre*uy*yr*tensor[1];
02775         val -= pre*uz*zr*tensor[1];
02776         val += pre*qxx*xr*xr*tensor[2];
02777         val += pre*qyy*yr*yr*tensor[2];
02778         val += pre*qzz*zr*zr*tensor[2];
02779         val += pre*2.0*qxy*xr*yr*tensor[2];
02780         val += pre*2.0*qxz*xr*zr*tensor[2];
02781         val += pre*2.0*qyz*yr*zr*tensor[2];
02782         gycf[IJKy(i,k,1)] += val;
02783     }
02784 }
02785
02786 /* the "k" boundaries (dirichlet) */
02787 for (j=0; j<ny; j++) {
02788     gpos[1] = yf[j];
02789     for (i=0; i<nx; i++) {
02790         gpos[0] = xf[i];
02791         gpos[2] = zf[0];
02792         xr = gpos[0] - apos[0];
02793         yr = gpos[1] - apos[1];
02794         zr = gpos[2] - apos[2];
02795         dist = VSQRT(VSQR(xr) + VSQR(yr) + VSQR(zr));
02796         multipolebc(dist, xkappa, eps_p, eps_w, size, tensor);
02797         val = pre*charge*tensor[0];
02798         val -= pre*ux*xr*tensor[1];
02799         val -= pre*uy*yr*tensor[1];
02800         val -= pre*uz*zr*tensor[1];
02801         val += pre*qxx*xr*xr*tensor[2];
02802         val += pre*qyy*yr*yr*tensor[2];
02803         val += pre*qzz*zr*zr*tensor[2];
02804         val += pre*2.0*qxy*xr*yr*tensor[2];
02805         val += pre*2.0*qxz*xr*zr*tensor[2];
02806         val += pre*2.0*qyz*yr*zr*tensor[2];
02807         gzcfc[IJKz(i,j,0)] += val;
02808
02809         gpos[2] = zf[nz-1];
02810         zr = gpos[2] - apos[2];
02811         dist = VSQRT(VSQR(xr) + VSQR(yr) + VSQR(zr));
02812         multipolebc(dist, xkappa, eps_p, eps_w, size, tensor);
02813         val = pre*charge*tensor[0];
02814         val -= pre*ux*xr*tensor[1];
02815         val -= pre*uy*yr*tensor[1];
02816         val -= pre*uz*zr*tensor[1];
02817         val += pre*qxx*xr*xr*tensor[2];
02818         val += pre*qyy*yr*yr*tensor[2];
02819         val += pre*qzz*zr*zr*tensor[2];
02820         val += pre*2.0*qxy*xr*yr*tensor[2];
02821         val += pre*2.0*qxz*xr*zr*tensor[2];
02822         val += pre*2.0*qyz*yr*zr*tensor[2];
02823         gzcfc[IJKz(i,j,1)] += val;
02824     }
02825 }
02826 }
02827
02828 VPRIVATE void bcCalcOrig(Vpmg *three) {
02829
02830     int nx, ny, nz;
02831     double size, *position, charge, xkappa, eps_w, T, prel;
02832     double *dipole, *quadrupole, debye, eps_p;
02833     double xr, yr, zr, qave, *apos;
02834     double sdhcharge, sdhdipole[3], traced[9], sdhquadrupole[9];
02835     int i, j, k, iatom;
02836     Vpbe *pbe;
02837     Vatom *atom;
02838     Valist *alist;
02839
02840     pbe = three->pbe;
02841     alist = three->pbe->alist;
02842     nx = three->pmgp->nx;
02843     ny = three->pmgp->ny;
02844     nz = three->pmgp->nz;

```

```

02845
02846 /* Zero out the boundaries */
02847 /* the "i" boundaries (dirichlet) */
02848 for (k=0; k<nz; k++) {
02849     for (j=0; j<ny; j++) {
02850         thee->gxcf[IJKx(j,k,0)] = 0.0;
02851         thee->gxcf[IJKx(j,k,1)] = 0.0;
02852         thee->gxcf[IJKx(j,k,2)] = 0.0;
02853         thee->gxcf[IJKx(j,k,3)] = 0.0;
02854     }
02855 }
02856
02857 /* the "j" boundaries (dirichlet) */
02858 for (k=0; k<nz; k++) {
02859     for (i=0; i<nx; i++) {
02860         thee->gyxf[IJKy(i,k,0)] = 0.0;
02861         thee->gyxf[IJKy(i,k,1)] = 0.0;
02862         thee->gyxf[IJKy(i,k,2)] = 0.0;
02863         thee->gyxf[IJKy(i,k,3)] = 0.0;
02864     }
02865 }
02866
02867 /* the "k" boundaries (dirichlet) */
02868 for (j=0; j<ny; j++) {
02869     for (i=0; i<nx; i++) {
02870         thee->gzcf[IJKz(i,j,0)] = 0.0;
02871         thee->gzcf[IJKz(i,j,1)] = 0.0;
02872         thee->gzcf[IJKz(i,j,2)] = 0.0;
02873         thee->gzcf[IJKz(i,j,3)] = 0.0;
02874     }
02875 }
02876
02877 /* For each "atom" (only one for bcfl=1), we use the following formula to
02878 * calculate the boundary conditions:
02879 *  $g(x) = \frac{q}{4\pi\epsilon_0\epsilon_w k_b T} \frac{\exp(-\kappa(d-a))}{1+\kappa a}$ 
02880 *  $\frac{1}{d}$ 
02881 * where  $d = ||x - x_0||$  (in m) and  $a$  is the size of the atom (in m).
02882 * We only need to evaluate some of these prefactors once:
02883 *  $prel = \frac{q}{4\pi\epsilon_0\epsilon_w k_b T}$ 
02884 * which gives the potential as
02885 *  $g(x) = prel * q/d * \frac{\exp(-\kappa(d-a))}{1+\kappa a}$ 
02886 */
02887 eps_w = Vpbe_getSolventDiel(pbe); /* Dimensionless */
02888 eps_p = Vpbe_getSoluteDiel(pbe); /* Dimensionless */
02889 T = Vpbe_getTemperature(pbe); /* K */
02890 prel = (Vunit_ec)/(4*VPI*Vunit_eps0*eps_w*Vunit_kb*T);
02891
02892 /* Finally, if we convert keep  $\kappa$  in  $\text{\AA}^{-1}$  and scale  $prel$  by
02893 * m/ $\text{\AA}$ , then we will only need to deal with distances and sizes in
02894 * Angstroms rather than meters. */
02895
02896  $\kappa$  = Vpbe_getXkappa(pbe); /*  $\text{\AA}^{-1}$  */
02897 prel = prel*(1.0e10);
02898
02899 switch (thee->pmgp->bcfl) {
02900     /* If we have zero boundary conditions, we're done */
02901     case BCFL_ZERO:
02902         return;
02903
02904     /* For single DH sphere BC's, we only have one "atom" to deal with;
02905     * get its information and */
02906     case BCFL_SDH:
02907         size = Vpbe_getSoluteRadius(pbe);
02908         position = Vpbe_getSoluteCenter(pbe);
02909
02910     /*
02911     For AMOEBA SDH boundary conditions, we need to find the
02912     total monopole, dipole and traceless quadrupole moments
02913     of either the permanent multipoles, induced dipoles or
02914     non-local induced dipoles.
02915     */
02916
02917     sdhcharge = 0.0;
02918     for (i=0; i<3; i++) sdhdipole[i] = 0.0;
02919     for (i=0; i<9; i++) sdhquadrupole[i] = 0.0;
02920
02921     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
02922         atom = Valist_getAtom(alist, iatom);
02923         apos = Vatom_getPosition(atom);
02924         xr = apos[0] - position[0];
02925         yr = apos[1] - position[1];

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02926         zr = apos[2] - position[2];
02927         switch (three->chargeSrc) {
02928             case VCM_CHARGE:
02929                 charge = Vatom_getCharge(atom);
02930                 sdhcharge += charge;
02931                 sdhdipole[0] += xr * charge;
02932                 sdhdipole[1] += yr * charge;
02933                 sdhdipole[2] += zr * charge;
02934                 traced[0] = xr*xr*charge;
02935                 traced[1] = xr*yr*charge;
02936                 traced[2] = xr*zr*charge;
02937                 traced[3] = yr*xr*charge;
02938                 traced[4] = yr*yr*charge;
02939                 traced[5] = yr*zr*charge;
02940                 traced[6] = zr*xr*charge;
02941                 traced[7] = zr*yr*charge;
02942                 traced[8] = zr*zr*charge;
02943                 qave = (traced[0] + traced[4] + traced[8]) / 3.0;
02944                 sdhquadrupole[0] += 1.5*(traced[0] - qave);
02945                 sdhquadrupole[1] += 1.5*(traced[1]);
02946                 sdhquadrupole[2] += 1.5*(traced[2]);
02947                 sdhquadrupole[3] += 1.5*(traced[3]);
02948                 sdhquadrupole[4] += 1.5*(traced[4] - qave);
02949                 sdhquadrupole[5] += 1.5*(traced[5]);
02950                 sdhquadrupole[6] += 1.5*(traced[6]);
02951                 sdhquadrupole[7] += 1.5*(traced[7]);
02952                 sdhquadrupole[8] += 1.5*(traced[8] - qave);
02953         #if defined(WITH_TINKER)
02954             case VCM_PERMANENT:
02955                 charge = Vatom_getCharge(atom);
02956                 dipole = Vatom_getDipole(atom);
02957                 quadrupole = Vatom_getQuadrupole(atom);
02958                 sdhcharge += charge;
02959                 sdhdipole[0] += xr * charge;
02960                 sdhdipole[1] += yr * charge;
02961                 sdhdipole[2] += zr * charge;
02962                 traced[0] = xr*xr*charge;
02963                 traced[1] = xr*yr*charge;
02964                 traced[2] = xr*zr*charge;
02965                 traced[3] = yr*xr*charge;
02966                 traced[4] = yr*yr*charge;
02967                 traced[5] = yr*zr*charge;
02968                 traced[6] = zr*xr*charge;
02969                 traced[7] = zr*yr*charge;
02970                 traced[8] = zr*zr*charge;
02971                 sdhdipole[0] += dipole[0];
02972                 sdhdipole[1] += dipole[1];
02973                 sdhdipole[2] += dipole[2];
02974                 traced[0] += 2.0*xr*dipole[0];
02975                 traced[1] += xr*dipole[1] + yr*dipole[0];
02976                 traced[2] += xr*dipole[2] + zr*dipole[0];
02977                 traced[3] += yr*dipole[0] + xr*dipole[1];
02978                 traced[4] += 2.0*yr*dipole[1];
02979                 traced[5] += yr*dipole[2] + zr*dipole[1];
02980                 traced[6] += zr*dipole[0] + xr*dipole[2];
02981                 traced[7] += zr*dipole[1] + yr*dipole[2];
02982                 traced[8] += 2.0*zr*dipole[2];
02983                 qave = (traced[0] + traced[4] + traced[8]) / 3.0;
02984                 sdhquadrupole[0] += 1.5*(traced[0] - qave);
02985                 sdhquadrupole[1] += 1.5*(traced[1]);
02986                 sdhquadrupole[2] += 1.5*(traced[2]);
02987                 sdhquadrupole[3] += 1.5*(traced[3]);
02988                 sdhquadrupole[4] += 1.5*(traced[4] - qave);
02989                 sdhquadrupole[5] += 1.5*(traced[5]);
02990                 sdhquadrupole[6] += 1.5*(traced[6]);
02991                 sdhquadrupole[7] += 1.5*(traced[7]);
02992                 sdhquadrupole[8] += 1.5*(traced[8] - qave);
02993                 sdhquadrupole[0] += quadrupole[0];
02994                 sdhquadrupole[1] += quadrupole[1];
02995                 sdhquadrupole[2] += quadrupole[2];
02996                 sdhquadrupole[3] += quadrupole[3];
02997                 sdhquadrupole[4] += quadrupole[4];
02998                 sdhquadrupole[5] += quadrupole[5];
02999                 sdhquadrupole[6] += quadrupole[6];
03000                 sdhquadrupole[7] += quadrupole[7];
03001                 sdhquadrupole[8] += quadrupole[8];
03002             case VCM_INDUCED:
03003                 dipole = Vatom_getInducedDipole(atom);
03004                 sdhdipole[0] += dipole[0];
03005                 sdhdipole[1] += dipole[1];
03006                 sdhdipole[2] += dipole[2];

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03007         traced[0] = 2.0*xr*dipole[0];
03008         traced[1] = xr*dipole[1] + yr*dipole[0];
03009         traced[2] = xr*dipole[2] + zr*dipole[0];
03010         traced[3] = yr*dipole[0] + xr*dipole[1];
03011         traced[4] = 2.0*yr*dipole[1];
03012         traced[5] = yr*dipole[2] + zr*dipole[1];
03013         traced[6] = zr*dipole[0] + xr*dipole[2];
03014         traced[7] = zr*dipole[1] + yr*dipole[2];
03015         traced[8] = 2.0*zr*dipole[2];
03016         qave = (traced[0] + traced[4] + traced[8]) / 3.0;
03017         sdhquadrupole[0] += 1.5*(traced[0] - qave);
03018         sdhquadrupole[1] += 1.5*(traced[1]);
03019         sdhquadrupole[2] += 1.5*(traced[2]);
03020         sdhquadrupole[3] += 1.5*(traced[3]);
03021         sdhquadrupole[4] += 1.5*(traced[4] - qave);
03022         sdhquadrupole[5] += 1.5*(traced[5]);
03023         sdhquadrupole[6] += 1.5*(traced[6]);
03024         sdhquadrupole[7] += 1.5*(traced[7]);
03025         sdhquadrupole[8] += 1.5*(traced[8] - qave);
03026     case VCM_NLINDUCED:
03027         dipole = Vatom_getNLInducedDipole(atom);
03028         sdhdipole[0] += dipole[0];
03029         sdhdipole[1] += dipole[1];
03030         sdhdipole[2] += dipole[2];
03031         traced[0] = 2.0*xr*dipole[0];
03032         traced[1] = xr*dipole[1] + yr*dipole[0];
03033         traced[2] = xr*dipole[2] + zr*dipole[0];
03034         traced[3] = yr*dipole[0] + xr*dipole[1];
03035         traced[4] = 2.0*yr*dipole[1];
03036         traced[5] = yr*dipole[2] + zr*dipole[1];
03037         traced[6] = zr*dipole[0] + xr*dipole[2];
03038         traced[7] = zr*dipole[1] + yr*dipole[2];
03039         traced[8] = 2.0*zr*dipole[2];
03040         qave = (traced[0] + traced[4] + traced[8]) / 3.0;
03041         sdhquadrupole[0] += 1.5*(traced[0] - qave);
03042         sdhquadrupole[1] += 1.5*(traced[1]);
03043         sdhquadrupole[2] += 1.5*(traced[2]);
03044         sdhquadrupole[3] += 1.5*(traced[3]);
03045         sdhquadrupole[4] += 1.5*(traced[4] - qave);
03046         sdhquadrupole[5] += 1.5*(traced[5]);
03047         sdhquadrupole[6] += 1.5*(traced[6]);
03048         sdhquadrupole[7] += 1.5*(traced[7]);
03049         sdhquadrupole[8] += 1.5*(traced[8] - qave);
03050         /*Added the else to kill a warning when building with clang*/
03051     #else
03052         case VCM_PERMANENT:;
03053         case VCM_INDUCED:;
03054         case VCM_NLINDUCED:;
03055     #endif /* if defined(WITH_TINKER) */
03056     }
03057 }
03058 /* SDH dipole and traceless quadrupole values
03059 were checked against similar routines in TINKER
03060 for large proteins.
03061
03062 debye=4.8033324;
03063 printf("%6.3f, %6.3f, %6.3f\n", sdhdipole[0]*debye,
03064 sdhdipole[1]*debye, sdhdipole[2]*debye);
03065 printf("%6.3f\n", sdhquadrupole[0]*debye);
03066 printf("%6.3f %6.3f\n", sdhquadrupole[3]*debye,
03067 sdhquadrupole[4]*debye);
03068 printf("%6.3f %6.3f %6.3f\n", sdhquadrupole[6]*debye,
03069 sdhquadrupole[7]*debye, sdhquadrupole[8]*debye);
03070 */
03071
03072 bcf12(size, position, sdhcharge, sdhdipole, sdhquadrupole,
03073 xkappa, eps_p, eps_w, T, thee->gxcf, thee->gycf,
03074 thee->gzcf, thee->xf, thee->yf, thee->zf, nx, ny, nz);
03075 break;
03076
03077 case BCF1_MDH:
03078     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
03079         atom = Valist_getAtom(alist, iatom);
03080         position = Vatom_getPosition(atom);
03081         charge = Vunit_ec*Vatom_getCharge(atom);
03082         dipole = VNULL;
03083         quadrupole = VNULL;
03084         size = Vatom_getRadius(atom);
03085         switch (thee->chargeSrc)
03086         {
03087             case VCM_CHARGE:

```

```

03088         ;
03089 #if defined(WITH_TINKER)
03090         case VCM_PERMANENT:
03091             dipole = Vatom_getDipole(atom);
03092             quadrupole = Vatom_getQuadrupole(atom);
03093
03094         case VCM_INDUCED:
03095             dipole = Vatom_getInducedDipole(atom);
03096
03097         case VCM_NLINDUCED:
03098             dipole = Vatom_getNLInducedDipole(atom);
03099 /*added this to kill a warning when building with clang (by Juan Brandi).*/
03100 #else
03101         case VCM_PERMANENT;;
03102         case VCM_INDUCED;;
03103         case VCM_NLINDUCED;;
03104 #endif
03105     }
03106     bcfl1(size, position, charge, xkappa, prel,
03107         thee->gxcf, thee->gycf, thee->gzcf,
03108         thee->xf, thee->yf, thee->zf, nx, ny, nz);
03109 }
03110 break;
03111
03112 case BCFL_UNUSED:
03113     Vnm_print(2, "bcCalc: Invalid bcfl (%d)!\n", thee->pmgp->bcfl);
03114     VASSERT(0);
03115
03116 case BCFL_FOCUS:
03117     Vnm_print(2, "VPMG::bcCalc -- not appropriate for focusing!\n");
03118     VASSERT(0);
03119
03120 default:
03121     Vnm_print(2, "VPMG::bcCalc -- invalid boundary condition \
03122 flag (%d)!\n", thee->pmgp->bcfl);
03123     VASSERT(0);
03124 }
03125 }
03126
03127 /*
03128 Used by bcflnew
03129 */
03130 VPRIVATE int gridPointIsValid(int i, int j, int k, int nx, int ny, int nz){
03131
03132     int isValid = 0;
03133
03134     if((k==0) || (k==nz-1)){
03135         isValid = 1;
03136     }else if((j==0) || (j==ny-1)){
03137         isValid = 1;
03138     }else if((i==0) || (i==nx-1)){
03139         isValid = 1;
03140     }
03141
03142     return isValid;
03143 }
03144
03145 /*
03146 Used by bcflnew
03147 */
03148 #ifdef DEBUG_MAC_OSX_OCL
03149 #include "mach_chud.h"
03150 VPRIVATE void packAtomsOpenCL(float *ax, float *ay, float *az,
03151     float *charge, float *size, Vpmg *thee){
03152
03153     int i;
03154     int natoms;
03155
03156     Vatom *atom = VNULL;
03157     Valist *alist = VNULL;
03158
03159     alist = thee->pbe->alist;
03160     natoms = Valist_getNumberAtoms(alist);
03161
03162     for(i=0;i<natoms;i++){
03163         atom = *(alist->atoms[i]);
03164         charge[i] = Vunit_ec*atom->charge;
03165         ax[i] = atom->position[0];
03166         ay[i] = atom->position[1];
03167         az[i] = atom->position[2];
03168         size[i] = atom->radius;

```

```

03169     }
03170 }
03171
03172 /*
03173  Used by bcflnew
03174 */
03175 VPRIVATE void packUnpackOpenCL(int nx, int ny, int nz, int ngrid,
03176                                float *gx, float *gy, float *gz, float *value,
03177                                Vpmg *thee, int pack){
03178
03179     int i,j,k,igrid;
03180     int x0,x1,y0,y1,z0,z1;
03181
03182     float gpos[3];
03183     double *xf, *yf, *zf;
03184     double *gxcf, *gycf, *gzcf;
03185
03186     xf = thee->xf;
03187     yf = thee->yf;
03188     zf = thee->zf;
03189
03190     gxcf = thee->gxcf;
03191     gycf = thee->gycf;
03192     gzcf = thee->gzcf;
03193
03194     igrid = 0;
03195     for(k=0;k<nz;k++){
03196         gpos[2] = zf[k];
03197         for(j=0;j<ny;j++){
03198             gpos[1] = yf[j];
03199             for(i=0;i<nx;i++){
03200                 gpos[0] = xf[i];
03201                 if(gridPointIsValid(i, j, k, nx, ny, nz)){
03202                     if(pack != 0){
03203                         gx[igrid] = gpos[0];
03204                         gy[igrid] = gpos[1];
03205                         gz[igrid] = gpos[2];
03206
03207                         value[igrid] = 0.0;
03208                     }else{
03209                         x0 = IJKx(j,k,0);
03210                         x1 = IJKx(j,k,1);
03211                         y0 = IJKy(i,k,0);
03212                         y1 = IJKy(i,k,1);
03213                         z0 = IJKz(i,j,0);
03214                         z1 = IJKz(i,j,1);
03215
03216                         if(i==0){
03217                             gxcf[x0] += value[igrid];
03218                         }
03219                         if(i==nx-1){
03220                             gxcf[x1] += value[igrid];
03221                         }
03222                         if(j==0){
03223                             gycf[y0] += value[igrid];
03224                         }
03225                         if(j==ny-1){
03226                             gycf[y1] += value[igrid];
03227                         }
03228                         if(k==0){
03229                             gzcf[z0] += value[igrid];
03230                         }
03231                         if(k==nz-1){
03232                             gzcf[z1] += value[igrid];
03233                         }
03234                     }
03235
03236                     igrid++;
03237                 } //end is valid point
03238             } //end i
03239         } //end j
03240     } //end k
03241
03242 }
03243
03244 /*
03245  bcflnew is an optimized replacement for bcfl1. bcfl1 is still used when TINKER
03246  support is compiled in.
03247  bcflnew uses: packUnpack, packAtoms, gridPointIsValid
03248 */
03249 VPRIVATE void bcflnewOpenCL(Vpmg *thee){

```

```

03250
03251     int i,j,k, iatom, igrd;
03252     int x0, x1, y0, y1, z0, z1;
03253
03254     int nx, ny, nz;
03255     int natoms, ngrid, ngadj;
03256
03257     float dist, prel, eps_w, eps_p, T, xkappa;
03258
03259     float *ax, *ay, *az;
03260     float *charge, *size, *val;
03261
03262     float *gx, *gy, *gz;
03263
03264     Vpbe *pbe = thee->pbe;
03265
03266     nx = thee->pmgp->nx;
03267     ny = thee->pmgp->ny;
03268     nz = thee->pmgp->nz;
03269
03270     eps_w = Vpbe_getSolventDiel(pbe);           /* Dimensionless */
03271     eps_p = Vpbe_getSoluteDiel(pbe);           /* Dimensionless */
03272     T = Vpbe_getTemperature(pbe);             /* K */
03273     prel = ((Vunit_ec)/(4*VPI*Vunit_eps0*eps_w*Vunit_kb*T))*(1.0e10);
03274     xkappa = Vpbe_getXkappa(pbe);
03275
03276     natoms = Valist_getNumberAtoms(thee->pbe->alist);
03277     ngrid = 2*((nx*ny) + (ny*nz) + (nx*nz));
03278     ngadj = ngrid + (512 - (ngrid & 511));
03279
03280     ax = (float*)malloc(natoms * sizeof(float));
03281     ay = (float*)malloc(natoms * sizeof(float));
03282     az = (float*)malloc(natoms * sizeof(float));
03283
03284     charge = (float*)malloc(natoms * sizeof(float));
03285     size = (float*)malloc(natoms * sizeof(float));
03286
03287     gx = (float*)malloc(ngrid * sizeof(float));
03288     gy = (float*)malloc(ngrid * sizeof(float));
03289     gz = (float*)malloc(ngrid * sizeof(float));
03290
03291     val = (float*)malloc(ngrid * sizeof(float));
03292
03293     packAtomsOpenCL(ax, ay, az, charge, size, thee);
03294     packUnpackOpenCL(nx, ny, nz, ngrid, gx, gy, gz, val, thee, 1);
03295
03296     runMDHCL(ngrid, natoms, ngadj, ax, ay, az, gx, gy, gz, charge, size, xkappa, prel, val);
03297
03298     packUnpackOpenCL(nx, ny, nz, ngrid, gx, gy, gz, val, thee, 0);
03299
03300     free(ax);
03301     free(ay);
03302     free(az);
03303     free(charge);
03304     free(size);
03305
03306     free(gx);
03307     free(gy);
03308     free(gz);
03309     free(val);
03310 }
03311 #endif
03312
03313 VPRIVATE void packAtoms(double *ax, double *ay, double *az,
03314                        double *charge, double *size, Vpmg *thee){
03315
03316     int i;
03317     int natoms;
03318
03319     Vatom *atom = VNULL;
03320     Valist *alist = VNULL;
03321
03322     alist = thee->pbe->alist;
03323     natoms = Valist_getNumberAtoms(alist);
03324
03325     for(i=0; i<natoms; i++){
03326         atom = &(alist->atoms[i]);
03327         charge[i] = Vunit_ec*atom->charge;
03328         ax[i] = atom->position[0];
03329         ay[i] = atom->position[1];
03330         az[i] = atom->position[2];

```



```

03331         size[i] = atom->radius;
03332     }
03333 }
03334
03335 /*
03336  Used by bcf1new
03337 */
03338 VPRIVATE void packUnpack(int nx, int ny, int nz, int ngrid,
03339     double *gx, double *gy, double *gz, double *value,
03340     Vpmg *thee, int pack){
03341
03342     int i,j,k,igrid;
03343     int x0,x1,y0,y1,z0,z1;
03344
03345     double gpos[3];
03346     double *xf, *yf, *zf;
03347     double *gxcf, *gycf, *gzcf;
03348
03349     xf = thee->xf;
03350     yf = thee->yf;
03351     zf = thee->zf;
03352
03353     gxcf = thee->gxcf;
03354     gycf = thee->gycf;
03355     gzcf = thee->gzcf;
03356
03357     igrid = 0;
03358     for(k=0;k<nz;k++){
03359         gpos[2] = zf[k];
03360         for(j=0;j<ny;j++){
03361             gpos[1] = yf[j];
03362             for(i=0;i<nx;i++){
03363                 gpos[0] = xf[i];
03364                 if(gridPointIsValid(i, j, k, nx, ny, nz)){
03365                     if(pack != 0){
03366                         gx[igrid] = gpos[0];
03367                         gy[igrid] = gpos[1];
03368                         gz[igrid] = gpos[2];
03369
03370                         value[igrid] = 0.0;
03371                     }else{
03372                         x0 = IJKx(j,k,0);
03373                         x1 = IJKx(j,k,1);
03374                         y0 = IJKy(i,k,0);
03375                         y1 = IJKy(i,k,1);
03376                         z0 = IJKz(i,j,0);
03377                         z1 = IJKz(i,j,1);
03378
03379                         if(i==0){
03380                             gxcf[x0] += value[igrid];
03381                         }
03382                         if(i==nx-1){
03383                             gxcf[x1] += value[igrid];
03384                         }
03385                         if(j==0){
03386                             gycf[y0] += value[igrid];
03387                         }
03388                         if(j==ny-1){
03389                             gycf[y1] += value[igrid];
03390                         }
03391                         if(k==0){
03392                             gzcf[z0] += value[igrid];
03393                         }
03394                         if(k==nz-1){
03395                             gzcf[z1] += value[igrid];
03396                         }
03397                     }
03398
03399                     igrid++;
03400                 } //end is valid point
03401             } //end i
03402         } //end j
03403     } //end k
03404 }
03405
03406
03407 VPRIVATE void bcf1new(Vpmg *thee){
03408
03409     int i,j,k, iatom, igrid;
03410     int x0, x1, y0, y1, z0, z1;
03411

```

```

03412     int nx, ny, nz;
03413     int natoms, ngrid;
03414
03415     double dist, prel, eps_w, eps_p, T, xkappa;
03416
03417     double *ax, *ay, *az;
03418     double *charge, *size, *val;
03419
03420     double *gx, *gy, *gz;
03421
03422     Vpbe *pbe = thee->pbe;
03423
03424     nx = thee->pmgp->nx;
03425     ny = thee->pmgp->ny;
03426     nz = thee->pmgp->nz;
03427
03428     eps_w = Vpbe_getSolventDiel(pbe);           /* Dimensionless */
03429     eps_p = Vpbe_getSoluteDiel(pbe);           /* Dimensionless */
03430     T = Vpbe_getTemperature(pbe);              /* K */
03431     prel = ((Vunit_ec)/(4*VPI*Vunit_eps0*eps_w*Vunit_kb*T))*(1.0e10);
03432     xkappa = Vpbe_getXkappa(pbe);
03433
03434     natoms = Valist_getNumberAtoms(thee->pbe->alist);
03435     ngrid = 2*((nx*ny) + (ny*nz) + (nx*nz));
03436
03437     ax = (double*)malloc(natoms * sizeof(double));
03438     ay = (double*)malloc(natoms * sizeof(double));
03439     az = (double*)malloc(natoms * sizeof(double));
03440
03441     charge = (double*)malloc(natoms * sizeof(double));
03442     size = (double*)malloc(natoms * sizeof(double));
03443
03444     gx = (double*)malloc(ngrid * sizeof(double));
03445     gy = (double*)malloc(ngrid * sizeof(double));
03446     gz = (double*)malloc(ngrid * sizeof(double));
03447
03448     val = (double*)malloc(ngrid * sizeof(double));
03449
03450     packAtoms(ax, ay, az, charge, size, thee);
03451     packUnpack(nx, ny, nz, ngrid, gx, gy, gz, val, thee, 1);
03452
03453     if(xkappa > VSMALL){
03454 #pragma omp parallel for default(shared) private(igrid, iatom, dist)
03455         for(igrid=0; igrid<ngrid; igrid++){
03456             for(iatom=0; iatom<natoms; iatom++){
03457                 dist = VSQRT(VSQR(gx[igrid]-ax[iatom]) + VSQR(gy[igrid]-ay[iatom])
03458                             + VSQR(gz[igrid]-az[iatom]));
03459                 val[igrid] += prel*(charge[iatom]/dist)*VEXP(-xkappa*(dist-size[iatom]))
03460                             / (1+xkappa*size[iatom]);
03461             }
03462         }
03463     }else{
03464 #pragma omp parallel for default(shared) private(igrid, iatom, dist)
03465         for(igrid=0; igrid<ngrid; igrid++){
03466             for(iatom=0; iatom<natoms; iatom++){
03467                 dist = VSQRT(VSQR(gx[igrid]-ax[iatom]) + VSQR(gy[igrid]-ay[iatom])
03468                             + VSQR(gz[igrid]-az[iatom]));
03469                 val[igrid] += prel*(charge[iatom]/dist);
03470             }
03471         }
03472     }
03473     packUnpack(nx, ny, nz, ngrid, gx, gy, gz, val, thee, 0);
03474
03475     free(ax);
03476     free(ay);
03477     free(az);
03478     free(charge);
03479     free(size);
03480
03481     free(gx);
03482     free(gy);
03483     free(gz);
03484     free(val);
03485 }
03486
03487 VPRIVATE void multipolebc(double r, double kappa, double eps_p,
03488                          double eps_w, double rad, double tsr[3]) {
03489     double r2, r3, r5;
03490     double eps_r;
03491     double ka, ka2, ka3;
03492     double kr, kr2, kr3;

```

```

03493
03494  /*
03495  Below an attempt is made to explain the potential outside of a
03496  multipole located at the center of spherical cavity of dielectric
03497  eps_p, with dielectric eps_w outside (and possibly kappa > 0).
03498
03499  First, eps_p = 1.0
03500  eps_w = 1.0
03501  kappa = 0.0
03502
03503  The general form for the potential of a traceless multipole tensor
03504  of rank n in vacuum is:
03505
03506  V(r) = (-1)^n * u . n . Del^n (1/r)
03507
03508  where
03509  u          is a multipole of order n (3^n components)
03510  u . n . Del^n (1/r)  is the contraction of u with the nth
03511  derivative of 1/r
03512
03513  for example, if n = 1, the dipole potential is
03514  V_vac(r) = (-1)*(ux*x + uy*y + uz*z)/r^3
03515
03516  This function returns the parts of V(r) for multipoles of
03517  order 0, 1 and 2 that are independent of the contraction.
03518
03519  For the vacuum example, this would be 1/r, -1/r^3 and 3/r^5
03520  respectively.
03521
03522  *** Note that this requires that the quadrupole is
03523  traceless. If not, the diagonal quadrupole potential changes
03524  from
03525  qaa * 3*a^2/r^5
03526  to
03527  qaa * (3*a^2/r^5 - 1/r^3a )
03528  where we sum over the trace; a = x, y and z.
03529
03530  (In other words, the -1/r^3 term cancels for a traceless quadrupole.
03531  qxx + qyy + qzz = 0
03532  such that
03533  -(qxx + qyy + qzz)/r^3 = 0
03534
03535  For quadrupole with trace:
03536  qxx + qyy + qzz != 0
03537  such that
03538  -(qxx + qyy + qzz)/r^3 != 0
03539  )
03540
03541  =====
03542
03543  eps_p != 1 or eps_w != 1
03544  kappa = 0.0
03545
03546  If the multipole is placed at the center of a sphere with
03547  dielectric eps_p in a solvent of dielectric eps_w, the potential
03548  outside the sphere is the solution to the Laplace equation:
03549
03550  V(r) = 1/eps_w * (2*n+1)*eps_r/(n*(n+1)*eps_r)
03551  * (-1)^n * u . n . Del^n (1/r)
03552  where
03553  eps_r = eps_w / eps_p
03554  is the ratio of solvent to solute dielectric
03555
03556  =====
03557
03558  kappa > 0
03559
03560  Finally, if the region outside the sphere is treated by the linearized
03561  PB equation with Debye-Huckel parameter kappa, the solution is:
03562
03563  V(r) = kappa/eps_w * alpha_n(kappa*a) * K_n(kappa*r) * r^(n+1)/a^n
03564  * (-1)^n * u . n . Del^n (1/r)
03565  where
03566  alpha_n(x) is [(2n + 1) / x] / [(n*K_n(x)/eps_r) - x*K_n'(x)]
03567  K_n(x) are modified spherical Bessel functions of the third kind.
03568  K_n'(x) is the derivative of K_n(x)
03569  */
03570
03571  eps_r = eps_w/eps_p;
03572  r2 = r*r;
03573

```

```

03574     r3 = r2*r;
03575     r5 = r3*r2;
03576     tsr[0] = (1.0/eps_w)/r;
03577     tsr[1] = (1.0/eps_w)*(-1.0)/r3;
03578     tsr[2] = (1.0/eps_w)*(3.0)/r5;
03579     if (kappa < VSMALL) {
03580         tsr[1] = (3.0*eps_r)/(1.0 + 2.0*eps_r)*tsr[1];
03581         tsr[2] = (5.0*eps_r)/(2.0 + 3.0*eps_r)*tsr[2];
03582     } else {
03583         ka = kappa*rad;
03584         ka2 = ka*ka;
03585         ka3 = ka2*ka;
03586         kr = kappa*r;
03587         kr2 = kr*kr;
03588         kr3 = kr2*kr;
03589         tsr[0] = exp(ka-kr) / (1.0 + ka) * tsr[0];
03590         tsr[1] = 3.0*eps_r*exp(ka-kr)*(1.0 + kr) * tsr[1];
03591         tsr[1] = tsr[1] / (1.0 + ka + eps_r*(2.0 + 2.0*ka + ka2));
03592         tsr[2] = 5.0*eps_r*exp(ka-kr)*(3.0 + 3.0*kr + kr2) * tsr[2];
03593         tsr[2] = tsr[2] / (6.0+6.0*ka+2.0*ka2+eps_r*(9.0+9.0*ka+4.0*ka2+ka3));
03594     }
03595 }
03596
03597 VPRIVATE void bcfl_sdh(Vpmg *thee){
03598
03599     int i,j,k,iatom;
03600     int nx, ny, nz;
03601
03602     double size, *position, charge, xkappa, eps_w, eps_p, T, pre, dist;
03603     double sdhcharge, sdhdipole[3], traced[9], sdhquadrupole[9];
03604     double *dipole, *quadrupole;
03605
03606     double val, *apos, gpos[3], tensor[3], qave;
03607     double ux, uy, uz, xr, yr, zr;
03608     double qxx,qxy,qxz,qyx,qyy,qyz,qzx,qzy,qzz;
03609
03610     double *xf, *yf, *zf;
03611     double *gxcf, *gycf, *gzcf;
03612
03613     Vpbe *pbe;
03614     Vatom *atom;
03615     Valist *alist;
03616
03617     pbe = thee->pbe;
03618     alist = thee->pbe->alist;
03619     nx = thee->pmgp->nx;
03620     ny = thee->pmgp->ny;
03621     nz = thee->pmgp->nz;
03622
03623     xf = thee->xf;
03624     yf = thee->yf;
03625     zf = thee->zf;
03626
03627     gxcf = thee->gxcf;
03628     gycf = thee->gycf;
03629     gzcf = thee->gzcf;
03630
03631     /* For each "atom" (only one for bcfl=1), we use the following formula to
03632      * calculate the boundary conditions:
03633      * 
$$g(x) = \frac{q}{4\pi\epsilon_0\epsilon_w k_b T} \frac{\exp(-x\kappa(d-a))}{1+x\kappa a}$$

03634      * where  $d = ||x - x_0||$  (in m) and  $a$  is the size of the atom (in m).
03635      * We only need to evaluate some of these prefactors once:
03636      *  $prel = \frac{q}{4\pi\epsilon_0\epsilon_w k_b T}$ 
03637      * which gives the potential as
03638      * 
$$g(x) = prel * q/d * \frac{\exp(-x\kappa(d-a))}{1+x\kappa a}$$

03639      */
03640     eps_w = Vpbe_getSolventDiel(pbe); /* Dimensionless */
03641     eps_p = Vpbe_getSoluteDiel(pbe); /* Dimensionless */
03642     T = Vpbe_getTemperature(pbe); /* K */
03643
03644     pre = (Vunit_ec*Vunit_ec)/(4*VPI*Vunit_eps0*Vunit_kb*T);
03645     pre = pre*(1.0e10);
03646
03647     /* Finally, if we convert keep xkappa in Å-1 and scale prel by
03648      * m/Å, then we will only need to deal with distances and sizes in
03649      * Angstroms rather than meters. */
03650     xkappa = Vpbe_getXkappa(pbe); /* Å-1 */
03651
03652     /* Solute size and position */

```

```
03655     size = Vpbe_getSoluteRadius(pbe);
03656     position = Vpbe_getSoluteCenter(pbe);
03657
03658     sdhcharge = 0.0;
03659     for (i=0; i<3; i++) sdhdipole[i] = 0.0;
03660     for (i=0; i<9; i++) sdhquadrupole[i] = 0.0;
03661
03662     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
03663         atom = Valist_getAtom(alist, iatom);
03664         apos = Vatom_getPosition(atom);
03665         xr = apos[0] - position[0];
03666         yr = apos[1] - position[1];
03667         zr = apos[2] - position[2];
03668         switch (three->chargeSrc) {
03669             case VCM_CHARGE:
03670                 charge = Vatom_getCharge(atom);
03671                 sdhcharge += charge;
03672                 sdhdipole[0] += xr * charge;
03673                 sdhdipole[1] += yr * charge;
03674                 sdhdipole[2] += zr * charge;
03675                 traced[0] = xr*xr*charge;
03676                 traced[1] = xr*yr*charge;
03677                 traced[2] = xr*zr*charge;
03678                 traced[3] = yr*xr*charge;
03679                 traced[4] = yr*yr*charge;
03680                 traced[5] = yr*zr*charge;
03681                 traced[6] = zr*xr*charge;
03682                 traced[7] = zr*yr*charge;
03683                 traced[8] = zr*zr*charge;
03684                 gave = (traced[0] + traced[4] + traced[8]) / 3.0;
03685                 sdhquadrupole[0] += 1.5*(traced[0] - gave);
03686                 sdhquadrupole[1] += 1.5*(traced[1]);
03687                 sdhquadrupole[2] += 1.5*(traced[2]);
03688                 sdhquadrupole[3] += 1.5*(traced[3]);
03689                 sdhquadrupole[4] += 1.5*(traced[4] - gave);
03690                 sdhquadrupole[5] += 1.5*(traced[5]);
03691                 sdhquadrupole[6] += 1.5*(traced[6]);
03692                 sdhquadrupole[7] += 1.5*(traced[7]);
03693                 sdhquadrupole[8] += 1.5*(traced[8] - gave);
03694 #if defined(WITH_TINKER)
03695                 case VCM_PERMANENT:
03696                     charge = Vatom_getCharge(atom);
03697                     dipole = Vatom_getDipole(atom);
03698                     quadrupole = Vatom_getQuadrupole(atom);
03699                     sdhcharge += charge;
03700                     sdhdipole[0] += xr * charge;
03701                     sdhdipole[1] += yr * charge;
03702                     sdhdipole[2] += zr * charge;
03703                     traced[0] = xr*xr*charge;
03704                     traced[1] = xr*yr*charge;
03705                     traced[2] = xr*zr*charge;
03706                     traced[3] = yr*xr*charge;
03707                     traced[4] = yr*yr*charge;
03708                     traced[5] = yr*zr*charge;
03709                     traced[6] = zr*xr*charge;
03710                     traced[7] = zr*yr*charge;
03711                     traced[8] = zr*zr*charge;
03712                     sdhdipole[0] += dipole[0];
03713                     sdhdipole[1] += dipole[1];
03714                     sdhdipole[2] += dipole[2];
03715                     traced[0] += 2.0*xr*dipole[0];
03716                     traced[1] += xr*dipole[1] + yr*dipole[0];
03717                     traced[2] += xr*dipole[2] + zr*dipole[0];
03718                     traced[3] += yr*dipole[0] + xr*dipole[1];
03719                     traced[4] += 2.0*yr*dipole[1];
03720                     traced[5] += yr*dipole[2] + zr*dipole[1];
03721                     traced[6] += zr*dipole[0] + xr*dipole[2];
03722                     traced[7] += zr*dipole[1] + yr*dipole[2];
03723                     traced[8] += 2.0*zr*dipole[2];
03724                     gave = (traced[0] + traced[4] + traced[8]) / 3.0;
03725                     sdhquadrupole[0] += 1.5*(traced[0] - gave);
03726                     sdhquadrupole[1] += 1.5*(traced[1]);
03727                     sdhquadrupole[2] += 1.5*(traced[2]);
03728                     sdhquadrupole[3] += 1.5*(traced[3]);
03729                     sdhquadrupole[4] += 1.5*(traced[4] - gave);
03730                     sdhquadrupole[5] += 1.5*(traced[5]);
03731                     sdhquadrupole[6] += 1.5*(traced[6]);
03732                     sdhquadrupole[7] += 1.5*(traced[7]);
03733                     sdhquadrupole[8] += 1.5*(traced[8] - gave);
03734                     sdhquadrupole[0] += quadrupole[0];
03735                     sdhquadrupole[1] += quadrupole[1];
```

```

03736         sdhquadrupole[2] += quadrupole[2];
03737         sdhquadrupole[3] += quadrupole[3];
03738         sdhquadrupole[4] += quadrupole[4];
03739         sdhquadrupole[5] += quadrupole[5];
03740         sdhquadrupole[6] += quadrupole[6];
03741         sdhquadrupole[7] += quadrupole[7];
03742         sdhquadrupole[8] += quadrupole[8];
03743     case VCM_INDUCED:
03744         dipole = Vatom_getInducedDipole(atom);
03745         sdhdipole[0] += dipole[0];
03746         sdhdipole[1] += dipole[1];
03747         sdhdipole[2] += dipole[2];
03748         traced[0] = 2.0*xr*dipole[0];
03749         traced[1] = xr*dipole[1] + yr*dipole[0];
03750         traced[2] = xr*dipole[2] + zr*dipole[0];
03751         traced[3] = yr*dipole[0] + xr*dipole[1];
03752         traced[4] = 2.0*yr*dipole[1];
03753         traced[5] = yr*dipole[2] + zr*dipole[1];
03754         traced[6] = zr*dipole[0] + xr*dipole[2];
03755         traced[7] = zr*dipole[1] + yr*dipole[2];
03756         traced[8] = 2.0*zr*dipole[2];
03757         gave = (traced[0] + traced[4] + traced[8]) / 3.0;
03758         sdhquadrupole[0] += 1.5*(traced[0] - gave);
03759         sdhquadrupole[1] += 1.5*(traced[1]);
03760         sdhquadrupole[2] += 1.5*(traced[2]);
03761         sdhquadrupole[3] += 1.5*(traced[3]);
03762         sdhquadrupole[4] += 1.5*(traced[4] - gave);
03763         sdhquadrupole[5] += 1.5*(traced[5]);
03764         sdhquadrupole[6] += 1.5*(traced[6]);
03765         sdhquadrupole[7] += 1.5*(traced[7]);
03766         sdhquadrupole[8] += 1.5*(traced[8] - gave);
03767     case VCM_NLINDUCED:
03768         dipole = Vatom_getNLInducedDipole(atom);
03769         sdhdipole[0] += dipole[0];
03770         sdhdipole[1] += dipole[1];
03771         sdhdipole[2] += dipole[2];
03772         traced[0] = 2.0*xr*dipole[0];
03773         traced[1] = xr*dipole[1] + yr*dipole[0];
03774         traced[2] = xr*dipole[2] + zr*dipole[0];
03775         traced[3] = yr*dipole[0] + xr*dipole[1];
03776         traced[4] = 2.0*yr*dipole[1];
03777         traced[5] = yr*dipole[2] + zr*dipole[1];
03778         traced[6] = zr*dipole[0] + xr*dipole[2];
03779         traced[7] = zr*dipole[1] + yr*dipole[2];
03780         traced[8] = 2.0*zr*dipole[2];
03781         gave = (traced[0] + traced[4] + traced[8]) / 3.0;
03782         sdhquadrupole[0] += 1.5*(traced[0] - gave);
03783         sdhquadrupole[1] += 1.5*(traced[1]);
03784         sdhquadrupole[2] += 1.5*(traced[2]);
03785         sdhquadrupole[3] += 1.5*(traced[3]);
03786         sdhquadrupole[4] += 1.5*(traced[4] - gave);
03787         sdhquadrupole[5] += 1.5*(traced[5]);
03788         sdhquadrupole[6] += 1.5*(traced[6]);
03789         sdhquadrupole[7] += 1.5*(traced[7]);
03790         sdhquadrupole[8] += 1.5*(traced[8] - gave);
03791     /*added this to kill a warning when building with clang (by Juan Brandi)*/
03792 #else
03793         case VCM_PERMANENT;;
03794         case VCM_INDUCED;;
03795         case VCM_NLINDUCED;;
03796 #endif /* if defined(WITH_TINKER) */
03797     }
03798 }
03799
03800 ux = sdhdipole[0];
03801 uy = sdhdipole[1];
03802 uz = sdhdipole[2];
03803
03804 /* The factor of 1/3 results from using a
03805 traceless quadrupole definition. See, for example,
03806 "The Theory of Intermolecular Forces" by A.J. Stone,
03807 Chapter 3. */
03808 qxx = sdhquadrupole[0] / 3.0;
03809 qxy = sdhquadrupole[1] / 3.0;
03810 qxz = sdhquadrupole[2] / 3.0;
03811 qyx = sdhquadrupole[3] / 3.0;
03812 qyy = sdhquadrupole[4] / 3.0;
03813 qyz = sdhquadrupole[5] / 3.0;
03814 qzx = sdhquadrupole[6] / 3.0;
03815 qzy = sdhquadrupole[7] / 3.0;
03816 qzz = sdhquadrupole[8] / 3.0;

```

```

03817
03818     for(k=0;k<nz;k++){
03819         gpos[2] = zf[k];
03820         for(j=0;j<ny;j++){
03821             gpos[1] = yf[j];
03822             for(i=0;i<nx;i++){
03823                 gpos[0] = xf[i];
03824                 if(gridPointIsValid(i, j, k, nx, ny, nz)){
03825                     xr = gpos[0] - position[0];
03826                     yr = gpos[1] - position[1];
03827                     zr = gpos[2] - position[2];
03828
03829                     dist = VSQRT(VSQR(xr) + VSQR(yr) + VSQR(zr));
03830                     multipolebc(dist, xkappa, eps_p, eps_w, size, tensor);
03831
03832                     val = pre*sdhcharge*tensor[0];
03833                     val -= pre*ux*xr*tensor[1];
03834                     val -= pre*uy*yr*tensor[1];
03835                     val -= pre*uz*zr*tensor[1];
03836                     val += pre*qxx*xr*xr*tensor[2];
03837                     val += pre*qyy*yr*yr*tensor[2];
03838                     val += pre*qzz*zr*zr*tensor[2];
03839                     val += pre*2.0*qxy*xr*yr*tensor[2];
03840                     val += pre*2.0*qxz*xr*zr*tensor[2];
03841                     val += pre*2.0*qyz*yr*zr*tensor[2];
03842
03843                     if(i==0){
03844                         gxcf[IJKx(j,k,0)] = val;
03845                     }
03846                     if(i==nx-1){
03847                         gxcf[IJKx(j,k,1)] = val;
03848                     }
03849                     if(j==0){
03850                         gycf[IJKy(i,k,0)] = val;
03851                     }
03852                     if(j==ny-1){
03853                         gycf[IJKy(i,k,1)] = val;
03854                     }
03855                     if(k==0){
03856                         gzcf[IJKz(i,j,0)] = val;
03857                     }
03858                     if(k==nz-1){
03859                         gzcf[IJKz(i,j,1)] = val;
03860                     }
03861                 } /* End grid point is valid */
03862             } /* End i loop */
03863         } /* End j loop */
03864     } /* End k loop */
03865 }
03866 }
03867
03868 VPRIVATE void bcfl_mdh(Vpmg *thee){
03869     int i,j,k,iatom;
03870     int nx, ny, nz;
03871
03872     double val, *apos, gpos[3];
03873     double *dipole, *quadrupole;
03874     double size, charge, xkappa, eps_w, eps_p, T, prel, dist;
03875
03876     double *xf, *yf, *zf;
03877     double *gxcf, *gycf, *gzcf;
03878
03879     Vpbe *pbe;
03880     Vatom *atom;
03881     Valist *alist;
03882
03883     pbe = thee->pbe;
03884     alist = thee->pbe->alist;
03885     nx = thee->pmgp->nx;
03886     ny = thee->pmgp->ny;
03887     nz = thee->pmgp->nz;
03888
03889     xf = thee->xf;
03890     yf = thee->yf;
03891     zf = thee->zf;
03892
03893     gxcf = thee->gxcf;
03894     gycf = thee->gycf;
03895     gzcf = thee->gzcf;
03896
03897

```

```

03898  /* For each "atom" (only one for bcf1=1), we use the following formula to
03899  * calculate the boundary conditions:
03900  *   
$$g(x) = \frac{q e_c}{4\pi\epsilon_0\epsilon_w\epsilon_b T} \frac{\exp(-\kappa(d-a))}{1+\kappa a}$$

03901  *   where  $d = ||x - x_0||$  (in m) and  $a$  is the size of the atom (in m).
03902  *   We only need to evaluate some of these prefactors once:
03903  *    $prel = \frac{e_c}{4\pi\epsilon_0\epsilon_w\epsilon_b T}$ 
03904  *   which gives the potential as
03905  *   
$$g(x) = prel * q/d * \frac{\exp(-\kappa(d-a))}{1+\kappa a}$$

03906  */
03907  eps_w = Vpbe_getSolventDiel(pbe);          /* Dimensionless */
03908  eps_p = Vpbe_getSoluteDiel(pbe);          /* Dimensionless */
03909  T = Vpbe_getTemperature(pbe);             /* K */
03910  prel = (Vunit_ec)/(4*VPI*Vunit_eps0*eps_w*Vunit_kb*T);
03911
03912  /* Finally, if we convert keep xkappa in A^{-1} and scale prel by
03913  * m/A, then we will only need to deal with distances and sizes in
03914  * Angstroms rather than meters. */
03915  xkappa = Vpbe_getXkappa(pbe);             /* A^{-1} */
03916  prel = prel*(1.0e10);
03917
03918  /* Finally, if we convert keep xkappa in A^{-1} and scale prel by
03919  * m/A, then we will only need to deal with distances and sizes in
03920  * Angstroms rather than meters. */
03921  xkappa = Vpbe_getXkappa(pbe);             /* A^{-1} */
03922
03923  for(k=0;k<nz;k++){
03924    gpos[2] = zf[k];
03925    for(j=0;j<ny;j++){
03926      gpos[1] = yf[j];
03927      for(i=0;i<nx;i++){
03928        gpos[0] = xf[i];
03929        if(gridPointIsValid(i, j, k, nx, ny, nz)){
03930          val = 0.0;
03931
03932          for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
03933            atom = Valist_getAtom(alist, iatom);
03934            apos = Vatom_getPosition(atom);
03935            charge = Vunit_ec*Vatom_getCharge(atom);
03936            size = Vatom_getRadius(atom);
03937
03938            dist = VSQRT(VSQR(gpos[0]-apos[0]) + VSQR(gpos[1]-apos[1])
03939                      + VSQR(gpos[2]-apos[2]));
03940            if (xkappa > VSMALL) {
03941              val += prel*(charge/dist)*VEXP(-xkappa*(dist-size))
03942                / (1+xkappa*size);
03943            } else {
03944              val += prel*(charge/dist);
03945            }
03946          }
03947
03948          if(i==0){
03949            gxcf[IJKx(j,k,0)] = val;
03950          }
03951          if(i==nx-1){
03952            gxcf[IJKx(j,k,1)] = val;
03953          }
03954          if(j==0){
03955            gycf[IJKy(i,k,0)] = val;
03956          }
03957          if(j==ny-1){
03958            gycf[IJKy(i,k,1)] = val;
03959          }
03960          if(k==0){
03961            gzcf[IJKz(i,j,0)] = val;
03962          }
03963          if(k==nz-1){
03964            gzcf[IJKz(i,j,1)] = val;
03965          }
03966        } /* End grid point is valid */
03967      } /* End i loop */
03968    } /* End j loop */
03969  } /* End k loop */
03970
03971  }
03972  // Routine: bcf1_mem

```



```

03979 //
03980 // Purpose: Increment all the boundary points by the
03981 //          analytic expression for a membrane system in
03982 //          the presence of a membrane potential. This
03983 //          Boundary flag should only be used for systems
03984 //          that explicitly have membranes in the dielectric
03985 //          and solvent maps.
03986 //
03987 //          There should be several input variables add to this
03988 //          function such as membrane potential, membrane thickness
03989 //          and height.
03990 //
03991 // Args:    apos is a 3-vector
03992 //
03993 // Author: Michael Grabe
03994 VPRIVATE void bcfl_mem(double zmem, double L, double eps_m, double eps_w,
03995                        double V, double xkappa, double *gxcf, double *gycf, double *gzcf,
03996                        double *xf, double *yf, double *zf, int nx, int ny, int nz) {
03997
03998     /* some definitions */
03999     /* L = total length of the membrane */
04000     /* xkappa = inverse Debeye length */
04001     /* zmem = z value of membrane bottom (Cytoplasm) */
04002     /* V = electrical potential inside the cell */
04003     int i, j, k;
04004     double dist, val, z_low, z_high, z_shift;
04005     double A, B, C, D, edge_L, l;
04006     double G, z_0, z_rel;
04007     double gpos[3];
04008
04009     Vnm_print(0, "Here is the value of kappa: %f\n", xkappa);
04010     Vnm_print(0, "Here is the value of L: %f\n", L);
04011     Vnm_print(0, "Here is the value of zmem: %f\n", zmem);
04012     Vnm_print(0, "Here is the value of mdie: %f\n", eps_m);
04013     Vnm_print(0, "Here is the value of memv: %f\n", V);
04014
04015     /* no salt symmetric BC's at +/- infinity */
04016     // B=V/(edge_L - l*(1-eps_w/eps_m));
04017     // A=V + B*edge_L;
04018     // D=eps_w/eps_m*B;
04019     z_low = zmem; /* this defines the bottom of the membrane */
04020     z_high = zmem + L; /* this is the top of the membrane */
04021
04022     /* proper boundary conditions for V = 0 extracellular */
04023     /* and psi=-V cytoplasm. */
04024     /* Implicit in this formulation is that the membrane */
04025     /* center be at z = 0 */
04026     /*
04027     *****
04028     l=L/2; /* half of the membrane length */
04029     z_0 = z_low + l; /* center of the membrane */
04030     G=l*eps_w/eps_m*xkappa;
04031     A=-V/2*(1/(G+l))*exp(xkappa*l);
04032     B=V/2;
04033     C=-V/2*eps_w/eps_m*xkappa*(1/(G+l));
04034     D=-A;
04035     /* The analytic expression for the boundary conditions */
04036     /* had the cytoplasmic surface of the membrane set to zero. */
04037     /* This requires an off-set of the BC equations. */
04038
04039     /* the "i" boundaries (dirichlet) */
04040     for (k=0; k<nz; k++) {
04041         gpos[2] = zf[k];
04042         z_rel = gpos[2] - z_0; /* relative position for BCs */
04043
04044         for (j=0; j<ny; j++) {
04045             if (gpos[2] <= z_low) { /* cytoplasmic */
04046                 val = A*exp(xkappa*z_rel) + V;
04047                 gxcf[IJKx(j,k,0)] += val; /* assign low side BC */
04048                 gxcf[IJKx(j,k,1)] += val; /* assign high side BC */
04049             }
04050             else if (gpos[2] > z_low && gpos[2] <= z_high) { /* in membrane */
04051                 val = B + C*z_rel;
04052                 gxcf[IJKx(j,k,0)] += val; /* assign low side BC */
04053                 gxcf[IJKx(j,k,1)] += val; /* assign high side BC */
04054             }
04055         }
04056     }
04057 }

```

```

04063     }
04064 }
04065
04066     else if (gpos[2] > z_high) {                                     /* extracellular */
04067
04068         val = D*exp(-xkappa*z_rel);
04069         gxcf[IJKx(j,k,0)] += val;    /* assign low side BC */
04070         gxcf[IJKx(j,k,1)] += val;    /* assign high side BC */
04071     }
04072 }
04073 }
04074 }
04075 }
04076
04077 /* the "j" boundaries (dirichlet) */
04078 for (k=0; k<nz; k++) {
04079     gpos[2] = zf[k];
04080     z_rel = gpos[2] - z_0;
04081     for (i=0; i<nx; i++) {
04082
04083         if (gpos[2] <= z_low) {                                     /* cytoplasmic */
04084
04085             val = A*exp(xkappa*z_rel) + V;
04086             gycf[IJKy(i,k,0)] += val;    /* assign low side BC */
04087             gycf[IJKy(i,k,1)] += val;    /* assign high side BC */
04088             //printf("%f \n",val);
04089         }
04090
04091         else if (gpos[2] > z_low && gpos[2] <= z_high) { /* in membrane */
04092
04093             val = B + C*z_rel;
04094             gycf[IJKy(i,k,0)] += val;    /* assign low side BC */
04095             gycf[IJKy(i,k,1)] += val;    /* assign high side BC */
04096             //printf("%f \n",val);
04097         }
04098
04099         else if (gpos[2] > z_high) {                                     /* extracellular */
04100
04101             val = D*exp(-xkappa*z_rel);
04102             gycf[IJKy(i,k,0)] += val;    /* assign low side BC */
04103             gycf[IJKy(i,k,1)] += val;    /* assign high side BC */
04104             //printf("%f \n",val);
04105         }
04106     }
04107 }
04108 }
04109 }
04110 }
04111
04112 /* the "k" boundaries (dirichlet) */
04113 for (j=0; j<ny; j++) {
04114     for (i=0; i<nx; i++) {
04115
04116         /* first assign the bottom boundary */
04117
04118         gpos[2] = zf[0];
04119         z_rel = gpos[2] - z_0;
04120
04121         if (gpos[2] <= z_low) {                                     /* cytoplasmic */
04122
04123             val = A*exp(xkappa*z_rel) + V;
04124             gzcfc[IJKz(i,j,0)] += val;    /* assign low side BC */
04125             //printf("%f \n",val);
04126         }
04127
04128         else if (gpos[2] > z_low && gpos[2] <= z_high) { /* in membrane */
04129
04130             val = B + C*z_rel;
04131             gzcfc[IJKz(i,j,0)] += val;    /* assign low side BC */
04132         }
04133
04134         else if (gpos[2] > z_high) {                                     /* extracellular */
04135
04136             val = D*exp(-xkappa*z_rel);
04137             gzcfc[IJKz(i,j,0)] += val;    /* assign low side BC */
04138         }
04139     }
04140 }
04141
04142 /* now assign the top boundary */
04143

```

```

04144
04145     gpos[2] = zf[nz-1];
04146     z_rel = gpos[2] - z_0;
04147
04148     if (gpos[2] <= z_low) {                                     /* cytoplasmic */
04149
04150         val = A*exp(xkappa*z_rel) + V;
04151         gzcfc[IJKz(i,j,1)] += val;    /* assign high side BC */
04152     }
04153
04154
04155     else if (gpos[2] > z_low && gpos[2] <= z_high) { /* in membrane */
04156
04157         val = B + C*z_rel;
04158         gzcfc[IJKz(i,j,1)] += val;    /* assign high side BC */
04159     }
04160
04161
04162     else if (gpos[2] > z_high) {                                 /* extracellular */
04163
04164         val = D*exp(-xkappa*z_rel);
04165         gzcfc[IJKz(i,j,1)] += val;    /* assign high side BC */
04166         //printf("%f \n",val);
04167     }
04168 }
04169 }
04170 }
04171 }
04172 }
04173
04174 VPRIVATE void bcfl_map(Vpmg *thee){
04175
04176     Vpbe *pbe;
04177     double position[3], pot, hx, hy, hzed;
04178     int i, j, k, nx, ny, nz, rc;
04179
04180
04181     VASSERT(thee != VNULL);
04182
04183     /* Mesh info */
04184     nx = thee->pmgp->nx;
04185     ny = thee->pmgp->ny;
04186     nz = thee->pmgp->nz;
04187     hx = thee->pmgp->hx;
04188     hy = thee->pmgp->hy;
04189     hzed = thee->pmgp->hzed;
04190
04191     /* Reset the potential array */
04192     for (i=0; i<(nx*ny*nz); i++) thee->pot[i] = 0.0;
04193
04194     /* Fill in the source term (atomic potentials) */
04195     Vnm_print(0, "Vpmg_fillco: filling in source term.\n");
04196     for (k=0; k<nz; k++) {
04197         for (j=0; j<ny; j++) {
04198             for (i=0; i<nx; i++) {
04199                 position[0] = thee->xf[i];
04200                 position[1] = thee->yf[j];
04201                 position[2] = thee->zf[k];
04202                 rc = Vgrid_value(thee->potMap, position, &pot);
04203                 if (!rc) {
04204                     Vnm_print(2, "fillcoChargeMap: Error -- fell off of potential map at (%g, %g,
04205 %g)!\n",
04206                             position[0], position[1], position[2]);
04207                     VASSERT(0);
04208                 }
04209                 thee->pot[IJK(i,j,k)] = pot;
04210             }
04211         }
04212     }
04213 }
04214
04215 #if defined(WITH_TINKER)
04216 VPRIVATE void bcfl_mdh_tinker(Vpmg *thee){
04217
04218     int i,j,k,iatom;
04219     int nx, ny, nz;
04220
04221     double val, *apos, gpos[3], tensor[9];
04222     double *dipole, *quadrupole;
04223     double size, charge, xkappa, eps_w, eps_p, T, pre1, dist;

```

```

04224
04225     double ux,uy,uz,xr,yr,zr;
04226     double qxx,qxy,qxz,qyx,qyy,qyz,qzx,qzy,qzz;
04227
04228     double *xf, *yf, *zf;
04229     double *gxcf, *gycf, *gzcf;
04230
04231     Vpbe *pbe;
04232     Vatom *atom;
04233     Valist *alist;
04234
04235     pbe = thee->pbe;
04236     alist = thee->pbe->alist;
04237     nx = thee->pmgp->nx;
04238     ny = thee->pmgp->ny;
04239     nz = thee->pmgp->nz;
04240
04241     xf = thee->xf;
04242     yf = thee->yf;
04243     zf = thee->zf;
04244
04245     gxcf = thee->gxcf;
04246     gycf = thee->gycf;
04247     gzcf = thee->gzcf;
04248
04249     /* For each "atom" (only one for bcfl=1), we use the following formula to
04250      * calculate the boundary conditions:
04251      *   
$$g(x) = \frac{q}{4\pi\epsilon_0\epsilon_w k_b T} \frac{\exp(-x\kappa(d-a))}{1+x\kappa a}$$

04252      *   where  $d = ||x - x_0||$  (in m) and  $a$  is the size of the atom (in m).
04253      *   We only need to evaluate some of these prefactors once:
04254      *   
$$prel = \frac{q}{4\pi\epsilon_0\epsilon_w k_b T}$$

04255      *   which gives the potential as
04256      *   
$$g(x) = prel * q/d * \frac{\exp(-x\kappa(d-a))}{1+x\kappa a}$$

04257      */
04258     eps_w = Vpbe_getSolventDiel(pbe);          /* Dimensionless */
04259     eps_p = Vpbe_getSoluteDiel(pbe);           /* Dimensionless */
04260     T = Vpbe_getTemperature(pbe);             /* K */
04261     prel = (Vunit_ec*Vunit_ec)/(4*VPI*Vunit_eps0*Vunit_kb*T);
04262
04263     /* Finally, if we convert keep xkappa in A-1 and scale prel by
04264      * m/A, then we will only need to deal with distances and sizes in
04265      * Angstroms rather than meters. */
04266     xkappa = Vpbe_getXkappa(pbe);             /* A-1 */
04267     prel = prel*(1.0e10);
04268
04269     /* Finally, if we convert keep xkappa in A-1 and scale prel by
04270      * m/A, then we will only need to deal with distances and sizes in
04271      * Angstroms rather than meters. */
04272     xkappa = Vpbe_getXkappa(pbe);             /* A-1 */
04273
04274     for(k=0;k<nz;k++){
04275         gpos[2] = zf[k];
04276         for(j=0;j<ny;j++){
04277             gpos[1] = yf[j];
04278             for(i=0;i<nx;i++){
04279                 gpos[0] = xf[i];
04280                 if(gridPointIsValid(i, j, k, nx, ny, nz)){
04281                     val = 0.0;
04282
04283                     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
04284                         atom = Valist_getAtom(alist, iatom);
04285                         apos = Vatom_getPosition(atom);
04286                         size = Vatom_getRadius(atom);
04287
04288                         charge = 0.0;
04289
04290                         dipole = VNULL;
04291                         quadrupole = VNULL;
04292
04293                         if (thee->chargeSrc == VCM_PERMANENT) {
04294                             charge = Vatom_getCharge(atom);
04295                             dipole = Vatom_getDipole(atom);
04296                             quadrupole = Vatom_getQuadrupole(atom);
04297                         } else if (thee->chargeSrc == VCM_INDUCED) {
04298                             dipole = Vatom_getInducedDipole(atom);
04299                         } else {
04300                             dipole = Vatom_getNLInducedDipole(atom);
04301                         }
04302                     }
04303                 }
04304             }
04305         }
04306     }

```

```

04305
04306         ux = dipole[0];
04307         uy = dipole[1];
04308         uz = dipole[2];
04309
04310         if (quadrupole != VNULL) {
04311             /* The factor of 1/3 results from using a
04312              * traceless quadrupole definition. See, for example,
04313              * "The Theory of Intermolecular Forces" by A.J. Stone,
04314              * Chapter 3. */
04315             qxx = quadrupole[0] / 3.0;
04316             qxy = quadrupole[1] / 3.0;
04317             qxz = quadrupole[2] / 3.0;
04318             qyx = quadrupole[3] / 3.0;
04319             qyy = quadrupole[4] / 3.0;
04320             qyz = quadrupole[5] / 3.0;
04321             qzx = quadrupole[6] / 3.0;
04322             qzy = quadrupole[7] / 3.0;
04323             qzz = quadrupole[8] / 3.0;
04324         } else {
04325             qxx = 0.0;
04326             qxy = 0.0;
04327             qxz = 0.0;
04328             qyx = 0.0;
04329             qyy = 0.0;
04330             qyz = 0.0;
04331             qzx = 0.0;
04332             qzy = 0.0;
04333             qzz = 0.0;
04334         }
04335
04336         xr = gpos[0] - apos[0];
04337         yr = gpos[1] - apos[1];
04338         zr = gpos[2] - apos[2];
04339
04340         dist = VSQRT(VSQR(xr) + VSQR(yr) + VSQR(zr));
04341         multipolebc(dist, xkappa, eps_p, eps_w, size, tensor);
04342
04343         val += prel*charge*tensor[0];
04344         val -= prel*ux*xr*tensor[1];
04345         val -= prel*uy*yr*tensor[1];
04346         val -= prel*uz*zr*tensor[1];
04347         val += prel*qxx*xr*xr*tensor[2];
04348         val += prel*qyy*yr*yr*tensor[2];
04349         val += prel*qzz*zr*zr*tensor[2];
04350         val += prel*2.0*qxy*xr*yr*tensor[2];
04351         val += prel*2.0*qxz*xr*zr*tensor[2];
04352         val += prel*2.0*qyz*yr*zr*tensor[2];
04353
04354     }
04355
04356     if(i==0){
04357         gxcf[IJKx(j,k,0)] = val;
04358     }
04359     if(i==nx-1){
04360         gxcf[IJKx(j,k,1)] = val;
04361     }
04362     if(j==0){
04363         gycf[IJKy(i,k,0)] = val;
04364     }
04365     if(j==ny-1){
04366         gycf[IJKy(i,k,1)] = val;
04367     }
04368     if(k==0){
04369         gzcf[IJKz(i,j,0)] = val;
04370     }
04371     if(k==nz-1){
04372         gzcf[IJKz(i,j,1)] = val;
04373     }
04374     } /* End grid point is valid */
04375     } /* End i loop */
04376     } /* End j loop */
04377 } /* End k loop */
04378 }
04379 }
04380 #endif
04381
04382 VPRIVATE void bcCalc(Vpmg *thee){
04383
04384     int i, j, k;
04385     int nx, ny, nz;

```

```

04386
04387     double zmem, eps_m, Lmem, memv, eps_w, xkappa;
04388
04389     nx = thee->pmgp->nx;
04390     ny = thee->pmgp->ny;
04391     nz = thee->pmgp->nz;
04392
04393     /* Zero out the boundaries */
04394     /* the "i" boundaries (dirichlet) */
04395     for (k=0; k<nz; k++) {
04396         for (j=0; j<ny; j++) {
04397             thee->gxcf[IJKx(j,k,0)] = 0.0;
04398             thee->gxcf[IJKx(j,k,1)] = 0.0;
04399             thee->gxcf[IJKx(j,k,2)] = 0.0;
04400             thee->gxcf[IJKx(j,k,3)] = 0.0;
04401         }
04402     }
04403
04404     /* the "j" boundaries (dirichlet) */
04405     for (k=0; k<nz; k++) {
04406         for (i=0; i<nx; i++) {
04407             thee->gycf[IJKy(i,k,0)] = 0.0;
04408             thee->gycf[IJKy(i,k,1)] = 0.0;
04409             thee->gycf[IJKy(i,k,2)] = 0.0;
04410             thee->gycf[IJKy(i,k,3)] = 0.0;
04411         }
04412     }
04413
04414     /* the "k" boundaries (dirichlet) */
04415     for (j=0; j<ny; j++) {
04416         for (i=0; i<nx; i++) {
04417             thee->gzcf[IJKz(i,j,0)] = 0.0;
04418             thee->gzcf[IJKz(i,j,1)] = 0.0;
04419             thee->gzcf[IJKz(i,j,2)] = 0.0;
04420             thee->gzcf[IJKz(i,j,3)] = 0.0;
04421         }
04422     }
04423
04424     switch (thee->pmgp->bcfl) {
04425         /* If we have zero boundary conditions, we're done */
04426         case BCFL_ZERO:
04427             return;
04428         case BCFL_SDH:
04429             bcfl_sdh(thee);
04430             break;
04431         case BCFL_MDH:
04432             #if defined(WITH_TINKER)
04433                 bcfl_mdh_tinker(thee);
04434             #else
04435
04436             #ifdef DEBUG_MAC_OSX_OCL
04437             #include "mach_chud.h"
04438                 uint64_t mbeg = mach_absolute_time();
04439
04440                 /*
04441                  * If OpenCL is available we use it, otherwise fall back to
04442                  * normal route (CPU multithreaded w/ OpenMP)
04443                  */
04444                 if (kOpenCLAvailable == 1) bcflnewOpenCL(thee);
04445                 else bcflnew(thee);
04446
04447                 mets_(&mbeg, "MDH");
04448             #else
04449                 /* bcfl_mdh(thee); */
04450                 bcflnew(thee);
04451             #endif /* DEBUG_MAC_OSX_OCL */
04452
04453             #endif /* WITH_TINKER */
04454             break;
04455         case BCFL_MEM:
04456
04457             zmem = Vpbe_getzmem(thee->pbe);
04458             Lmem = Vpbe_getLmem(thee->pbe);
04459             eps_m = Vpbe_getmembraneDiel(thee->pbe);
04460             memv = Vpbe_getmemv(thee->pbe);
04461
04462             eps_w = Vpbe_getSolventDiel(thee->pbe);
04463             xkappa = Vpbe_getXkappa(thee->pbe);
04464
04465             bcfl_mem(zmem, Lmem, eps_m, eps_w, memv, xkappa,
04466                 thee->gxcf, thee->gycf, thee->gzcf,

```

```

04467         thee->xf, thee->yf, thee->zf, nx, ny, nz);
04468         break;
04469     case BCFL_UNUSED:
04470         Vnm_print(2, "bcCalc: Invalid bcfl (%d)!\n", thee->pmgp->bcfl);
04471         VASSERT(0);
04472         break;
04473     case BCFL_FOCUS:
04474         Vnm_print(2, "VPMG::bcCalc -- not appropriate for focusing!\n");
04475         VASSERT(0);
04476         break;
04477     case BCFL_MAP:
04478         bcfl_map(thee);
04479         focusFillBound(thee, VNULL);
04480         break;
04481     default:
04482         Vnm_print(2, "VPMG::bcCalc -- invalid boundary condition \
04483                 flag (%d)!\n", thee->pmgp->bcfl);
04484         VASSERT(0);
04485         break;
04486     }
04487 }
04488
04489 VPRIVATE void fillcoCoefMap(Vpmg *thee) {
04490     Vpbe *pbe;
04491     double ionstr, position[3], tkappa, eps, pot, hx, hy, hzed;
04492     int i, j, k, nx, ny, nz;
04493     double kappamax;
04494     VASSERT(thee != VNULL);
04495
04496     /* Get PBE info */
04497     pbe = thee->pbe;
04498     ionstr = Vpbe_getBulkIonicStrength(pbe);
04499
04500     /* Mesh info */
04501     nx = thee->pmgp->nx;
04502     ny = thee->pmgp->ny;
04503     nz = thee->pmgp->nz;
04504     hx = thee->pmgp->hx;
04505     hy = thee->pmgp->hy;
04506     hzed = thee->pmgp->hzed;
04507
04508     if ((!thee->useDielXMap) || (!thee->useDielYMap)
04509         || (!thee->useDielZMap) || ((!thee->useKappaMap) && (ionstr > VPMGSMALL))) {
04510         Vnm_print(2, "fillcoCoefMap: You need to use all coefficient maps!\n");
04511         VASSERT(0);
04512     }
04513
04514     /* Scale the kappa map to values between 0 and 1
04515     Thus get the maximum value in the map - this
04516     is theoretically unnecessary, but a good check.*/
04517     kappamax = -1.00;
04518     for (k=0; k<nz; k++) {
04519         for (j=0; j<ny; j++) {
04520             for (i=0; i<nx; i++) {
04521                 if (ionstr > VPMGSMALL) {
04522                     position[0] = thee->xf[i];
04523                     position[1] = thee->yf[j];
04524                     position[2] = thee->zf[k];
04525                     if (!Vgrid_value(thee->kappaMap, position, &tkappa)) {
04526                         Vnm_print(2, "Vpmg_fillco: Off kappaMap at:\n");
04527                         Vnm_print(2, "Vpmg_fillco: (x,y,z) = (%g,%g %g)\n",
04528                             position[0], position[1], position[2]);
04529                         VASSERT(0);
04530                     }
04531                     if (tkappa > kappamax) {
04532                         kappamax = tkappa;
04533                     }
04534                     if (tkappa < 0.0) {
04535                         Vnm_print(2, "Vpmg_fillcoCoefMap: Kappa map less than 0\n");
04536                         Vnm_print(2, "Vpmg_fillcoCoefMap: at (x,y,z) = (%g,%g %g)\n",
04537                             position[0], position[1], position[2]);
04538                         VASSERT(0);
04539                     }
04540                 }
04541             }
04542         }
04543     }
04544 }
04545 }
04546 }
04547

```

```

04548     if (kappamax > 1.0){
04549         Vnm_print(2, "Vpmg_fillcoCoefMap: Maximum Kappa value\n");
04550         Vnm_print(2, "%g is greater than 1 - will scale appropriately!\n",
04551             kappamax);
04552     }
04553     else {
04554         kappamax = 1.0;
04555     }
04556
04557     for (k=0; k<nz; k++) {
04558         for (j=0; j<ny; j++) {
04559             for (i=0; i<nx; i++) {
04560
04561                 if (ionstr > VPMGSMALL) {
04562                     position[0] = thee->xf[i];
04563                     position[1] = thee->yf[j];
04564                     position[2] = thee->zf[k];
04565                     if (!Vgrid_value(thee->kappaMap, position, &tkappa)) {
04566                         Vnm_print(2, "Vpmg_fillco: Off kappaMap at:\n");
04567                         Vnm_print(2, "Vpmg_fillco: (x,y,z) = (%g,%g %g)\n",
04568                             position[0], position[1], position[2]);
04569                         VASSERT(0);
04570                     }
04571                     if (tkappa < VPMGSMALL) tkappa = 0.0;
04572                     thee->kappa[IJK(i,j,k)] = (tkappa / kappamax);
04573                 }
04574
04575                 position[0] = thee->xf[i] + 0.5*hx;
04576                 position[1] = thee->yf[j];
04577                 position[2] = thee->zf[k];
04578                 if (!Vgrid_value(thee->dielXMap, position, &eps)) {
04579                     Vnm_print(2, "Vpmg_fillco: Off dielXMap at:\n");
04580                     Vnm_print(2, "Vpmg_fillco: (x,y,z) = (%g,%g %g)\n",
04581                         position[0], position[1], position[2]);
04582                     VASSERT(0);
04583                 }
04584                 thee->epsx[IJK(i,j,k)] = eps;
04585
04586                 position[0] = thee->xf[i];
04587                 position[1] = thee->yf[j] + 0.5*hy;
04588                 position[2] = thee->zf[k];
04589                 if (!Vgrid_value(thee->dielYMap, position, &eps)) {
04590                     Vnm_print(2, "Vpmg_fillco: Off dielYMap at:\n");
04591                     Vnm_print(2, "Vpmg_fillco: (x,y,z) = (%g,%g %g)\n",
04592                         position[0], position[1], position[2]);
04593                     VASSERT(0);
04594                 }
04595                 thee->epsy[IJK(i,j,k)] = eps;
04596
04597                 position[0] = thee->xf[i];
04598                 position[1] = thee->yf[j];
04599                 position[2] = thee->zf[k] + 0.5*hzed;
04600                 if (!Vgrid_value(thee->dielZMap, position, &eps)) {
04601                     Vnm_print(2, "Vpmg_fillco: Off dielZMap at:\n");
04602                     Vnm_print(2, "Vpmg_fillco: (x,y,z) = (%g,%g %g)\n",
04603                         position[0], position[1], position[2]);
04604                     VASSERT(0);
04605                 }
04606                 thee->epsz[IJK(i,j,k)] = eps;
04607             }
04608         }
04609     }
04610 }
04611
04612 VPRIVATE void fillcoCoefMol(Vpmg *thee) {
04613
04614     if (thee->useDielXMap || thee->useDielYMap || thee->useDielZMap ||
04615         thee->useKappaMap) {
04616
04617         fillcoCoefMap(thee);
04618     } else {
04619
04620         fillcoCoefMolDiel(thee);
04621         fillcoCoefMolIon(thee);
04622     }
04623 }
04624
04625 }
04626 }
04627
04628 VPRIVATE void fillcoCoefMolIon(Vpmg *thee) {

```



```

04629
04630     Vaccum *acc;
04631     Valist *alist;
04632     Vpbe *pbe;
04633     Vatom *atom;
04634     double xmin, xmax, ymin, ymax, zmin, zmax, ionmask, ionstr;
04635     double xlen, ylen, zlen, irad;
04636     double hx, hy, hzed, *apos, arad;
04637     int i, nx, ny, nz, iatom;
04638     Vsurf_Meth surfMeth;
04639
04640     VASSERT(thee != VNULL);
04641     surfMeth = thee->surfMeth;
04642
04643     /* Get PBE info */
04644     pbe = thee->pbe;
04645     acc = pbe->acc;
04646     alist = pbe->alist;
04647     irad = Vpbe_getMaxIonRadius(pbe);
04648     ionstr = Vpbe_getBulkIonicStrength(pbe);
04649
04650     /* Mesh info */
04651     nx = thee->pmgp->nx;
04652     ny = thee->pmgp->ny;
04653     nz = thee->pmgp->nz;
04654     hx = thee->pmgp->hx;
04655     hy = thee->pmgp->hy;
04656     hzed = thee->pmgp->hzed;
04657
04658     /* Define the total domain size */
04659     xlen = thee->pmgp->xlen;
04660     ylen = thee->pmgp->ylen;
04661     zlen = thee->pmgp->zlen;
04662
04663     /* Define the min/max dimensions */
04664     xmin = thee->pmgp->xcent - (xlen/2.0);
04665     ymin = thee->pmgp->ycent - (ylen/2.0);
04666     zmin = thee->pmgp->zcent - (zlen/2.0);
04667     xmax = thee->pmgp->xcent + (xlen/2.0);
04668     ymax = thee->pmgp->ycent + (ylen/2.0);
04669     zmax = thee->pmgp->zcent + (zlen/2.0);
04670
04671     /* This is a floating point parameter related to the non-zero nature of the
04672      * bulk ionic strength. If the ionic strength is greater than zero; this
04673      * parameter is set to 1.0 and later scaled by the appropriate pre-factors.
04674      * Otherwise, this parameter is set to 0.0 */
04675     if (ionstr > VPMGSMALL) ionmask = 1.0;
04676     else ionmask = 0.0;
04677
04678     /* Reset the kappa array, marking everything accessible */
04679     for (i=0; i<(nx*ny*nz); i++) thee->kappa[i] = ionmask;
04680
04681     if (ionstr < VPMGSMALL) return;
04682
04683     /* Loop through the atoms and set kappa = 0.0 (inaccessible) if a point
04684      * is inside the ion-inflated van der Waals radii */
04685     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
04686
04687         atom = Valist_getAtom(alist, iatom);
04688         apos = Vatom_getPosition(atom);
04689         arad = Vatom_getRadius(atom);
04690
04691         if (arad > VSMALL) {
04692
04693             /* Make sure we're on the grid */
04694             if ((apos[0]<(xmin-irad-arad)) || (apos[0]>(xmax+irad+arad)) || \
04695                 (apos[1]<(ymin-irad-arad)) || (apos[1]>(ymax+irad+arad)) || \
04696                 (apos[2]<(zmin-irad-arad)) || (apos[2]>(zmax+irad+arad))) {
04697                 if ((thee->pmgp->bconf1 != BCFL_FOCUS) &&
04698                     (thee->pmgp->bconf1 != BCFL_MAP)) {
04699                     Vnm_print(2,
04700 "Vpmg_fillco: Atom #d at (%4.3f, %4.3f, %4.3f) is off the mesh (ignoring):\n",
04701 iatom, apos[0], apos[1], apos[2]);
04702                     Vnm_print(2, "Vpmg_fillco:  xmin = %g, xmax = %g\n",
04703 xmin, xmax);
04704                     Vnm_print(2, "Vpmg_fillco:  ymin = %g, ymax = %g\n",
04705 ymin, ymax);
04706                     Vnm_print(2, "Vpmg_fillco:  zmin = %g, zmax = %g\n",
04707 zmin, zmax);
04708                 }
04709                 fflush(stderr);

```

```

04710
04711     } else { /* if we're on the mesh */
04712
04713         /* Mark ions */
04714         markSphere((irad+arad), apos,
04715                 nx, ny, nz,
04716                 hx, hy, hzed,
04717                 xmin, ymin, zmin,
04718                 thee->kappa, 0.0);
04719
04720     } /* endif (on the mesh) */
04721 }
04722 } /* endfor (over all atoms) */
04723
04724 }
04725
04726 VPRIVATE void fillcoCoefMolDiel(Vpmg *thee) {
04727
04728     /* Always call NoSmooth to fill the epsilon arrays */
04729     fillcoCoefMolDielNoSmooth(thee);
04730
04731     /* Call the smoothing algorithm as needed */
04732     if (thee->surfMeth == VSM_MOLSMOOTH) {
04733         fillcoCoefMolDielSmooth(thee);
04734     }
04735 }
04736
04737 VPRIVATE void fillcoCoefMolDielNoSmooth(Vpmg *thee) {
04738
04739     Vacc *acc;
04740     VaccSurf *asurf;
04741     Valist *alist;
04742     Vpbe *pbe;
04743     Vatom *atom;
04744     double xmin, xmax, ymin, ymax, zmin, zmax;
04745     double xlen, ylen, zlen, position[3];
04746     double srad, epsw, epsp, deps, area;
04747     double hx, hy, hzed, *apos, arad;
04748     int i, nx, ny, nz, ntot, iatom, ipt;
04749
04750     /* Get PBE info */
04751     pbe = thee->pbe;
04752     acc = pbe->acc;
04753     alist = pbe->alist;
04754     srad = Vpbe_getSolventRadius(pbe);
04755     epsw = Vpbe_getSolventDiel(pbe);
04756     epsp = Vpbe_getSoluteDiel(pbe);
04757
04758     /* Mesh info */
04759     nx = thee->pmgp->nx;
04760     ny = thee->pmgp->ny;
04761     nz = thee->pmgp->nz;
04762     hx = thee->pmgp->hx;
04763     hy = thee->pmgp->hy;
04764     hzed = thee->pmgp->hzed;
04765
04766     /* Define the total domain size */
04767     xlen = thee->pmgp->xlen;
04768     ylen = thee->pmgp->ylen;
04769     zlen = thee->pmgp->zlen;
04770
04771     /* Define the min/max dimensions */
04772     xmin = thee->pmgp->xcent - (xlen/2.0);
04773     ymin = thee->pmgp->ycent - (ylen/2.0);
04774     zmin = thee->pmgp->zcent - (zlen/2.0);
04775     xmax = thee->pmgp->xcent + (xlen/2.0);
04776     ymax = thee->pmgp->ycent + (ylen/2.0);
04777     zmax = thee->pmgp->zcent + (zlen/2.0);
04778
04779     /* Reset the arrays */
04780     ntot = nx*ny*nz;
04781     for (i=0; i<ntot; i++) {
04782         thee->epsx[i] = epsw;
04783         thee->epsy[i] = epsw;
04784         thee->epsz[i] = epsw;
04785     }
04786
04787     /* Loop through the atoms and set a{123}cf = 0.0 (inaccessible)
04788      * if a point is inside the solvent-inflated van der Waals radii */
04789     #pragma omp parallel for default(shared) private(iatom,atom,apos,arad)
04790     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {

```

```

04791
04792     atom = Valist_getAtom(alist, iatom);
04793     apos = Vatom_getPosition(atom);
04794     arad = Vatom_getRadius(atom);
04795
04796     /* Make sure we're on the grid */
04797     if ((apos[0]<=xmin) || (apos[0]>=xmax) || \
04798         (apos[1]<=ymin) || (apos[1]>=ymax) || \
04799         (apos[2]<=zmin) || (apos[2]>=zmax)) {
04800         if ((thee->pmgp->bcfl != BCFL_FOCUS) &&
04801             (thee->pmgp->bcfl != BCFL_MAP)) {
04802             Vnm_print(2, "Vpmg_fillco: Atom #d at (%4.3f, %4.3f, \
04803 %4.3f) is off the mesh (ignoring):\n",
04804                 iatom, apos[0], apos[1], apos[2]);
04805             Vnm_print(2, "Vpmg_fillco: xmin = %g, xmax = %g\n",
04806                 xmin, xmax);
04807             Vnm_print(2, "Vpmg_fillco: ymin = %g, ymax = %g\n",
04808                 ymin, ymax);
04809             Vnm_print(2, "Vpmg_fillco: zmin = %g, zmax = %g\n",
04810                 zmin, zmax);
04811         }
04812         fflush(stderr);
04813
04814     } else { /* if we're on the mesh */
04815
04816         if (arad > VSMALL) {
04817             /* Mark x-shifted dielectric */
04818             markSphere((arad+srad), apos,
04819                 nx, ny, nz,
04820                 hx, hy, hzed,
04821                 (xmin+0.5*hx), ymin, zmin,
04822                 thee->epsx, epsp);
04823
04824             /* Mark y-shifted dielectric */
04825             markSphere((arad+srad), apos,
04826                 nx, ny, nz,
04827                 hx, hy, hzed,
04828                 xmin, (ymin+0.5*hy), zmin,
04829                 thee->epsy, epsp);
04830
04831             /* Mark z-shifted dielectric */
04832             markSphere((arad+srad), apos,
04833                 nx, ny, nz,
04834                 hx, hy, hzed,
04835                 xmin, ymin, (zmin+0.5*hzed),
04836                 thee->epsz, epsp);
04837         }
04838
04839     } /* endif (on the mesh) */
04840 } /* endfor (over all atoms) */
04841
04842 area = Vacc_SASA(acc, srad);
04843
04844 /* We only need to do the next step for non-zero solvent radii */
04845 if (srad > VSMALL) {
04846
04847     /* Now loop over the solvent accessible surface points */
04848
04849 #pragma omp parallel for default(shared) private(iatom,atom,area,asurf,ipt,position)
04850     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
04851         atom = Valist_getAtom(alist, iatom);
04852         area = Vacc_atomSASA(acc, srad, atom);
04853         if (area > 0.0 ) {
04854             asurf = Vacc_atomSASPoints(acc, srad, atom);
04855
04856             /* Use each point on the SAS to reset the solvent accessibility */
04857             /* TODO: Make sure we're not still wasting time here. */
04858             for (ipt=0; ipt<(asurf->npts); ipt++) {
04859
04860                 position[0] = asurf->xpts[ipt];
04861                 position[1] = asurf->ypts[ipt];
04862                 position[2] = asurf->zpts[ipt];
04863
04864                 /* Mark x-shifted dielectric */
04865                 markSphere(srads, position,
04866                     nx, ny, nz,
04867                     hx, hy, hzed,
04868                     (xmin+0.5*hx), ymin, zmin,
04869                     thee->epsx, epsw);
04870
04871                 /* Mark y-shifted dielectric */

```

```

04872         markSphere(srad, position,
04873                     nx, ny, nz,
04874                     hx, hy, hzed,
04875                     xmin, (ymin+0.5*hy), zmin,
04876                     thee->epsy, epsw);
04877
04878         /* Mark z-shifted dielectric */
04879         markSphere(srad, position,
04880                     nx, ny, nz,
04881                     hx, hy, hzed,
04882                     xmin, ymin, (zmin+0.5*hzed),
04883                     thee->epsz, epsw);
04884
04885     }
04886 }
04887 }
04888 }
04889 }
04890
04891 VPRIVATE void fillcoCoefMolDielSmooth(Vpmg *thee) {
04892
04893     /* This function smoothes using a 9 point method based on
04894        Bruccoleri, et al. J Comput Chem 18 268-276 (1997). The nine points
04895        used are the shifted grid point and the 8 points that are 1/sqrt(2)
04896        grid spacings away. The harmonic mean of the 9 points is then used to
04897        find the overall dielectric value for the point in question. The use of
04898        this function assumes that the non-smoothed values were placed in the
04899        dielectric arrays by the fillcoCoefMolDielNoSmooth function.*/
04900
04901     Vpbe *pbe;
04902     double frac, epsw;
04903     int i, j, k, nx, ny, nz, numpts;
04904
04905     /* Mesh info */
04906     nx = thee->pmgp->nx;
04907     ny = thee->pmgp->ny;
04908     nz = thee->pmgp->nz;
04909
04910     pbe = thee->pbe;
04911     epsw = Vpbe_getSolventDiel(pbe);
04912
04913     /* Copy the existing diel arrays to work arrays */
04914     for (i=0; i<(nx*ny*nz); i++) {
04915         thee->alcx[i] = thee->epsx[i];
04916         thee->a2cf[i] = thee->epsy[i];
04917         thee->a3cf[i] = thee->epsz[i];
04918         thee->epsx[i] = epsw;
04919         thee->epsy[i] = epsw;
04920         thee->epsz[i] = epsw;
04921     }
04922
04923     /* Smooth the dielectric values */
04924     for (i=0; i<nx; i++) {
04925         for (j=0; j<ny; j++) {
04926             for (k=0; k<nz; k++) {
04927
04928                 /* Get the 8 points that are 1/sqrt(2) grid spacings away */
04929
04930                 /* Points for the X-shifted array */
04931                 frac = 1.0/thee->a2cf[IJK(i,j,k)];
04932                 frac += 1.0/thee->a2cf[IJK(i,j,k)];
04933                 frac += 1.0/thee->a3cf[IJK(i,j,k)];
04934                 numpts = 3;
04935
04936                 if (j > 0) {
04937                     frac += 1.0/thee->a2cf[IJK(i,j-1,k)];
04938                     numpts += 1;
04939                 }
04940                 if (k > 0) {
04941                     frac += 1.0/thee->a3cf[IJK(i,j,k-1)];
04942                     numpts += 1;
04943                 }
04944                 if (i < (nx-1)) {
04945                     frac += 1.0/thee->a2cf[IJK(i+1,j,k)];
04946                     frac += 1.0/thee->a3cf[IJK(i+1,j,k)];
04947                     numpts += 2;
04948                     if (j > 0) {
04949                         frac += 1.0/thee->a2cf[IJK(i+1,j-1,k)];
04950                         numpts += 1;
04951                     }
04952                     if (k > 0) {

```

```

04953         frac += 1.0/thee->a3cf[IJK(i+1,j,k-1)];
04954         numpts += 1;
04955     }
04956 }
04957 thee->epsx[IJK(i,j,k)] = numpts/frac;
04958
04959 /* Points for the Y-shifted array */
04960 frac = 1.0/thee->a2cf[IJK(i,j,k)];
04961 frac += 1.0/thee->a1cf[IJK(i,j,k)];
04962 frac += 1.0/thee->a3cf[IJK(i,j,k)];
04963 numpts = 3;
04964
04965 if (i > 0) {
04966     frac += 1.0/thee->a1cf[IJK(i-1,j,k)];
04967     numpts += 1;
04968 }
04969 if (k > 0) {
04970     frac += 1.0/thee->a3cf[IJK(i,j,k-1)];
04971     numpts += 1;
04972 }
04973 if (j < (ny-1)){
04974     frac += 1.0/thee->a1cf[IJK(i,j+1,k)];
04975     frac += 1.0/thee->a3cf[IJK(i,j+1,k)];
04976     numpts += 2;
04977     if (i > 0) {
04978         frac += 1.0/thee->a1cf[IJK(i-1,j+1,k)];
04979         numpts += 1;
04980     }
04981     if (k > 0) {
04982         frac += 1.0/thee->a3cf[IJK(i,j+1,k-1)];
04983         numpts += 1;
04984     }
04985 }
04986 thee->epsy[IJK(i,j,k)] = numpts/frac;
04987
04988 /* Points for the Z-shifted array */
04989 frac = 1.0/thee->a3cf[IJK(i,j,k)];
04990 frac += 1.0/thee->a1cf[IJK(i,j,k)];
04991 frac += 1.0/thee->a2cf[IJK(i,j,k)];
04992 numpts = 3;
04993
04994 if (i > 0) {
04995     frac += 1.0/thee->a1cf[IJK(i-1,j,k)];
04996     numpts += 1;
04997 }
04998 if (j > 0) {
04999     frac += 1.0/thee->a2cf[IJK(i,j-1,k)];
05000     numpts += 1;
05001 }
05002 if (k < (nz-1)){
05003     frac += 1.0/thee->a1cf[IJK(i,j,k+1)];
05004     frac += 1.0/thee->a2cf[IJK(i,j,k+1)];
05005     numpts += 2;
05006     if (i > 0) {
05007         frac += 1.0/thee->a1cf[IJK(i-1,j,k+1)];
05008         numpts += 1;
05009     }
05010     if (j > 0) {
05011         frac += 1.0/thee->a2cf[IJK(i,j-1,k+1)];
05012         numpts += 1;
05013     }
05014 }
05015 thee->epsz[IJK(i,j,k)] = numpts/frac;
05016 }
05017 }
05018 }
05019 }
05020
05021
05022 VPRIVATE void fillCoefSpline(Vpmg *thee) {
05023     Valist *alist;
05024     Vpbe *pbe;
05025     Vatom *atom;
05026     double xmin, xmax, ymin, ymax, zmin, zmax, ionmask, ionstr, dist2;
05027     double xlen, ylen, zlen, position[3], itot, stot, ictot, ictot2, sctot;
05028     double irad, dx, dy, dz, epsw, epsp, w2i;
05029     double hx, hy, hzed, *apos, arad, sctot2;
05030     double dx2, dy2, dz2, stot2, itot2, rtot, rtot2, splineWin, w3i;
05031     double dist, value, sm, sm2;
05032     int i, j, k, nx, ny, nz, iatom;

```

```

05034     int imin, imax, jmin, jmax, kmin, kmax;
05035
05036     VASSERT(thee != VNULL);
05037     splineWin = thee->splineWin;
05038     w2i = 1.0/(splineWin*splineWin);
05039     w3i = 1.0/(splineWin*splineWin*splineWin);
05040
05041     /* Get PBE info */
05042     pbe = thee->pbe;
05043     alist = pbe->alist;
05044     irad = Vpbe_getMaxIonRadius(pbe);
05045     ionstr = Vpbe_getBulkIonicStrength(pbe);
05046     epsw = Vpbe_getSolventDiel(pbe);
05047     epsp = Vpbe_getSoluteDiel(pbe);
05048
05049     /* Mesh info */
05050     nx = thee->pmgp->nx;
05051     ny = thee->pmgp->ny;
05052     nz = thee->pmgp->nz;
05053     hx = thee->pmgp->hx;
05054     hy = thee->pmgp->hy;
05055     hzed = thee->pmgp->hzed;
05056
05057     /* Define the total domain size */
05058     xlen = thee->pmgp->xlen;
05059     ylen = thee->pmgp->ylen;
05060     zlen = thee->pmgp->zlen;
05061
05062     /* Define the min/max dimensions */
05063     xmin = thee->pmgp->xcent - (xlen/2.0);
05064     ymin = thee->pmgp->ycent - (ylen/2.0);
05065     zmin = thee->pmgp->zcent - (zlen/2.0);
05066     xmax = thee->pmgp->xcent + (xlen/2.0);
05067     ymax = thee->pmgp->ycent + (ylen/2.0);
05068     zmax = thee->pmgp->zcent + (zlen/2.0);
05069
05070     /* This is a floating point parameter related to the non-zero nature of the
05071      * bulk ionic strength. If the ionic strength is greater than zero; this
05072      * parameter is set to 1.0 and later scaled by the appropriate pre-factors.
05073      * Otherwise, this parameter is set to 0.0 */
05074     if (ionstr > VPMGSMALL) ionmask = 1.0;
05075     else ionmask = 0.0;
05076
05077     /* Reset the kappa, epsx, epsy, and epsz arrays */
05078     for (i=0; i<(nx*ny*nz); i++) {
05079         thee->kappa[i] = 1.0;
05080         thee->epsx[i] = 1.0;
05081         thee->epsy[i] = 1.0;
05082         thee->epsz[i] = 1.0;
05083     }
05084
05085     /* Loop through the atoms and do assign the dielectric */
05086     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
05087
05088         atom = Valist_getAtom(alist, iatom);
05089         apos = Vatom_getPosition(atom);
05090         arad = Vatom_getRadius(atom);
05091
05092         /* Make sure we're on the grid */
05093         if ((apos[0]<=xmin) || (apos[0]>=xmax) || \
05094             (apos[1]<=ymin) || (apos[1]>=ymax) || \
05095             (apos[2]<=zmin) || (apos[2]>=zmax)) {
05096             if ((thee->pmgp->bcfl != BCFL_FOCUS) &&
05097                 (thee->pmgp->bcfl != BCFL_MAP)) {
05098                 Vnm_print(2, "Vpmg_fillco: Atom #d at (%4.3f, %4.3f,\n
05099 %4.3f) is off the mesh (ignoring):\n",
05100                     iatom, apos[0], apos[1], apos[2]);
05101                 Vnm_print(2, "Vpmg_fillco:      xmin = %g, xmax = %g\n",
05102                     xmin, xmax);
05103                 Vnm_print(2, "Vpmg_fillco:      ymin = %g, ymax = %g\n",
05104                     ymin, ymax);
05105                 Vnm_print(2, "Vpmg_fillco:      zmin = %g, zmax = %g\n",
05106                     zmin, zmax);
05107             }
05108             fflush(stderr);
05109
05110             } else if (arad > VPMGSMALL) { /* if we're on the mesh */
05111
05112                 /* Convert the atom position to grid reference frame */
05113                 position[0] = apos[0] - xmin;
05114                 position[1] = apos[1] - ymin;

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05115     position[2] = apos[2] - zmin;
05116
05117     /* MARK ION ACCESSIBILITY AND DIELECTRIC VALUES FOR LATER
05118      * ASSIGNMENT (Steps #1-3) */
05119     itot = irad + arad + splineWin;
05120     itot2 = VSQR(itot);
05121     ictot = VMAX2(0, (irad + arad - splineWin));
05122     ictot2 = VSQR(ictot);
05123     stot = arad + splineWin;
05124     stot2 = VSQR(stot);
05125     sctot = VMAX2(0, (arad - splineWin));
05126     sctot2 = VSQR(sctot);
05127
05128     /* We'll search over grid points which are in the greater of
05129      * these two radii */
05130     rtot = VMAX2(itot, stot);
05131     rtot2 = VMAX2(itot2, stot2);
05132     dx = rtot + 0.5*hx;
05133     dy = rtot + 0.5*hy;
05134     dz = rtot + 0.5*hzed;
05135     imin = VMAX2(0, (int)floor((position[0] - dx)/hx));
05136     imax = VMIN2(nx-1, (int)ceil((position[0] + dx)/hx));
05137     jmin = VMAX2(0, (int)floor((position[1] - dy)/hy));
05138     jmax = VMIN2(ny-1, (int)ceil((position[1] + dy)/hy));
05139     kmin = VMAX2(0, (int)floor((position[2] - dz)/hzed));
05140     kmax = VMIN2(nz-1, (int)ceil((position[2] + dz)/hzed));
05141     for (i=imin; i<=imax; i++) {
05142         dx2 = VSQR(position[0] - hx*i);
05143         for (j=jmin; j<=jmax; j++) {
05144             dy2 = VSQR(position[1] - hy*j);
05145             for (k=kmin; k<=kmax; k++) {
05146                 dz2 = VSQR(position[2] - k*hzed);
05147
05148                 /* ASSIGN CCF */
05149                 if (thee->kappa[IJK(i,j,k)] > VPMGSMALL) {
05150                     dist2 = dz2 + dy2 + dx2;
05151                     if (dist2 >= itot2) {
05152                         ;
05153                     }
05154                     if (dist2 <= ictot2) {
05155                         thee->kappa[IJK(i,j,k)] = 0.0;
05156                     }
05157                     if ((dist2 < itot2) && (dist2 > ictot2)) {
05158                         dist = VSQRT(dist2);
05159                         sm = dist - (arad + irad) + splineWin;
05160                         sm2 = VSQR(sm);
05161                         value = 0.75*sm2*w2i - 0.25*sm*sm2*w3i;
05162                         thee->kappa[IJK(i,j,k)] *= value;
05163                     }
05164                 }
05165
05166                 /* ASSIGN A1CF */
05167                 if (thee->epsx[IJK(i,j,k)] > VPMGSMALL) {
05168                     dist2 = dz2+dy2+VSQR(position[0]-(i+0.5)*hx);
05169                     if (dist2 >= stot2) {
05170                         thee->epsx[IJK(i,j,k)] *= 1.0;
05171                     }
05172                     if (dist2 <= sctot2) {
05173                         thee->epsx[IJK(i,j,k)] = 0.0;
05174                     }
05175                     if ((dist2 > sctot2) && (dist2 < stot2)) {
05176                         dist = VSQRT(dist2);
05177                         sm = dist - arad + splineWin;
05178                         sm2 = VSQR(sm);
05179                         value = 0.75*sm2*w2i - 0.25*sm*sm2*w3i;
05180                         thee->epsx[IJK(i,j,k)] *= value;
05181                     }
05182                 }
05183
05184                 /* ASSIGN A2CF */
05185                 if (thee->epsy[IJK(i,j,k)] > VPMGSMALL) {
05186                     dist2 = dz2+dx2+VSQR(position[1]-(j+0.5)*hy);
05187                     if (dist2 >= stot2) {
05188                         thee->epsy[IJK(i,j,k)] *= 1.0;
05189                     }
05190                     if (dist2 <= sctot2) {
05191                         thee->epsy[IJK(i,j,k)] = 0.0;
05192                     }
05193                     if ((dist2 > sctot2) && (dist2 < stot2)) {
05194                         dist = VSQRT(dist2);
05195                         sm = dist - arad + splineWin;

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```

05196             sm2 = VSQR(sm);
05197             value = 0.75*sm2*w2i - 0.25*sm*sm2*w3i;
05198             thee->epsy[IJK(i,j,k)] *= value;
05199         }
05200     }
05201
05202     /* ASSIGN A3CF */
05203     if (thee->epsz[IJK(i,j,k)] > VPMGSMALL) {
05204         dist2 = dy2+dx2+VSQR(position[2]-(k+0.5)*hzd);
05205         if (dist2 >= stot2) {
05206             thee->epsz[IJK(i,j,k)] *= 1.0;
05207         }
05208         if (dist2 <= sctot2) {
05209             thee->epsz[IJK(i,j,k)] = 0.0;
05210         }
05211         if ((dist2 > sctot2) && (dist2 < stot2)) {
05212             dist = VSQR(dist2);
05213             sm = dist - arad + splineWin;
05214             sm2 = VSQR(sm);
05215             value = 0.75*sm2*w2i - 0.25*sm*sm2*w3i;
05216             thee->epsz[IJK(i,j,k)] *= value;
05217         }
05218     }
05219
05220     } /* k loop */
05221 } /* j loop */
05222 } /* i loop */
05223 } /* endif (on the mesh) */
05224 } /* endfor (over all atoms) */
05225
05226 Vnm_print(0, "Vpmg_fillco: filling coefficient arrays\n");
05227 /* Interpret markings and fill the coefficient arrays */
05228 for (k=0; k<nz; k++) {
05229     for (j=0; j<ny; j++) {
05230         for (i=0; i<nx; i++) {
05231             thee->kappa[IJK(i,j,k)] = ionmask*thee->kappa[IJK(i,j,k)];
05232             thee->epsx[IJK(i,j,k)] = (epsw-epsp)*thee->epsx[IJK(i,j,k)]
05233             + epsp;
05234             thee->epsy[IJK(i,j,k)] = (epsw-epsp)*thee->epsy[IJK(i,j,k)]
05235             + epsp;
05236             thee->epsz[IJK(i,j,k)] = (epsw-epsp)*thee->epsz[IJK(i,j,k)]
05237             + epsp;
05238         } /* i loop */
05239     } /* j loop */
05240 } /* k loop */
05241
05242 }
05243
05244 VPRIVATE void fillcoCoef(Vpmg *thee) {
05245     VASSERT(thee != VNULL);
05246
05247     if (thee->useDielXMap || thee->useDielYMap ||
05248         thee->useDielZMap || thee->useKappaMap) {
05249         fillcoCoefMap(thee);
05250         return;
05251     }
05252
05253     switch(thee->surfMeth) {
05254     case VSM_MOL:
05255         Vnm_print(0, "fillcoCoef: Calling fillcoCoefMol...\n");
05256         fillcoCoefMol(thee);
05257         break;
05258     case VSM_MOLSMOOTH:
05259         Vnm_print(0, "fillcoCoef: Calling fillcoCoefMol...\n");
05260         fillcoCoefMol(thee);
05261         break;
05262     case VSM_SPLINE:
05263         Vnm_print(0, "fillcoCoef: Calling fillcoCoefSpline...\n");
05264         fillcoCoefSpline(thee);
05265         break;
05266     case VSM_SPLINE3:
05267         Vnm_print(0, "fillcoCoef: Calling fillcoCoefSpline3...\n");
05268         fillcoCoefSpline3(thee);
05269         break;
05270     case VSM_SPLINE4:
05271         Vnm_print(0, "fillcoCoef: Calling fillcoCoefSpline4...\n");
05272         fillcoCoefSpline4(thee);
05273     }
05274 }

```



```

05277         break;
05278     default:
05279         Vnm_print(2, "fillcoCoef: Invalid surfMeth (%d)!\n",
05280             thee->surfMeth);
05281         VASSERT(0);
05282         break;
05283     }
05284 }
05285
05286
05287 VPRIVATE Vrc_Codes fillcoCharge(Vpmg *thee) {
05288     Vrc_Codes rc;
05289
05290     VASSERT(thee != VNULL);
05291
05292     if (thee->useChargeMap) {
05293         return fillcoChargeMap(thee);
05294     }
05295
05296     switch(thee->chargeMeth) {
05297     case VCM_TRIL:
05298         Vnm_print(0, "fillcoCharge: Calling fillcoChargeSpline1...\n");
05299         fillcoChargeSpline1(thee);
05300         break;
05301     case VCM_BSPL2:
05302         Vnm_print(0, "fillcoCharge: Calling fillcoChargeSpline2...\n");
05303         fillcoChargeSpline2(thee);
05304         break;
05305     case VCM_BSPL4:
05306         switch (thee->chargeSrc) {
05307         case VCM_CHARGE:
05308             Vnm_print(0, "fillcoCharge: Calling fillcoPermanentMultipole...\n");
05309             fillcoPermanentMultipole(thee);
05310             break;
05311         #if defined(WITH_TINKER)
05312         case VCM_PERMANENT:
05313             Vnm_print(0, "fillcoCharge: Calling fillcoPermanentMultipole...\n");
05314             fillcoPermanentMultipole(thee);
05315             break;
05316         case VCM_INDUCED:
05317             Vnm_print(0, "fillcoCharge: Calling fillcoInducedDipole...\n");
05318             fillcoInducedDipole(thee);
05319             break;
05320         case VCM_NLINDUCED:
05321             Vnm_print(0, "fillcoCharge: Calling fillcoNLInducedDipole...\n");
05322             fillcoNLInducedDipole(thee);
05323             break;
05324         #endif /* if defined(WITH_TINKER) */
05325         default:
05326             Vnm_print(2, "fillcoCharge: Invalid chargeSource (%d)!\n",
05327                 thee->chargeSrc);
05328             return VRC_FAILURE;
05329             break;
05330         }
05331     }
05332     break;
05333     default:
05334         Vnm_print(2, "fillcoCharge: Invalid chargeMeth (%d)!\n",
05335             thee->chargeMeth);
05336         return VRC_FAILURE;
05337         break;
05338     }
05339
05340     return VRC_SUCCESS;
05341 }
05342
05343 VPRIVATE Vrc_Codes fillcoChargeMap(Vpmg *thee) {
05344     Vpbe *pbe;
05345     double position[3], charge, zmagic, hx, hy, hzed;
05346     int i, j, k, nx, ny, nz, rc;
05347
05348     VASSERT(thee != VNULL);
05349
05350     /* Get PBE info */
05351     pbe = thee->pbe;
05352     zmagic = Vpbe_getZmagic(pbe);
05353
05354     /* Mesh info */
05355     nx = thee->pmgp->nx;

```

```

05358     ny = thee->pmgp->ny;
05359     nz = thee->pmgp->nz;
05360     hx = thee->pmgp->hx;
05361     hy = thee->pmgp->hy;
05362     hzed = thee->pmgp->hzed;
05363
05364     /* Reset the charge array */
05365     for (i=0; i<(nx*ny*nz); i++) thee->charge[i] = 0.0;
05366
05367     /* Fill in the source term (atomic charges) */
05368     Vnm_print(0, "Vpmg_fillco: filling in source term.\n");
05369     for (k=0; k<nz; k++) {
05370         for (j=0; j<ny; j++) {
05371             for (i=0; i<nx; i++) {
05372                 position[0] = thee->xf[i];
05373                 position[1] = thee->yf[j];
05374                 position[2] = thee->zf[k];
05375                 rc = Vgrid_value(thee->chargeMap, position, &charge);
05376                 if (!rc) {
05377                     Vnm_print(2, "fillcoChargeMap: Error -- fell off of charge map at (%g, %g, %g)!\n",
05378                             position[0], position[1], position[2]);
05379                     return VRC_FAILURE;
05380                 }
05381                 /* Scale the charge to internal units */
05382                 charge = charge*zmagic;
05383                 thee->charge[IJK(i,j,k)] = charge;
05384             }
05385         }
05386     }
05387
05388     return VRC_SUCCESS;
05389 }
05390
05391 VPRIVATE void fillcoChargeSpline1(Vpmg *thee) {
05392
05393     Valist *alist;
05394     Vpbe *pbe;
05395     Vatom *atom;
05396     double xmin, xmax, ymin, ymax, zmin, zmax;
05397     double xlen, ylen, zlen, position[3], ifloat, jfloat, kfloat;
05398     double charge, dx, dy, dz, zmagic, hx, hy, hzed, *apos;
05399     int i, nx, ny, nz, iatom, ihi, ilo, jhi, jlo, khi, klo;
05400
05401
05402     VASSERT(thee != VNULL);
05403
05404     /* Get PBE info */
05405     pbe = thee->pbe;
05406     alist = pbe->alist;
05407     zmagic = Vpbe_getZmagic(pbe);
05408
05409     /* Mesh info */
05410     nx = thee->pmgp->nx;
05411     ny = thee->pmgp->ny;
05412     nz = thee->pmgp->nz;
05413     hx = thee->pmgp->hx;
05414     hy = thee->pmgp->hy;
05415     hzed = thee->pmgp->hzed;
05416
05417     /* Define the total domain size */
05418     xlen = thee->pmgp->xlen;
05419     ylen = thee->pmgp->ylen;
05420     zlen = thee->pmgp->zlen;
05421
05422     /* Define the min/max dimensions */
05423     xmin = thee->pmgp->xcent - (xlen/2.0);
05424     ymin = thee->pmgp->ycent - (ylen/2.0);
05425     zmin = thee->pmgp->zcent - (zlen/2.0);
05426     xmax = thee->pmgp->xcent + (xlen/2.0);
05427     ymax = thee->pmgp->ycent + (ylen/2.0);
05428     zmax = thee->pmgp->zcent + (zlen/2.0);
05429
05430     /* Reset the charge array */
05431     for (i=0; i<(nx*ny*nz); i++) thee->charge[i] = 0.0;
05432
05433     /* Fill in the source term (atomic charges) */
05434     Vnm_print(0, "Vpmg_fillco: filling in source term.\n");
05435     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
05436
05437         atom = Valist_getAtom(alist, iatom);
05438         apos = Vatom_getPosition(atom);

```

```

05439     charge = Vatom_getCharge(atom);
05440
05441     /* Make sure we're on the grid */
05442     if ((apos[0]<=xmin) || (apos[0]>=xmax) || \
05443         (apos[1]<=ymin) || (apos[1]>=ymax) || \
05444         (apos[2]<=zmin) || (apos[2]>=zmax)) {
05445         if ((thee->pmgp->bcfl != BCFL_FOCUS) &&
05446             (thee->pmgp->bcfl != BCFL_MAP)) {
05447             Vnm_print(2, "Vpmg_fillco: Atom #d at (%4.3f, %4.3f, \
05448 %4.3f) is off the mesh (ignoring):\n",
05449                 iatom, apos[0], apos[1], apos[2]);
05450             Vnm_print(2, "Vpmg_fillco:   xmin = %g, xmax = %g\n",
05451                 xmin, xmax);
05452             Vnm_print(2, "Vpmg_fillco:   ymin = %g, ymax = %g\n",
05453                 ymin, ymax);
05454             Vnm_print(2, "Vpmg_fillco:   zmin = %g, zmax = %g\n",
05455                 zmin, zmax);
05456         }
05457         fflush(stderr);
05458     } else {
05459
05460         /* Convert the atom position to grid reference frame */
05461         position[0] = apos[0] - xmin;
05462         position[1] = apos[1] - ymin;
05463         position[2] = apos[2] - zmin;
05464
05465         /* Scale the charge to be a delta function */
05466         charge = charge*zmagic/(hx*hy*hzed);
05467
05468         /* Figure out which vertices we're next to */
05469         ifloat = position[0]/hx;
05470         jfloat = position[1]/hy;
05471         kfloat = position[2]/hzed;
05472
05473         ihi = (int)ceil(ifloat);
05474         ilo = (int)floor(ifloat);
05475         jhi = (int)ceil(jfloat);
05476         jlo = (int)floor(jfloat);
05477         khi = (int)ceil(kfloat);
05478         klo = (int)floor(kfloat);
05479
05480         /* Now assign fractions of the charge to the nearby verts */
05481         dx = ifloat - (double)(ilo);
05482         dy = jfloat - (double)(jlo);
05483         dz = kfloat - (double)(klo);
05484         thee->charge[IJK(ihi, jhi, khi)] += (dx*dy*dz*charge);
05485         thee->charge[IJK(ihi, jlo, khi)] += (dx*(1.0-dy)*dz*charge);
05486         thee->charge[IJK(ihi, jhi, klo)] += (dx*dy*(1.0-dz)*charge);
05487         thee->charge[IJK(ihi, jlo, klo)] += (dx*(1.0-dy)*(1.0-dz)*charge);
05488         thee->charge[IJK(ilo, jhi, khi)] += ((1.0-dx)*dy*dz *charge);
05489         thee->charge[IJK(ilo, jlo, khi)] += ((1.0-dx)*(1.0-dy)*dz *charge);
05490         thee->charge[IJK(ilo, jhi, klo)] += ((1.0-dx)*dy*(1.0-dz)*charge);
05491         thee->charge[IJK(ilo, jlo, klo)] += ((1.0-dx)*(1.0-dy)*(1.0-dz)*charge);
05492     } /* endif (on the mesh) */
05493 } /* endfor (each atom) */
05494 }
05495
05496 VPRIVATE double bspline2(double x) {
05497     double m2m, m2, m3;
05498
05499     if ((x >= 0.0) && (x <= 2.0)) m2m = 1.0 - VABS(x - 1.0);
05500     else m2m = 0.0;
05501     if ((x >= 1.0) && (x <= 3.0)) m2 = 1.0 - VABS(x - 2.0);
05502     else m2 = 0.0;
05503
05504     if ((x >= 0.0) && (x <= 3.0)) m3 = 0.5*x*m2m + 0.5*(3.0-x)*m2;
05505     else m3 = 0.0;
05506
05507     return m3;
05508 }
05509
05510 }
05511
05512 VPRIVATE double dbspline2(double x) {
05513     double m2m, m2, dm3;
05514
05515     if ((x >= 0.0) && (x <= 2.0)) m2m = 1.0 - VABS(x - 1.0);
05516     else m2m = 0.0;
05517     if ((x >= 1.0) && (x <= 3.0)) m2 = 1.0 - VABS(x - 2.0);
05518     else m2 = 0.0;

```

```

05520
05521     dm3 = m2m - m2;
05522
05523     return dm3;
05524
05525 }
05526
05527
05528 VPRIVATE void fillcoChargeSpline2(Vpmg *thee) {
05529
05530     Valist *alist;
05531     Vpbe *pbe;
05532     Vatom *atom;
05533     double xmin, xmax, ymin, ymax, zmin, zmax, zmagic;
05534     double xlen, ylen, zlen, position[3], ifloat, jfloat, kfloat;
05535     double charge, hx, hy, hzed, *apos, mx, my, mz;
05536     int i, ii, jj, kk, nx, ny, nz, iatom;
05537     int im2, im1, ip1, ip2, jm2, jm1, jp1, jp2, km2, km1, kp1, kp2;
05538
05539
05540     VASSERT(thee != VNULL);
05541
05542     /* Get PBE info */
05543     pbe = thee->pbe;
05544     alist = pbe->alist;
05545     zmagic = Vpbe_getZmagic(pbe);
05546
05547     /* Mesh info */
05548     nx = thee->pmgp->nx;
05549     ny = thee->pmgp->ny;
05550     nz = thee->pmgp->nz;
05551     hx = thee->pmgp->hx;
05552     hy = thee->pmgp->hy;
05553     hzed = thee->pmgp->hzed;
05554
05555     /* Define the total domain size */
05556     xlen = thee->pmgp->xlen;
05557     ylen = thee->pmgp->ylen;
05558     zlen = thee->pmgp->zlen;
05559
05560     /* Define the min/max dimensions */
05561     xmin = thee->pmgp->xcent - (xlen/2.0);
05562     ymin = thee->pmgp->ycent - (ylen/2.0);
05563     zmin = thee->pmgp->zcent - (zlen/2.0);
05564     xmax = thee->pmgp->xcent + (xlen/2.0);
05565     ymax = thee->pmgp->ycent + (ylen/2.0);
05566     zmax = thee->pmgp->zcent + (zlen/2.0);
05567
05568     /* Reset the charge array */
05569     for (i=0; i<(nx*ny*nz); i++) thee->charge[i] = 0.0;
05570
05571     /* Fill in the source term (atomic charges) */
05572     Vnm_print(0, "Vpmg_fillco: filling in source term.\n");
05573     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
05574
05575         atom = Valist_getAtom(alist, iatom);
05576         apos = Vatom_getPosition(atom);
05577         charge = Vatom_getCharge(atom);
05578
05579         /* Make sure we're on the grid */
05580         if ((apos[0]<=(xmin-hx)) || (apos[0]>=(xmax+hx)) || \
05581             (apos[1]<=(ymin-hy)) || (apos[1]>=(ymax+hy)) || \
05582             (apos[2]<=(zmin-hzed)) || (apos[2]>=(zmax+hzed))) {
05583             if ((thee->pmgp->bcfl != BCFL_FOCUS) &&
05584                 (thee->pmgp->bcfl != BCFL_MAP)) {
05585                 Vnm_print(2, "Vpmg_fillco: Atom #d at (%4.3f, %4.3f, \
05586 %4.3f) is off the mesh (for cubic splines!!) (ignoring this atom):\n",
05587                     iatom, apos[0], apos[1], apos[2]);
05588                 Vnm_print(2, "Vpmg_fillco:      xmin = %g, xmax = %g\n",
05589                     xmin, xmax);
05590                 Vnm_print(2, "Vpmg_fillco:      ymin = %g, ymax = %g\n",
05591                     ymin, ymax);
05592                 Vnm_print(2, "Vpmg_fillco:      zmin = %g, zmax = %g\n",
05593                     zmin, zmax);
05594             }
05595             fflush(stderr);
05596         } else {
05597
05598             /* Convert the atom position to grid reference frame */
05599             position[0] = apos[0] - xmin;
05600             position[1] = apos[1] - ymin;

```

```

05601         position[2] = apos[2] - zmin;
05602
05603         /* Scale the charge to be a delta function */
05604         charge = charge*zmagic/(hx*hy*hzed);
05605
05606         /* Figure out which vertices we're next to */
05607         ifloat = position[0]/hx;
05608         jfloat = position[1]/hy;
05609         kfloat = position[2]/hzed;
05610
05611         ip1 = (int)ceil(ifloat);
05612         ip2 = ip1 + 1;
05613         im1 = (int)floor(ifloat);
05614         im2 = im1 - 1;
05615         jp1 = (int)ceil(jfloat);
05616         jp2 = jp1 + 1;
05617         jm1 = (int)floor(jfloat);
05618         jm2 = jm1 - 1;
05619         kp1 = (int)ceil(kfloat);
05620         kp2 = kp1 + 1;
05621         km1 = (int)floor(kfloat);
05622         km2 = km1 - 1;
05623
05624         /* This step shouldn't be necessary, but it saves nasty debugging
05625          * later on if something goes wrong */
05626         ip2 = VMIN2(ip2,nx-1);
05627         ip1 = VMIN2(ip1,nx-1);
05628         im1 = VMAX2(im1,0);
05629         im2 = VMAX2(im2,0);
05630         jp2 = VMIN2(jp2,ny-1);
05631         jp1 = VMIN2(jp1,ny-1);
05632         jm1 = VMAX2(jm1,0);
05633         jm2 = VMAX2(jm2,0);
05634         kp2 = VMIN2(kp2,nz-1);
05635         kp1 = VMIN2(kp1,nz-1);
05636         km1 = VMAX2(km1,0);
05637         km2 = VMAX2(km2,0);
05638
05639         /* Now assign fractions of the charge to the nearby verts */
05640         for (ii=im2; ii<=ip2; ii++) {
05641             mx = bspline2(VFCHI(ii,ifloat));
05642             for (jj=jm2; jj<=jp2; jj++) {
05643                 my = bspline2(VFCHI(jj,jfloat));
05644                 for (kk=km2; kk<=kp2; kk++) {
05645                     mz = bspline2(VFCHI(kk,kfloat));
05646                     thee->charge[IJK(ii,jj,kk)] += (charge*mx*my*mz);
05647                 }
05648             }
05649         }
05650     } /* endif (on the mesh) */
05651 } /* endfor (each atom) */
05652 }
05653
05654
05655 VPUBLIC int Vpmg_fillco(Vpmg *thee,
05656                        Vsurf_Meth surfMeth,
05657                        double splineWin,
05658                        Vchrg_Meth chargeMeth,
05659                        int useDielXMap,
05660                        Vgrid *dielXMap,
05661                        int useDielYMap,
05662                        Vgrid *dielYMap,
05663                        int useDielZMap,
05664                        Vgrid *dielZMap,
05665                        int useKappaMap,
05666                        Vgrid *kappaMap,
05667                        int usePotMap,
05668                        Vgrid *potMap,
05669                        int useChargeMap,
05670                        Vgrid *chargeMap
05671                ) {
05672
05673     Vpbe *pbe;
05674     double xmin,
05675            xmax,
05676            ymin,
05677            ymax,
05678            zmin,
05679            zmax,
05680            xlen,
05681            ylen,

```

```

05682         zlen,
05683         hx,
05684         hy,
05685         hzed,
05686         epsw,
05687         epsp,
05688         ionstr;
05689     int i,
05690         nx,
05691         ny,
05692         nz,
05693         islap;
05694     Vrc_Codes rc;
05695
05696     if (thee == VNULL) {
05697         Vnm_print(2, "Vpmg_fillco: got NULL thee!\n");
05698         return 0;
05699     }
05700
05701     thee->surfMeth = surfMeth;
05702     thee->splineWin = splineWin;
05703     thee->chargeMeth = chargeMeth;
05704     thee->useDielXMap = useDielXMap;
05705     if (thee->useDielXMap) thee->dielXMap = dielXMap;
05706     thee->useDielYMap = useDielYMap;
05707     if (thee->useDielYMap) thee->dielYMap = dielYMap;
05708     thee->useDielZMap = useDielZMap;
05709     if (thee->useDielZMap) thee->dielZMap = dielZMap;
05710     thee->useKappaMap = useKappaMap;
05711     if (thee->useKappaMap) thee->kappaMap = kappaMap;
05712     thee->usePotMap = usePotMap;
05713     if (thee->usePotMap) thee->potMap = potMap;
05714     thee->useChargeMap = useChargeMap;
05715     if (thee->useChargeMap) thee->chargeMap = chargeMap;
05716
05717     /* Get PBE info */
05718     pbe = thee->pbe;
05719     ionstr = Vpbe_getBulkIonicStrength(pbe);
05720     epsw = Vpbe_getSolventDiel(pbe);
05721     epsp = Vpbe_getSoluteDiel(pbe);
05722
05723     /* Mesh info */
05724     nx = thee->pmgp->nx;
05725     ny = thee->pmgp->ny;
05726     nz = thee->pmgp->nz;
05727     hx = thee->pmgp->hx;
05728     hy = thee->pmgp->hy;
05729     hzed = thee->pmgp->hzed;
05730
05731     /* Define the total domain size */
05732     xlen = thee->pmgp->xlen;
05733     ylen = thee->pmgp->ylen;
05734     zlen = thee->pmgp->zlen;
05735
05736     /* Define the min/max dimensions */
05737     xmin = thee->pmgp->xcent - (xlen/2.0);
05738     thee->pmgp->xmin = xmin;
05739     ymin = thee->pmgp->ycent - (ylen/2.0);
05740     thee->pmgp->ymin = ymin;
05741     zmin = thee->pmgp->zcent - (zlen/2.0);
05742     thee->pmgp->zmin = zmin;
05743     xmax = thee->pmgp->xcent + (xlen/2.0);
05744     thee->pmgp->xmax = xmax;
05745     ymax = thee->pmgp->ycent + (ylen/2.0);
05746     thee->pmgp->ymax = ymax;
05747     zmax = thee->pmgp->zcent + (zlen/2.0);
05748     thee->pmgp->zmax = zmax;
05749     thee->rparm[2] = xmin;
05750     thee->rparm[3] = xmax;
05751     thee->rparm[4] = ymin;
05752     thee->rparm[5] = ymax;
05753     thee->rparm[6] = zmin;
05754     thee->rparm[7] = zmax;
05755
05756     /* This is a flag that gets set if the operator is a simple Laplacian;
05757      * i.e., in the case of a homogenous dielectric and zero ionic strength
05758      * The operator cannot be a simple Laplacian if maps are read in. */
05759     if (thee->useDielXMap || thee->useDielYMap || thee->useDielZMap ||
05760         thee->useKappaMap || thee->usePotMap){
05761         islap = 0;
05762     }else if ( (ionstr < VPMGSMALL) && (VABS(epsp-epsw) < VPMGSMALL) ){

```

```

05763     islap = 1;
05764 }else{
05765     islap = 0;
05766 }
05767
05768 /* Fill the mesh point coordinate arrays */
05769 for (i=0; i<nx; i++) thee->xf[i] = xmin + i*hx;
05770 for (i=0; i<ny; i++) thee->yf[i] = ymin + i*hy;
05771 for (i=0; i<nz; i++) thee->zf[i] = zmin + i*hzed;
05772
05773 /* Reset the tcf array */
05774 for (i=0; i<(nx*ny*nz); i++) thee->tcf[i] = 0.0;
05775
05776 /* Fill in the source term (atomic charges) */
05777 Vnm_print(0, "Vpmg_fillco: filling in source term.\n");
05778 rc = fillcoCharge(thee);
05779 switch(rc) {
05780     case VRC_SUCCESS:
05781         break;
05782     case VRC_WARNING:
05783         Vnm_print(2, "Vpmg_fillco: non-fatal errors while filling charge map!\n");
05784         break;
05785     case VRC_FAILURE:
05786         Vnm_print(2, "Vpmg_fillco: fatal errors while filling charge map!\n");
05787         return 0;
05788         break;
05789 }
05790
05791 /* THE FOLLOWING NEEDS TO BE DONE IF WE'RE NOT USING A SIMPLE LAPLACIAN
05792  * OPERATOR */
05793 if (!islap) {
05794     Vnm_print(0, "Vpmg_fillco: marking ion and solvent accessibility.\n");
05795     fillcoCoef(thee);
05796     Vnm_print(0, "Vpmg_fillco: done filling coefficient arrays\n");
05797 } else { /* else (!islap) ==> It's a Laplacian operator! */
05798
05799     for (i=0; i<(nx*ny*nz); i++) {
05800         thee->kappa[i] = 0.0;
05801         thee->epsx[i] = epsp;
05802         thee->epsy[i] = epsp;
05803         thee->epsz[i] = epsp;
05804     }
05805 }
05806
05807 } /* endif (!islap) */
05808
05809 /* Fill the boundary arrays (except when focusing, bcfl = 4) */
05810 if (thee->pmp->bcfl != BCFI_FOCUS) {
05811     Vnm_print(0, "Vpmg_fillco: filling boundary arrays\n");
05812     bcCalc(thee);
05813     Vnm_print(0, "Vpmg_fillco: done filling boundary arrays\n");
05814 }
05815
05816 thee->filled = 1;
05817
05818 return 1;
05819 }
05820
05821
05822 VPUBLIC int Vpmg_force(Vpmg *thee, double *force, int atomID,
05823     Vsurf_Meth srfm, Vchrg_Meth chgm) {
05824
05825     int rc = 1;
05826     double qfF[3]; /* Charge-field force */
05827     double dbF[3]; /* Dielectric boundary force */
05828     double ibF[3]; /* Ion boundary force */
05829     double npF[3]; /* Non-polar boundary force */
05830
05831     VASSERT(thee != VNULL);
05832
05833     rc = rc && Vpmg_dbForce(thee, qfF, atomID, srfm);
05834     rc = rc && Vpmg_ibForce(thee, dbF, atomID, srfm);
05835     rc = rc && Vpmg_qfForce(thee, ibF, atomID, chgm);
05836
05837     force[0] = qfF[0] + dbF[0] + ibF[0];
05838     force[1] = qfF[1] + dbF[1] + ibF[1];
05839     force[2] = qfF[2] + dbF[2] + ibF[2];
05840
05841     return rc;
05842 }
05843 }

```

```

05844
05845 VPUBLIC int Vpmg_ibForce(Vpmg *thee, double *force, int atomID,
05846     Vsurf_Meth srfm) {
05847
05848     Valist *alist;
05849     Vacc *acc;
05850     Vpbe *pbe;
05851     Vatom *atom;
05852
05853     double *apos, position[3], arad, irad, zkappa2, hx, hy, hzed;
05854     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax, rtot2;
05855     double rtot, dx, dx2, dy, dy2, dz, dz2, gpos[3], tgrad[3], fmag;
05856     double izmagic;
05857     int i, j, k, nx, ny, nz, imin, imax, jmin, jmax, kmin, kmax;
05858
05859     /* For nonlinear forces */
05860     int ichop, nchop, nion, m;
05861     double ionConc[MAXION], ionRadii[MAXION], ionQ[MAXION], ionstr;
05862
05863     VASSERT(thee != VNULL);
05864
05865     acc = thee->pbe->acc;
05866     atom = Valist_getAtom(thee->pbe->alist, atomID);
05867     apos = Vatom_getPosition(atom);
05868     arad = Vatom_getRadius(atom);
05869
05870     /* Reset force */
05871     force[0] = 0.0;
05872     force[1] = 0.0;
05873     force[2] = 0.0;
05874
05875     /* Check surface definition */
05876     if ((srfm != VSM_SPLINE) && (srfm!=VSM_SPLINE3) && (srfm!=VSM_SPLINE4)) {
05877         Vnm_print(2, "Vpmg_ibForce: Forces *must* be calculated with \
05878 spline-based surfaces!\n");
05879         Vnm_print(2, "Vpmg_ibForce: Skipping ionic boundary force \
05880 calculation!\n");
05881         return 0;
05882     }
05883
05884     /* If we aren't in the current position, then we're done */
05885     if (atom->partID == 0) return 1;
05886
05887     /* Get PBE info */
05888     pbe = thee->pbe;
05889     acc = pbe->acc;
05890     alist = pbe->alist;
05891     irad = Vpbe_getMaxIonRadius(pbe);
05892     zkappa2 = Vpbe_getZkappa2(pbe);
05893     izmagic = 1.0/Vpbe_getZmagic(pbe);
05894
05895     ionstr = Vpbe_getBulkIonicStrength(pbe);
05896     Vpbe_getIons(pbe, &nion, ionConc, ionRadii, ionQ);
05897
05898     /* Mesh info */
05899     nx = thee->pmgp->nx;
05900     ny = thee->pmgp->ny;
05901     nz = thee->pmgp->nz;
05902     hx = thee->pmgp->hx;
05903     hy = thee->pmgp->hy;
05904     hzed = thee->pmgp->hzed;
05905     xlen = thee->pmgp->xlen;
05906     ylen = thee->pmgp->ylen;
05907     zlen = thee->pmgp->zlen;
05908     xmin = thee->pmgp->xmin;
05909     ymin = thee->pmgp->ymin;
05910     zmin = thee->pmgp->zmin;
05911     xmax = thee->pmgp->xmax;
05912     ymax = thee->pmgp->ymax;
05913     zmax = thee->pmgp->zmax;
05914
05915     /* Sanity check: there is no force if there is zero ionic strength */
05916     if (zkappa2 < VPMGSMALL) {
05917 #ifndef VAPBSQUIET
05918         Vnm_print(2, "Vpmg_ibForce: No force for zero ionic strength!\n");
05919 #endif
05920         return 1;
05921     }
05922
05923     /* Make sure we're on the grid */
05924     if ((apos[0]<=xmin) || (apos[0]>=xmax) || \

```



```

05925     (apos[1]<=ymin) || (apos[1]>=ymax) || \
05926     (apos[2]<=zmin) || (apos[2]>=zmax)) {
05927         if ((thee->pmgp->bcfl != BCFL_FOCUS) &&
05928             (thee->pmgp->bcfl != BCFL_MAP)) {
05929             Vnm_print(2, "Vpmg_ibForce: Atom #d at (%4.3f, %4.3f, %4.3f) is off the mesh (ignoring):\n",
05930                 atom, apos[0], apos[1], apos[2]);
05931             Vnm_print(2, "Vpmg_ibForce:      xmin = %g, xmax = %g\n",
05932                 xmin, xmax);
05933             Vnm_print(2, "Vpmg_ibForce:      ymin = %g, ymax = %g\n",
05934                 ymin, ymax);
05935             Vnm_print(2, "Vpmg_ibForce:      zmin = %g, zmax = %g\n",
05936                 zmin, zmax);
05937         }
05938         fflush(stderr);
05939     } else {
05940
05941         /* Convert the atom position to grid reference frame */
05942         position[0] = apos[0] - xmin;
05943         position[1] = apos[1] - ymin;
05944         position[2] = apos[2] - zmin;
05945
05946         /* Integrate over points within this atom's (inflated) radius */
05947         rtot = (irad + arad + thee->splineWin);
05948         rtot2 = VSQR(rtot);
05949         dx = rtot + 0.5*hx;
05950         imin = VMAX2(0, (int)ceil((position[0] - dx)/hx));
05951         imax = VMIN2(nx-1, (int)floor((position[0] + dx)/hx));
05952         for (i=imin; i<=imax; i++) {
05953             dx2 = VSQR(position[0] - hx*i);
05954             if (rtot2 > dx2) dy = VSQR(rtot2 - dx2) + 0.5*hy;
05955             else dy = 0.5*hy;
05956             jmin = VMAX2(0, (int)ceil((position[1] - dy)/hy));
05957             jmax = VMIN2(ny-1, (int)floor((position[1] + dy)/hy));
05958             for (j=jmin; j<=jmax; j++) {
05959                 dy2 = VSQR(position[1] - hy*j);
05960                 if (rtot2 > (dx2+dy2)) dz = VSQR(rtot2-dx2-dy2)+0.5*hzed;
05961                 else dz = 0.5*hzed;
05962                 kmin = VMAX2(0, (int)ceil((position[2] - dz)/hzed));
05963                 kmax = VMIN2(nz-1, (int)floor((position[2] + dz)/hzed));
05964                 for (k=kmin; k<=kmax; k++) {
05965                     dz2 = VSQR(k*hzed - position[2]);
05966                     /* See if grid point is inside ivdw radius and set kappa
05967                        * accordingly (do spline assignment here) */
05968                     if ((dz2 + dy2 + dx2) <= rtot2) {
05969                         gpos[0] = i*hx + xmin;
05970                         gpos[1] = j*hy + ymin;
05971                         gpos[2] = k*hzed + zmin;
05972
05973                         /* Select the correct function based on the surface definition
05974                            * (now including the 7th order polynomial) */
05975                         Vpmg_splineSelect(srffm, acc, gpos, thee->splineWin, irad, atom, tgrad);
05976
05977                         if (thee->pmgp->nonlin) {
05978                             /* Nonlinear forces */
05979                             fmag = 0.0;
05980                             nchop = 0;
05981                             for (m=0; m<nion; m++) {
05982                                 fmag +=
05983                                     (thee->kappa[IJK(i, j, k)]) * ionConc[m] * (Vcap_exp(-ionQ[m]*thee->u[IJK(i, j, k)], &ichop)-1.0)/ionstr;
05984                                 nchop += ichop;
05985                             }
05986                             /* if (nchop > 0) Vnm_print(2, "Vpmg_ibForece: Chopped EXP %d
05987                                 times!\n", nchop);*/
05988                             force[0] += (zkappa2*fmag*tgrad[0]);
05989                             force[1] += (zkappa2*fmag*tgrad[1]);
05990                             force[2] += (zkappa2*fmag*tgrad[2]);
05991                         } else {
05992                             /* Use of bulk factor (zkappa2) OK here becuase
05993                                * LPBE force approximation */
05994                             /* NAB -- did we forget a kappa factor here??? */
05995                             fmag = VSQR(thee->u[IJK(i, j, k)]) * (thee->kappa[IJK(i, j, k)]);
05996                             force[0] += (zkappa2*fmag*tgrad[0]);
05997                             force[1] += (zkappa2*fmag*tgrad[1]);
05998                             force[2] += (zkappa2*fmag*tgrad[2]);
05999                         }
06000                     } /* k loop */
06001                 } /* j loop */
06002             } /* i loop */
06003         }
06004         force[0] = force[0] * 0.5 * hx * hy * hzed * izmagic;

```

```

06004     force[1] = force[1] * 0.5 * hx * hy * hzed * izmagic;
06005     force[2] = force[2] * 0.5 * hx * hy * hzed * izmagic;
06006
06007     return 1;
06008 }
06009
06010 VPUBLIC int Vpmg_dbForce(Vpmg *thee, double *dbForce, int atomID,
06011                        Vsurf_Meth srfm) {
06012
06013     Vacc *acc;
06014     Vpbe *pbe;
06015     Vatom *atom;
06016
06017     double *apos, position[3], arad, srad, hx, hy, hzed, izmagic, deps, deps;
06018     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax, rtot2, epsp;
06019     double rtot, dx, gpos[3], tgrad[3], dbFmag, epsw, kT;
06020     double *u, Hxijk, Hyijk, Hzijk, Hximljk, Hyijmlk, Hzijkm1;
06021     double dHxijk[3], dHyijk[3], dHzijk[3], dHximljk[3], dHyijmlk[3];
06022     double dHzijkm1[3];
06023     int i, j, k, l, nx, ny, nz, imin, imax, jmin, jmax, kmin, kmax;
06024
06025     VASSERT(thee != VNULL);
06026     if (!thee->filled) {
06027         Vnm_print(2, "Vpmg_dbForce: Need to callVpmg_fillco!\n");
06028         return 0;
06029     }
06030
06031     acc = thee->pbe->acc;
06032     atom = Valist_getAtom(thee->pbe->alist, atomID);
06033     apos = Vatom_getPosition(atom);
06034     arad = Vatom_getRadius(atom);
06035     srad = Vpbe_getSolventRadius(thee->pbe);
06036
06037     /* Reset force */
06038     dbForce[0] = 0.0;
06039     dbForce[1] = 0.0;
06040     dbForce[2] = 0.0;
06041
06042     /* Check surface definition */
06043     if ((srfm != VSM_SPLINE) && (srfm!=VSM_SPLINE3) && (srfm!=VSM_SPLINE4)) {
06044         Vnm_print(2, "Vpmg_dbForce: Forces *must* be calculated with \
06045 spline-based surfaces!\n");
06046         Vnm_print(2, "Vpmg_dbForce: Skipping dielectric/apolar boundary \
06047 force calculation!\n");
06048         return 0;
06049     }
06050
06051
06052     /* If we aren't in the current position, then we're done */
06053     if (atom->partID == 0) return 1;
06054
06055     /* Get PBE info */
06056     pbe = thee->pbe;
06057     acc = pbe->acc;
06058     epsp = Vpbe_getSoluteDiel(pbe);
06059     epsw = Vpbe_getSolventDiel(pbe);
06060     kT = Vpbe_getTemperature(pbe)*(1e-3)*Vunit_Na*Vunit_kb;
06061     izmagic = 1.0/Vpbe_getZmagic(pbe);
06062
06063     /* Mesh info */
06064     nx = thee->pmgp->nx;
06065     ny = thee->pmgp->ny;
06066     nz = thee->pmgp->nz;
06067     hx = thee->pmgp->hx;
06068     hy = thee->pmgp->hy;
06069     hzed = thee->pmgp->hzed;
06070     xlen = thee->pmgp->xlen;
06071     ylen = thee->pmgp->ylen;
06072     zlen = thee->pmgp->zlen;
06073     xmin = thee->pmgp->xmin;
06074     ymin = thee->pmgp->ymin;
06075     zmin = thee->pmgp->zmin;
06076     xmax = thee->pmgp->xmax;
06077     ymax = thee->pmgp->ymax;
06078     zmax = thee->pmgp->zmax;
06079     u = thee->u;
06080
06081     /* Sanity check: there is no force if there is zero ionic strength */
06082     if (VABS(epsp-epsw) < VPMGSMALL) {
06083         Vnm_print(0, "Vpmg_dbForce: No force for uniform dielectric!\n");
06084         return 1;

```

```

06085     }
06086     deps = (epsw - epsp);
06087     depsi = 1.0/deps;
06088     rtot = (arad + thee->splineWin + srad);
06089
06090     /* Make sure we're on the grid */
06091     /* Grid checking modified by Matteo Rotter */
06092     if ((apos[0]<=xmin + rtot) || (apos[0]>=xmax - rtot) || \
06093         (apos[1]<=ymin + rtot) || (apos[1]>=ymax - rtot) || \
06094         (apos[2]<=zmin + rtot) || (apos[2]>=zmax - rtot)) {
06095         if ((thee->pmgp->bcfl != BCFL_FOCUS) &&
06096             (thee->pmgp->bcfl != BCFL_MAP)) {
06097             Vnm_print(2, "Vpmg_dbForce: Atom #%d at (%4.3f, %4.3f, %4.3f) is off the mesh (ignoring):\n",
06098                 atomID, apos[0], apos[1], apos[2]);
06099             Vnm_print(2, "Vpmg_dbForce:      xmin = %g, xmax = %g\n",
06100                 xmin, xmax);
06101             Vnm_print(2, "Vpmg_dbForce:      ymin = %g, ymax = %g\n",
06102                 ymin, ymax);
06103             Vnm_print(2, "Vpmg_dbForce:      zmin = %g, zmax = %g\n",
06104                 zmin, zmax);
06105         }
06106         fflush(stderr);
06107     } else {
06108
06109         /* Convert the atom position to grid reference frame */
06110         position[0] = apos[0] - xmin;
06111         position[1] = apos[1] - ymin;
06112         position[2] = apos[2] - zmin;
06113
06114         /* Integrate over points within this atom's (inflated) radius */
06115         rtot2 = VSQR(rtot);
06116         dx = rtot/hx;
06117         imin = (int)floor((position[0]-rtot)/hx);
06118         if (imin < 1) {
06119             Vnm_print(2, "Vpmg_dbForce: Atom %d off grid!\n", atomID);
06120             return 0;
06121         }
06122         imax = (int)ceil((position[0]+rtot)/hx);
06123         if (imax > (nx-2)) {
06124             Vnm_print(2, "Vpmg_dbForce: Atom %d off grid!\n", atomID);
06125             return 0;
06126         }
06127         jmin = (int)floor((position[1]-rtot)/hy);
06128         if (jmin < 1) {
06129             Vnm_print(2, "Vpmg_dbForce: Atom %d off grid!\n", atomID);
06130             return 0;
06131         }
06132         jmax = (int)ceil((position[1]+rtot)/hy);
06133         if (jmax > (ny-2)) {
06134             Vnm_print(2, "Vpmg_dbForce: Atom %d off grid!\n", atomID);
06135             return 0;
06136         }
06137         kmin = (int)floor((position[2]-rtot)/hz);
06138         if (kmin < 1) {
06139             Vnm_print(2, "Vpmg_dbForce: Atom %d off grid!\n", atomID);
06140             return 0;
06141         }
06142         kmax = (int)ceil((position[2]+rtot)/hz);
06143         if (kmax > (nz-2)) {
06144             Vnm_print(2, "Vpmg_dbForce: Atom %d off grid!\n", atomID);
06145             return 0;
06146         }
06147         for (i=imin; i<=imax; i++) {
06148             for (j=jmin; j<=jmax; j++) {
06149                 for (k=kmin; k<=kmax; k++) {
06150                     /* i,j,k */
06151                     gpos[0] = (i+0.5)*hx + xmin;
06152                     gpos[1] = j*hy + ymin;
06153                     gpos[2] = k*hz + zmin;
06154                     Hxijk = (thee->epsx[IJK(i,j,k)] - epsp)*depsi;
06155
06156                     /* Select the correct function based on the surface definition
06157                      * (now including the 7th order polynomial) */
06158                     Vpmg_splineSelect(srffm,acc, gpos, thee->splineWin, 0.,atom, dHxijk);
06159                     /*
06160                     switch (srffm) {
06161                         case VSM_SPLINE :
06162                             Vacc_splineAccGradAtomNorm(acc, gpos, thee->splineWin, 0.,
06163                                 atom, dHxijk);
06164                             break;
06165                         case VSM_SPLINE4 :

```

```

06166         Vacc_splineAccGradAtomNorm4(acc, gpos, thee->splineWin, 0.,
06167                                     atom, dHxijk);
06168         break;
06169     default:
06170         Vnm_print(2, "Vpmg_dbnbForce: Unknown surface method.\n");
06171         return;
06172     }
06173     */
06174     for (l=0; l<3; l++) dHxijk[l] *= Hxijk;
06175     gpos[0] = i*hx + xmin;
06176     gpos[1] = (j+0.5)*hy + ymin;
06177     gpos[2] = k*hzed + zmin;
06178     Hyijk = (thee->epsy[IJK(i,j,k)] - epsp)*depsi;
06179
06180     /* Select the correct function based on the surface definition
06181      * (now including the 7th order polynomial) */
06182     Vpmg_splineSelect(srfm,acc, gpos, thee->splineWin, 0.,atom, dHyijk);
06183
06184     for (l=0; l<3; l++) dHyijk[l] *= Hyijk;
06185     gpos[0] = i*hx + xmin;
06186     gpos[1] = j*hy + ymin;
06187     gpos[2] = (k+0.5)*hzed + zmin;
06188     Hzijk = (thee->epsz[IJK(i,j,k)] - epsp)*depsi;
06189
06190     /* Select the correct function based on the surface definition
06191      * (now including the 7th order polynomial) */
06192     Vpmg_splineSelect(srfm,acc, gpos, thee->splineWin, 0.,atom, dHzijk);
06193
06194     for (l=0; l<3; l++) dHzijk[l] *= Hzijk;
06195     /* i-1,j,k */
06196     gpos[0] = (i-0.5)*hx + xmin;
06197     gpos[1] = j*hy + ymin;
06198     gpos[2] = k*hzed + zmin;
06199     Hximljk = (thee->epsx[IJK(i-1,j,k)] - epsp)*depsi;
06200
06201     /* Select the correct function based on the surface definition
06202      * (now including the 7th order polynomial) */
06203     Vpmg_splineSelect(srfm,acc, gpos, thee->splineWin, 0.,atom, dHximljk);
06204
06205     for (l=0; l<3; l++) dHximljk[l] *= Hximljk;
06206     /* i,j-1,k */
06207     gpos[0] = i*hx + xmin;
06208     gpos[1] = (j-0.5)*hy + ymin;
06209     gpos[2] = k*hzed + zmin;
06210     Hyijmlk = (thee->epsy[IJK(i,j-1,k)] - epsp)*depsi;
06211
06212     /* Select the correct function based on the surface definition
06213      * (now including the 7th order polynomial) */
06214     Vpmg_splineSelect(srfm,acc, gpos, thee->splineWin, 0.,atom, dHyijmlk);
06215
06216     for (l=0; l<3; l++) dHyijmlk[l] *= Hyijmlk;
06217     /* i,j,k-1 */
06218     gpos[0] = i*hx + xmin;
06219     gpos[1] = j*hy + ymin;
06220     gpos[2] = (k-0.5)*hzed + zmin;
06221     Hzijkml = (thee->epsz[IJK(i,j,k-1)] - epsp)*depsi;
06222
06223     /* Select the correct function based on the surface definition
06224      * (now including the 7th order polynomial) */
06225     Vpmg_splineSelect(srfm,acc, gpos, thee->splineWin, 0.,atom, dHzijkml);
06226
06227     for (l=0; l<3; l++) dHzijkml[l] *= Hzijkml;
06228     /* *** CALCULATE DIELECTRIC BOUNDARY FORCES *** */
06229     dbFmag = u[IJK(i,j,k)];
06230     tgrad[0] =
06231         (dHxijk[0] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)])
06232          + dHximljk[0] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) /VSQR(hx)
06233         + (dHyijk[0] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)])
06234          + dHyijmlk[0] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) /VSQR(hy)
06235         + (dHzijk[0] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)])
06236          + dHzijkml[0] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) /VSQR(hzed);
06237     tgrad[1] =
06238         (dHxijk[1] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)])
06239          + dHximljk[1] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) /VSQR(hx)
06240         + (dHyijk[1] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)])
06241          + dHyijmlk[1] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) /VSQR(hy)
06242         + (dHzijk[1] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)])
06243          + dHzijkml[1] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) /VSQR(hzed);
06244     tgrad[2] =
06245         (dHxijk[2] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)])
06246          + dHximljk[2] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) /VSQR(hx)

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```

06247         + (dHyijk[2] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)]))
06248         + dHyijm1k[2] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) /VSQR(hy)
06249         + (dHzijk[2] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)]))
06250         + dHzijkml[2] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) /VSQR(hzed);
06251         dbForce[0] += (dbFmag*tgrad[0]);
06252         dbForce[1] += (dbFmag*tgrad[1]);
06253         dbForce[2] += (dbFmag*tgrad[2]);
06254
06255     } /* k loop */
06256 } /* j loop */
06257 } /* i loop */
06258
06259     dbForce[0] = -dbForce[0]*hx*hy*hzed*deps*0.5*izmagic;
06260     dbForce[1] = -dbForce[1]*hx*hy*hzed*deps*0.5*izmagic;
06261     dbForce[2] = -dbForce[2]*hx*hy*hzed*deps*0.5*izmagic;
06262 }
06263
06264     return 1;
06265 }
06266
06267 VPUBLIC int Vpmg_qfForce(Vpmg *thee, double *force, int atomID,
06268     Vchrg_Meth chgm) {
06269
06270     double tforce[3];
06271
06272     /* Reset force */
06273     force[0] = 0.0;
06274     force[1] = 0.0;
06275     force[2] = 0.0;
06276
06277     /* Check surface definition */
06278     if (chgm != VCM_BSPL2) {
06279         Vnm_print(2, "Vpmg_qfForce: It is recommended that forces be \
06280 calculated with the\n");
06281         Vnm_print(2, "Vpmg_qfForce: cubic spline charge discretization \
06282 scheme\n");
06283     }
06284
06285     switch (chgm) {
06286     case VCM_TRIL:
06287         qfForceSpline1(thee, tforce, atomID);
06288         break;
06289     case VCM_BSPL2:
06290         qfForceSpline2(thee, tforce, atomID);
06291         break;
06292     case VCM_BSPL4:
06293         qfForceSpline4(thee, tforce, atomID);
06294         break;
06295     default:
06296         Vnm_print(2, "Vpmg_qfForce: Undefined charge discretization \
06297 method (%d)\n", chgm);
06298         Vnm_print(2, "Vpmg_qfForce: Forces not calculated!\n");
06299         return 0;
06300     }
06301
06302     /* Assign forces */
06303     force[0] = tforce[0];
06304     force[1] = tforce[1];
06305     force[2] = tforce[2];
06306
06307     return 1;
06308 }
06309
06310
06311 VPRIVATE void qfForceSpline1(Vpmg *thee, double *force, int atomID) {
06312
06313     Vatom *atom;
06314
06315     double *apos, position[3], hx, hy, hzed;
06316     double xmin, ymin, zmin, xmax, ymax, zmax;
06317     double dx, dy, dz;
06318     double *u, charge, ifloat, jfloat, kfloat;
06319     int nx, ny, nz, ihi, ilo, jhi, jlo, khi, klo;
06320
06321     VASSERT(thee != VNULL);
06322
06323     atom = Valist_getAtom(thee->pbe->alist, atomID);
06324     apos = Vatom_getPosition(atom);
06325     charge = Vatom_getCharge(atom);
06326
06327     /* Reset force */

```

```

06328     force[0] = 0.0;
06329     force[1] = 0.0;
06330     force[2] = 0.0;
06331
06332     /* If we aren't in the current position, then we're done */
06333     if (atom->partID == 0) return;
06334
06335     /* Mesh info */
06336     nx = thee->pmgp->nx;
06337     ny = thee->pmgp->ny;
06338     nz = thee->pmgp->nz;
06339     hx = thee->pmgp->hx;
06340     hy = thee->pmgp->hy;
06341     hzed = thee->pmgp->hzed;
06342     xmin = thee->pmgp->xmin;
06343     ymin = thee->pmgp->ymin;
06344     zmin = thee->pmgp->zmin;
06345     xmax = thee->pmgp->xmax;
06346     ymax = thee->pmgp->ymax;
06347     zmax = thee->pmgp->zmax;
06348     u = thee->u;
06349
06350     /* Make sure we're on the grid */
06351     if ((apos[0]<=xmin) || (apos[0]>=xmax) || (apos[1]<=ymin) || \
06352         (apos[1]>=ymax) || (apos[2]<=zmin) || (apos[2]>=zmax)) {
06353         if ((thee->pmgp->bcfl != BCFL_FOCUS) &&
06354             (thee->pmgp->bcfl != BCFL_MAP)) {
06355             Vnm_print(2, "Vpmg_qfForce: Atom #%d at (%4.3f, %4.3f, %4.3f) is off the mesh (ignoring):\n",
06356 atomID, apos[0], apos[1], apos[2]);
06356             Vnm_print(2, "Vpmg_qfForce:      xmin = %g, xmax = %g\n", xmin, xmax);
06357             Vnm_print(2, "Vpmg_qfForce:      ymin = %g, ymax = %g\n", ymin, ymax);
06358             Vnm_print(2, "Vpmg_qfForce:      zmin = %g, zmax = %g\n", zmin, zmax);
06359         }
06360         fflush(stderr);
06361     } else {
06362
06363         /* Convert the atom position to grid coordinates */
06364         position[0] = apos[0] - xmin;
06365         position[1] = apos[1] - ymin;
06366         position[2] = apos[2] - zmin;
06367         ifloat = position[0]/hx;
06368         jfloat = position[1]/hy;
06369         kfloat = position[2]/hzed;
06370         ihi = (int)ceil(ifloat);
06371         ilo = (int)floor(ifloat);
06372         jhi = (int)ceil(jfloat);
06373         jlo = (int)floor(jfloat);
06374         khi = (int)ceil(kfloat);
06375         klo = (int)floor(kfloat);
06376         VASSERT((ihi < nx) && (ihi >=0));
06377         VASSERT((ilo < nx) && (ilo >=0));
06378         VASSERT((jhi < ny) && (jhi >=0));
06379         VASSERT((jlo < ny) && (jlo >=0));
06380         VASSERT((khi < nz) && (khi >=0));
06381         VASSERT((klo < nz) && (klo >=0));
06382         dx = ifloat - (double)(ilo);
06383         dy = jfloat - (double)(jlo);
06384         dz = kfloat - (double)(klo);
06385
06386
06387     #if 0
06388         Vnm_print(1, "Vpmg_qfForce: (DEBUG) u ~ %g\n",
06389             dx *dy *dz *u[IJK(ihi,jhi,khi)]
06390             +dx *dy *(1-dz)*u[IJK(ihi,jhi,klo)]
06391             +dx *(1-dy)*dz *u[IJK(ihi,jlo,khi)]
06392             +dx *(1-dy)*(1-dz)*u[IJK(ihi,jlo,klo)]
06393             +(1-dx)*dy *dz *u[IJK(ilo,jhi,khi)]
06394             +(1-dx)*dy *(1-dz)*u[IJK(ilo,jhi,klo)]
06395             +(1-dx)*(1-dy)*dz *u[IJK(ilo,jlo,khi)]
06396             +(1-dx)*(1-dy)*(1-dz)*u[IJK(ilo,jlo,klo)]);
06397     #endif
06398
06399
06400     if ((dx > VPMGSMALL) && (VABS(1.0-dx) > VPMGSMALL)) {
06401         force[0] =
06402             -charge*(dy *dz *u[IJK(ihi,jhi,khi)]
06403                 + dy *(1-dz)*u[IJK(ihi,jhi,klo)]
06404                 + (1-dy)*dz *u[IJK(ihi,jlo,khi)]
06405                 + (1-dy)*(1-dz)*u[IJK(ihi,jlo,klo)]
06406                 - dy *dz *u[IJK(ilo,jhi,khi)]
06407                 - dy *(1-dz)*u[IJK(ilo,jhi,klo)]

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```

06408             - (1-dy)*dz      *u[IJK(ilo,jlo,khi)]
06409             - (1-dy)*(1-dz)*u[IJK(ilo,jlo,klo)])/hx;
06410     } else {
06411         force[0] = 0;
06412         Vnm_print(0,
06413             "Vpmg_qfForce: Atom %d on x gridline; zero x-force\n", atomID);
06414     }
06415     if ((dy > VPMGSMALL) && (VABS(1.0-dy) > VPMGSMALL)) {
06416         force[1] =
06417             -charge*(dx      *dz      *u[IJK(ihi,jhi,khi)]
06418                 + dx      *(1-dz)*u[IJK(ihi,jhi,klo)]
06419                 - dx      *dz      *u[IJK(ihi,jlo,khi)]
06420                 - dx      *(1-dz)*u[IJK(ihi,jlo,klo)]
06421                 + (1-dx)*dz      *u[IJK(ilo,jhi,khi)]
06422                 + (1-dx)*(1-dz)*u[IJK(ilo,jhi,klo)]
06423                 - (1-dx)*dz      *u[IJK(ilo,jlo,khi)]
06424                 - (1-dx)*(1-dz)*u[IJK(ilo,jlo,klo)])/hy;
06425     } else {
06426         force[1] = 0;
06427         Vnm_print(0,
06428             "Vpmg_qfForce: Atom %d on y gridline; zero y-force\n", atomID);
06429     }
06430     if ((dz > VPMGSMALL) && (VABS(1.0-dz) > VPMGSMALL)) {
06431         force[2] =
06432             -charge*(dy      *dx      *u[IJK(ihi,jhi,khi)]
06433                 - dy      *dx      *u[IJK(ihi,jhi,klo)]
06434                 + (1-dy)*dx      *u[IJK(ihi,jlo,khi)]
06435                 - (1-dy)*dx      *u[IJK(ihi,jlo,klo)]
06436                 + dy      *(1-dx)*u[IJK(ilo,jhi,khi)]
06437                 - dy      *(1-dx)*u[IJK(ilo,jhi,klo)]
06438                 + (1-dy)*(1-dx)*u[IJK(ilo,jlo,khi)]
06439                 - (1-dy)*(1-dx)*u[IJK(ilo,jlo,klo)])/hz;
06440     } else {
06441         force[2] = 0;
06442         Vnm_print(0,
06443             "Vpmg_qfForce: Atom %d on z gridline; zero z-force\n", atomID);
06444     }
06445 }
06446 }
06447
06448 VPRIVATE void qfForceSpline2(Vpmg *thee, double *force, int atomID) {
06449
06450     Vatom *atom;
06451
06452     double *apos, position[3], hx, hy, hzed;
06453     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax;
06454     double mx, my, mz, dmx, dmy, dmz;
06455     double *u, charge, ifloat, jfloat, kfloat;
06456     int nx, ny, nz, im2, im1, ip1, ip2, jm2, jml, jp1, jp2, km2, kml;
06457     int kpl, kp2, ii, jj, kk;
06458
06459     VASSERT(thee != VNULL);
06460
06461     atom = Valist_getAtom(thee->pbe->alist, atomID);
06462     apos = Vatom_getPosition(atom);
06463     charge = Vatom_getCharge(atom);
06464
06465     /* Reset force */
06466     force[0] = 0.0;
06467     force[1] = 0.0;
06468     force[2] = 0.0;
06469
06470     /* If we aren't in the current position, then we're done */
06471     if (atom->partID == 0) return;
06472
06473     /* Mesh info */
06474     nx = thee->pmgp->nx;
06475     ny = thee->pmgp->ny;
06476     nz = thee->pmgp->nz;
06477     hx = thee->pmgp->hx;
06478     hy = thee->pmgp->hy;
06479     hzed = thee->pmgp->hzed;
06480     xlen = thee->pmgp->xlen;
06481     ylen = thee->pmgp->ylen;
06482     zlen = thee->pmgp->zlen;
06483     xmin = thee->pmgp->xmin;
06484     ymin = thee->pmgp->ymin;
06485     zmin = thee->pmgp->zmin;
06486     xmax = thee->pmgp->xmax;
06487     ymax = thee->pmgp->ymax;
06488     zmax = thee->pmgp->zmax;

```

```

06489     u = thee->u;
06490
06491     /* Make sure we're on the grid */
06492     if ((apos[0]<=(xmin+hx)) || (apos[0]>=(xmax-hx)) \
06493         || (apos[1]<=(ymin+hy)) || (apos[1]>=(ymax-hy)) \
06494         || (apos[2]<=(zmin+hzed)) || (apos[2]>=(zmax-hzed))) {
06495         if ((thee->pmgp->bcfl != BCFL_FOCUS) &&
06496             (thee->pmgp->bcfl != BCFL_MAP)) {
06497             Vnm_print(2, "qfForceSpline2: Atom #%d off the mesh \
06498                 (ignoring)\n", atomID);
06499         }
06500         fflush(stderr);
06501     } else {
06502
06503         /* Convert the atom position to grid coordinates */
06504         position[0] = apos[0] - xmin;
06505         position[1] = apos[1] - ymin;
06506         position[2] = apos[2] - zmin;
06507         ifloat = position[0]/hx;
06508         jfloat = position[1]/hy;
06509         kfloat = position[2]/hzed;
06510         ip1 = (int)ceil(ifloat);
06511         ip2 = ip1 + 1;
06512         im1 = (int)floor(ifloat);
06513         im2 = im1 - 1;
06514         jp1 = (int)ceil(jfloat);
06515         jp2 = jp1 + 1;
06516         jm1 = (int)floor(jfloat);
06517         jm2 = jm1 - 1;
06518         kp1 = (int)ceil(kfloat);
06519         kp2 = kp1 + 1;
06520         km1 = (int)floor(kfloat);
06521         km2 = km1 - 1;
06522
06523         /* This step shouldn't be necessary, but it saves nasty debugging
06524          * later on if something goes wrong */
06525         ip2 = VMIN2(ip2,nx-1);
06526         ip1 = VMIN2(ip1,nx-1);
06527         im1 = VMAX2(im1,0);
06528         im2 = VMAX2(im2,0);
06529         jp2 = VMIN2(jp2,ny-1);
06530         jp1 = VMIN2(jp1,ny-1);
06531         jm1 = VMAX2(jm1,0);
06532         jm2 = VMAX2(jm2,0);
06533         kp2 = VMIN2(kp2,nz-1);
06534         kp1 = VMIN2(kp1,nz-1);
06535         km1 = VMAX2(km1,0);
06536         km2 = VMAX2(km2,0);
06537
06538         for (ii=im2; ii<=ip2; ii++) {
06539             mx = bspline2(VFCHI(ii,ifloat));
06540             dmx = dbspline2(VFCHI(ii,ifloat));
06541             for (jj=jm2; jj<=jp2; jj++) {
06542                 my = bspline2(VFCHI(jj,jfloat));
06543                 dmy = dbspline2(VFCHI(jj,jfloat));
06544                 for (kk=km2; kk<=kp2; kk++) {
06545                     mz = bspline2(VFCHI(kk,kfloat));
06546                     dmz = dbspline2(VFCHI(kk,kfloat));
06547
06548                     force[0] += (charge*dmx*my*mz*u[IJK(ii,jj,kk)])/hx;
06549                     force[1] += (charge*mx*dmy*mz*u[IJK(ii,jj,kk)])/hy;
06550                     force[2] += (charge*mx*my*dmz*u[IJK(ii,jj,kk)])/hzed;
06551                 }
06552             }
06553         }
06554     }
06555 }
06556 }
06557
06558 }
06559 }
06560
06561 VPRIVATE void qfForceSpline4(Vpmg *thee, double *force, int atomID) {
06562     Vatom *atom;
06563     double f, c, *u, *apos, position[3];
06564
06565     /* Grid variables */
06566     int nx,ny,nz;
06567     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax;
06568     double hx, hy, hzed, ifloat, jfloat, kfloat;

```



```

06570
06571 /* B-spline weights */
06572 double mx, my, mz, dmX, dmy, dmz;
06573 double mi, mj, mk;
06574
06575 /* Loop indeces */
06576 int i, j, k, ii, jj, kk;
06577 int im2, im1, ip1, ip2, jm2, jm1, jp1, jp2, km2, km1, kp1, kp2;
06578
06579 /* field */
06580 double e[3];
06581
06582 VASSERT(thee != VNULL);
06583 VASSERT(thee->filled);
06584
06585 atom = Valist_getAtom(thee->pbe->alist, atomID);
06586 apos = Vatom_getPosition(atom);
06587 c = Vatom_getCharge(atom);
06588
06589 for (i=0;i<3;i++){
06590     e[i] = 0.0;
06591 }
06592
06593 /* Mesh info */
06594 nx = thee->pmgp->nx;
06595 ny = thee->pmgp->ny;
06596 nz = thee->pmgp->nz;
06597 hx = thee->pmgp->hx;
06598 hy = thee->pmgp->hy;
06599 hzed = thee->pmgp->hzed;
06600 xlen = thee->pmgp->xlen;
06601 ylen = thee->pmgp->ylen;
06602 zlen = thee->pmgp->zlen;
06603 xmin = thee->pmgp->xmin;
06604 ymin = thee->pmgp->ymin;
06605 zmin = thee->pmgp->zmin;
06606 xmax = thee->pmgp->xmax;
06607 ymax = thee->pmgp->ymax;
06608 zmax = thee->pmgp->zmax;
06609 u = thee->u;
06610
06611 /* Make sure we're on the grid */
06612 if ((apos[0]<=(xmin+2*hx)) || (apos[0]>=(xmax-2*hx)) \
06613     || (apos[1]<=(ymin+2*hy)) || (apos[1]>=(ymax-2*hy)) \
06614     || (apos[2]<=(zmin+2*hzed)) || (apos[2]>=(zmax-2*hzed))) {
06615     Vnm_print(2, "qfForceSpline4: Atom off the mesh \
06616         (ignoring) %6.3f %6.3f %6.3f\n", apos[0], apos[1], apos[2]);
06617     fflush(stderr);
06618 } else {
06619
06620     /* Convert the atom position to grid coordinates */
06621     position[0] = apos[0] - xmin;
06622     position[1] = apos[1] - ymin;
06623     position[2] = apos[2] - zmin;
06624     ifloat = position[0]/hx;
06625     jfloat = position[1]/hy;
06626     kfloat = position[2]/hzed;
06627     ip1 = (int)ceil(ifloat);
06628     ip2 = ip1 + 2;
06629     im1 = (int)floor(ifloat);
06630     im2 = im1 - 2;
06631     jp1 = (int)ceil(jfloat);
06632     jp2 = jp1 + 2;
06633     jm1 = (int)floor(jfloat);
06634     jm2 = jm1 - 2;
06635     kp1 = (int)ceil(kfloat);
06636     kp2 = kp1 + 2;
06637     km1 = (int)floor(kfloat);
06638     km2 = km1 - 2;
06639
06640     /* This step shouldn't be necessary, but it saves nasty debugging
06641      * later on if something goes wrong */
06642     ip2 = VMIN2(ip2,nx-1);
06643     ip1 = VMIN2(ip1,nx-1);
06644     im1 = VMAX2(im1,0);
06645     im2 = VMAX2(im2,0);
06646     jp2 = VMIN2(jp2,ny-1);
06647     jp1 = VMIN2(jp1,ny-1);
06648     jm1 = VMAX2(jm1,0);
06649     jm2 = VMAX2(jm2,0);
06650     kp2 = VMIN2(kp2,nz-1);

```

```

06651         kp1 = VMIN2(kp1,nz-1);
06652         km1 = VMAX2(km1,0);
06653         km2 = VMAX2(km2,0);
06654
06655         for (ii=im2; ii<=ip2; ii++) {
06656             mi = VFCHI4(ii,ifloat);
06657             mx = bspline4(mi);
06658             dmx = dbspline4(mi);
06659             for (jj=jm2; jj<=jp2; jj++) {
06660                 mj = VFCHI4(jj,jfloat);
06661                 my = bspline4(mj);
06662                 dmy = dbspline4(mj);
06663                 for (kk=km2; kk<=kp2; kk++) {
06664                     mk = VFCHI4(kk,kfloat);
06665                     mz = bspline4(mk);
06666                     dmz = dbspline4(mk);
06667                     f = u[IJK(ii,jj,kk)];
06668                     /* Field */
06669                     e[0] += f*dmx*my*mz/hx;
06670                     e[1] += f*mx*dmy*mz/hy;
06671                     e[2] += f*mx*my*dmz/hzed;
06672                 }
06673             }
06674         }
06675     }
06676
06677     /* Monopole Force */
06678     force[0] = e[0]*c;
06679     force[1] = e[1]*c;
06680     force[2] = e[2]*c;
06681 }
06682 }
06683
06684 VPRIVATE void markFrac(
06685     double rtot, double *tpos,
06686     int nx, int ny, int nz,
06687     double hx, double hy, double hzed,
06688     double xmin, double ymin, double zmin,
06689     double *xarray, double *yarray, double *zarray) {
06690
06691     int i, j, k, imin, imax, jmin, jmax, kmin, kmax;
06692     double dx, dx2, dy, dy2, dz, dz2, a000, a001, a010, a100, r2;
06693     double x, xp, xm, y, yp, ym, zp, z, zm, xspan, yspan, zspan;
06694     double rtot2, pos[3];
06695
06696     /* Convert to grid reference frame */
06697     pos[0] = tpos[0] - xmin;
06698     pos[1] = tpos[1] - ymin;
06699     pos[2] = tpos[2] - zmin;
06700
06701     rtot2 = VSQR(rtot);
06702
06703     xspan = rtot + 2*hx;
06704     imin = VMAX2(0, (int)ceil((pos[0] - xspan)/hx));
06705     imax = VMIN2(nx-1, (int)floor((pos[0] + xspan)/hx));
06706     for (i=imin; i<=imax; i++) {
06707         x = hx*i;
06708         dx2 = VSQR(pos[0] - x);
06709         if (rtot2 > dx2) {
06710             yspan = VSQRT(rtot2 - dx2) + 2*hy;
06711         } else {
06712             yspan = 2*hy;
06713         }
06714         jmin = VMAX2(0, (int)ceil((pos[1] - yspan)/hy));
06715         jmax = VMIN2(ny-1, (int)floor((pos[1] + yspan)/hy));
06716         for (j=jmin; j<=jmax; j++) {
06717             y = hy*j;
06718             dy2 = VSQR(pos[1] - y);
06719             if (rtot2 > (dx2+dy2)) {
06720                 zspan = VSQRT(rtot2-dx2-dy2) + 2*hzed;
06721             } else {
06722                 zspan = 2*hzed;
06723             }
06724             kmin = VMAX2(0, (int)ceil((pos[2] - zspan)/hzed));
06725             kmax = VMIN2(nz-1, (int)floor((pos[2] + zspan)/hzed));
06726             for (k=kmin; k<=kmax; k++) {
06727                 z = hzed*k;
06728                 dz2 = VSQR(pos[2] - z);
06729
06730                 r2 = dx2 + dy2 + dz2;
06731

```

```

06732         /* We need to determine the inclusion value a000 at (i,j,k) */
06733         if (r2 < rtot2) a000 = 1.0;
06734         else a000 = 0.0;
06735
06736         /* We need to evaluate the values of x which intersect the
06737          * sphere and determine if these are in the interval
06738          * [(i,j,k), (i+1,j,k)] */
06739         if (r2 < (rtot2 - hx*hx)) a100 = 1.0;
06740         else if (r2 > (rtot2 + hx*hx)) a100 = 0.0;
06741         else if (rtot2 > (dy2 + dz2)) {
06742             dx = VSQRT(rtot2 - dy2 - dz2);
06743             xm = pos[0] - dx;
06744             xp = pos[0] + dx;
06745             if ((xm < x+hx) && (xm > x)) {
06746                 a100 = (xm - x)/hx;
06747             } else if ((xp < x+hx) && (xp > x)) {
06748                 a100 = (xp - x)/hx;
06749             }
06750         } else a100 = 0.0;
06751
06752         /* We need to evaluate the values of y which intersect the
06753          * sphere and determine if these are in the interval
06754          * [(i,j,k), (i,j+1,k)] */
06755         if (r2 < (rtot2 - hy*hy)) a010 = 1.0;
06756         else if (r2 > (rtot2 + hy*hy)) a010 = 0.0;
06757         else if (rtot2 > (dx2 + dz2)) {
06758             dy = VSQRT(rtot2 - dx2 - dz2);
06759             ym = pos[1] - dy;
06760             yp = pos[1] + dy;
06761             if ((ym < y+hy) && (ym > y)) {
06762                 a010 = (ym - y)/hy;
06763             } else if ((yp < y+hy) && (yp > y)) {
06764                 a010 = (yp - y)/hy;
06765             }
06766         } else a010 = 0.0;
06767
06768         /* We need to evaluate the values of z which intersect the
06769          * sphere and determine if these are in the interval
06770          * [(i,j,k), (i,j,k+1)] */
06771         if (r2 < (rtot2 - hzed*hzed)) a001 = 1.0;
06772         else if (r2 > (rtot2 + hzed*hzed)) a001 = 0.0;
06773         else if (rtot2 > (dx2 + dy2)) {
06774             dz = VSQRT(rtot2 - dx2 - dy2);
06775             zm = pos[2] - dz;
06776             zp = pos[2] + dz;
06777             if ((zm < z+hzed) && (zm > z)) {
06778                 a001 = (zm - z)/hzed;
06779             } else if ((zp < z+hzed) && (zp > z)) {
06780                 a001 = (zp - z)/hzed;
06781             }
06782         } else a001 = 0.0;
06783
06784         if (a100 < xarray[IJK(i,j,k)]) xarray[IJK(i,j,k)] = a100;
06785         if (a010 < yarray[IJK(i,j,k)]) yarray[IJK(i,j,k)] = a010;
06786         if (a001 < zarray[IJK(i,j,k)]) zarray[IJK(i,j,k)] = a001;
06787     } /* k loop */
06788 } /* j loop */
06789 } /* i loop */
06790 }
06791
06792 /*
06793 NOTE: This is the original version of the markSphere function. It's in here
06794 for reference and in case a reversion to the original code is needed.
06795 D. Gohara (2/14/08)
06796 */
06797
06798 /*
06799 PRIVATE void markSphere(
06800     double rtot, double *tpos,
06801     int nx, int ny, int nz,
06802     double hx, double hy, double hzed,
06803     double xmin, double ymin, double zmin,
06804     double *array, double markVal) {
06805
06806     int i, j, k, imin, imax, jmin, jmax, kmin, kmax;
06807     double dx, dx2, dy, dy2, dz, dz2;
06808     double rtot2, pos[3];
06809
06810     // Convert to grid reference frame
06811     pos[0] = tpos[0] - xmin;

```

```

06813     pos[1] = tpos[1] - ymin;
06814     pos[2] = tpos[2] - zmin;
06815
06816     rtot2 = VSQR(rtot);
06817
06818     dx = rtot + 0.5*hx;
06819     imin = VMAX2(0, (int)ceil((pos[0] - dx)/hx));
06820     imax = VMIN2(nx-1, (int)floor((pos[0] + dx)/hx));
06821     for (i=imin; i<=imax; i++) {
06822         dx2 = VSQR(pos[0] - hx*i);
06823         if (rtot2 > dx2) {
06824             dy = VSQRT(rtot2 - dx2) + 0.5*hy;
06825         } else {
06826             dy = 0.5*hy;
06827         }
06828         jmin = VMAX2(0, (int)ceil((pos[1] - dy)/hy));
06829         jmax = VMIN2(ny-1, (int)floor((pos[1] + dy)/hy));
06830         for (j=jmin; j<=jmax; j++) {
06831             dy2 = VSQR(pos[1] - hy*j);
06832             if (rtot2 > (dx2+dy2)) {
06833                 dz = VSQRT(rtot2-dx2-dy2)+0.5*hzed;
06834             } else {
06835                 dz = 0.5*hzed;
06836             }
06837             kmin = VMAX2(0, (int)ceil((pos[2] - dz)/hzed));
06838             kmax = VMIN2(nz-1, (int)floor((pos[2] + dz)/hzed));
06839             for (k=kmin; k<=kmax; k++) {
06840                 dz2 = VSQR(k*hzed - pos[2]);
06841                 if ((dz2 + dy2 + dx2) <= rtot2) {
06842                     array[IJK(i,j,k)] = markVal;
06843                 }
06844             } // k loop
06845         } // j loop
06846     } // i loop
06847 }
06848 */
06849 VPRIVATE void markSphere(double rtot, double *tpos,
06850                          int nx, int ny, int nz,
06851                          double hx, double hy, double hz,
06852                          double xmin, double ymin, double zmin,
06853                          double *array, double markVal) {
06854
06855     int i, j, k;
06856     double fi, fj, fk;
06857     int imin, imax;
06858     int jmin, jmax;
06859     int kmin, kmax;
06860     double dx2, dy2, dz2;
06861     double xrange, yrange, zrange;
06862     double rtot2, posx, posy, posz;
06863
06864     /* Convert to grid reference frame */
06865     posx = tpos[0] - xmin;
06866     posy = tpos[1] - ymin;
06867     posz = tpos[2] - zmin;
06868
06869     rtot2 = VSQR(rtot);
06870
06871     xrange = rtot + 0.5 * hx;
06872     yrange = rtot + 0.5 * hy;
06873     zrange = rtot + 0.5 * hz;
06874
06875     imin = VMAX2(0, (int)ceil((posx - xrange)/hx));
06876     jmin = VMAX2(0, (int)ceil((posy - yrange)/hy));
06877     kmin = VMAX2(0, (int)ceil((posz - zrange)/hz));
06878
06879     imax = VMIN2(nx-1, (int)floor((posx + xrange)/hx));
06880     jmax = VMIN2(ny-1, (int)floor((posy + yrange)/hy));
06881     kmax = VMIN2(nz-1, (int)floor((posz + zrange)/hz));
06882
06883     for (i=imin, fi=imin; i<=imax; i++, fi+=1.) {
06884         dx2 = VSQR(posx - hx*fi);
06885         for (j=jmin, fj=jmin; j<=jmax; j++, fj+=1.) {
06886             dy2 = VSQR(posy - hy*fj);
06887             if ((dx2 + dy2) > rtot2) continue;
06888             for (k=kmin, fk=kmin; k<=kmax; k++, fk+=1.) {
06889                 dz2 = VSQR(posz - hz*fk);
06890                 if ((dz2 + dy2 + dx2) <= rtot2) {
06891                     array[IJK(i,j,k)] = markVal;
06892                 }
06893             }
06894         }
06895     }

```

```

06894     }
06895     }
06896 }
06897
06898 VPRIVATE void zlapSolve(
06899     Vpmg *thee,
06900     double **solution,
06901     double **source,
06902     double **work1
06903 ) {
06904
06905     /* NOTE: this is an incredibly inefficient algorithm. The next
06906      * improvement is to focus on only non-zero entries in the source term.
06907      * The best improvement is to use a fast sine transform */
06908
06909     int n, nx, ny, nz, i, j, k, kx, ky, kz;
06910     double hx, hy, hzed, wx, wy, wz, xlen, ylen, zlen;
06911     double phix, phixpl, phixml, phiy, phiyml, phiypl, phiz, phizml, phizpl;
06912     double norm, coef, proj, eigx, eigy, eigz;
06913     double ihx2, ihy2, ihzed2;
06914     double *u, *f, *phi;
06915
06916     /* Snarf grid parameters */
06917     nx = thee->pmgp->nx;
06918     ny = thee->pmgp->ny;
06919     nz = thee->pmgp->nz;
06920     n = nx*ny*nz;
06921     hx = thee->pmgp->hx;
06922     ihx2 = 1.0/hx/hx;
06923     hy = thee->pmgp->hy;
06924     ihy2 = 1.0/hy/hy;
06925     hzed = thee->pmgp->hzed;
06926     ihzed2 = 1.0/hzed/hzed;
06927     xlen = thee->pmgp->xlen;
06928     ylen = thee->pmgp->ylen;
06929     zlen = thee->pmgp->zlen;
06930
06931     /* Set solution and source array pointers */
06932     u = *solution;
06933     f = *source;
06934     phi = *work1;
06935
06936     /* Zero out the solution vector */
06937     for (i=0; i<n; i++) thee->u[i] = 0.0;
06938
06939     /* Iterate through the wavenumbers */
06940     for (kx=1; kx<(nx-1); kx++) {
06941
06942         wx = (VPI*(double)kx)/((double)nx - 1.0);
06943         eigx = 2.0*ihx2*(1.0 - cos(wx));
06944
06945         for (ky=1; ky<(ny-1); ky++) {
06946
06947             wy = (VPI*(double)ky)/((double)ny - 1.0);
06948             eigy = 2.0*ihy2*(1.0 - cos(wy));
06949
06950             for (kz=1; kz<(nz-1); kz++) {
06951
06952                 wz = (VPI*(double)kz)/((double)nz - 1.0);
06953                 eigz = 2.0*ihzed2*(1.0 - cos(wz));
06954
06955                 /* Calculate the basis function.
06956                  * We could calculate each basis function as
06957                  *   phix(i) = sin(wx*i)
06958                  *   phiy(j) = sin(wy*j)
06959                  *   phiz(k) = sin(wz*k)
06960                  * However, this is likely to be very expensive.
06961                  * Therefore, we can use the fact that
06962                  *   phix(i+1) = (2-hx*hx*eigx)*phix(i) - phix(i-1)
06963                  */
06964                 for (i=1; i<(nx-1); i++) {
06965                     if (i == 1) {
06966                         phix = sin(wx*(double)i);
06967                         phixml = 0.0;
06968                     } else {
06969                         phixpl = (2.0-hx*hx*eigx)*phix - phixml;
06970                         phixml = phix;
06971                         phix = phixpl;
06972                     }
06973                     /* phix = sin(wx*(double)i); */
06974                     for (j=1; j<(ny-1); j++) {

```

```

06975         if (j == 1) {
06976             phiy = sin(wy*(double)j);
06977             phiyml = 0.0;
06978         } else {
06979             phiypl = (2.0-hy*hy*eigy)*phiy - phiyml;
06980             phiyml = phiy;
06981             phiy = phiypl;
06982         }
06983         /* phiy = sin(wy*(double)j); */
06984         for (k=1; k<(nz-1); k++) {
06985             if (k == 1) {
06986                 phiz = sin(wz*(double)k);
06987                 phizml = 0.0;
06988             } else {
06989                 phizpl = (2.0-hzed*hzed*eigz)*phiz - phizml;
06990                 phizml = phiz;
06991                 phiz = phizpl;
06992             }
06993             /* phiz = sin(wz*(double)k); */
06994
06995             phi[IJK(i,j,k)] = phix*phiy*phiz;
06996         }
06997     }
06998 }
06999
07000
07001 /* Calculate the projection of the source function on this
07002  * basis function */
07003 proj = 0.0;
07004 for (i=1; i<(nx-1); i++) {
07005     for (j=1; j<(ny-1); j++) {
07006         for (k=1; k<(nz-1); k++) {
07007
07008             proj += f[IJK(i,j,k)]*phi[IJK(i,j,k)];
07009
07010         } /* k loop */
07011     } /* j loop */
07012 } /* i loop */
07013
07014 /* Assemble the coefficient to weight the contribution of this
07015  * basis function to the solution */
07016 /* The first contribution is the projection */
07017 coef = proj;
07018 /* The second contribution is the eigenvalue */
07019 coef = coef/(eigx + eigy + eigz);
07020 /* The third contribution is the normalization factor */
07021 coef = (8.0/xlen/ylen/zlen)*coef;
07022 /* The fourth contribution is from scaling the diagonal */
07023 /* coef = hx*hy*hzed*coef; */
07024
07025 /* Evaluate the basis function at each grid point */
07026 for (i=1; i<(nx-1); i++) {
07027     for (j=1; j<(ny-1); j++) {
07028         for (k=1; k<(nz-1); k++) {
07029
07030             u[IJK(i,j,k)] += coef*phi[IJK(i,j,k)];
07031
07032         } /* k loop */
07033     } /* j loop */
07034 } /* i loop */
07035
07036     } /* kz loop */
07037 } /* ky loop */
07038 } /* kx loop */
07039 }
07040 }
07041
07042 VPUBLIC int Vpmg_solveLaplace(Vpmg *thee) {
07043
07044     int i, j, k, ijk, nx, ny, nz, n, dilo, dihi, djlo, djhi, dklo, dkhi;
07045     double hx, hy, hzed, epsw, iepsw, scal, scalx, scaly, scalz;
07046
07047     nx = thee->pmgp->nx;
07048     ny = thee->pmgp->ny;
07049     nz = thee->pmgp->nz;
07050     n = nx*ny*nz;
07051     hx = thee->pmgp->hx;
07052     hy = thee->pmgp->hy;
07053     hzed = thee->pmgp->hzed;
07054     epsw = Vpbe_getSolventDiel(thee->pbe);
07055     iepsw = 1.0/epsw;

```

```

07056     scal = hx*hy*hzed;
07057     scalx = hx*hy/hzed;
07058     scaly = hx*hzed/hy;
07059     scalz = hx*hy/hzed;
07060
07061     if (!(thee->filled)) {
07062         Vnm_print(2, "Vpmg_solve: Need to call Vpmg_fillco()!\n");
07063         return 0;
07064     }
07065
07066     /* Load boundary conditions into the RHS array */
07067     for (i=1; i<(nx-1); i++) {
07068
07069         if (i == 1) dilo = 1;
07070         else dilo = 0;
07071         if (i == nx-2) dihi = 1;
07072         else dihi = 0;
07073
07074         for (j=1; j<(ny-1); j++) {
07075
07076             if (j == 1) djlo = 1;
07077             else djlo = 0;
07078             if (j == ny-2) djhi = 1;
07079             else djhi = 0;
07080
07081             for (k=1; k<(nz-1); k++) {
07082
07083                 if (k == 1) dklo = 1;
07084                 else dklo = 0;
07085                 if (k == nz-2) dkhi = 1;
07086                 else dkhi = 0;
07087
07088                 thee->fcf[IJK(i,j,k)] = \
07089                     iepsw*scal*thee->charge[IJK(i,j,k)] \
07090                     + dilo*scalx*thee->gxcf[IJKx(j,k,0)] \
07091                     + dihi*scalx*thee->gxcf[IJKx(j,k,1)] \
07092                     + djlo*scaly*thee->gycf[IJKy(i,k,0)] \
07093                     + djhi*scaly*thee->gycf[IJKy(i,k,1)] \
07094                     + dklo*scalz*thee->gzcf[IJKz(i,j,0)] \
07095                     + dkhi*scalz*thee->gzcf[IJKz(i,j,1)] ;
07096
07097             }
07098         }
07099     }
07100 }
07101
07102 /* Solve */
07103 zlapSolve( thee, &(thee->u), &(thee->fcf), &(thee->tcf) );
07104
07105 /* Add boundary conditions to solution */
07106 /* i faces */
07107 for (j=0; j<ny; j++) {
07108     for (k=0; k<nz; k++) {
07109         thee->u[IJK(0,j,k)] = thee->gxcf[IJKx(j,k,0)];
07110         thee->u[IJK(nx-1,j,k)] = thee->gycf[IJKx(j,k,1)];
07111     }
07112 }
07113 /* j faces */
07114 for (i=0; i<nx; i++) {
07115     for (k=0; k<nz; k++) {
07116         thee->u[IJK(i,0,k)] = thee->gycf[IJKy(i,k,0)];
07117         thee->u[IJK(i,ny-1,k)] = thee->gycf[IJKy(i,k,1)];
07118     }
07119 }
07120 /* k faces */
07121 for (i=0; i<nx; i++) {
07122     for (j=0; j<ny; j++) {
07123         thee->u[IJK(i,j,0)] = thee->gzcf[IJKz(i,j,0)];
07124         thee->u[IJK(i,j,nz-1)] = thee->gzcf[IJKz(i,j,1)];
07125     }
07126 }
07127
07128 return 1;
07129
07130 }
07131
07132 VPRIVATE double VFCH14(int i, double f) {
07133     return (2.5+((double) (i)-(f)));
07134 }
07135
07136 VPRIVATE double bspline4(double x) {
07137

```

```

07138     double m, m2;
07139     static double one6 = 1.0/6.0;
07140     static double one8 = 1.0/8.0;
07141     static double one24 = 1.0/24.0;
07142     static double thirteen24 = 13.0/24.0;
07143     static double fortyseven24 = 47.0/24.0;
07144     static double seventeen24 = 17.0/24.0;
07145
07146     if ((x > 0.0) && (x <= 1.0)){
07147         m = x*x;
07148         return one24*m*m;
07149     } else if ((x > 1.0) && (x <= 2.0)){
07150         m = x - 1.0;
07151         m2 = m*m;
07152         return -one8 + one6*x + m2*(0.25 + one6*m - one6*m2);
07153     } else if ((x > 2.0) && (x <= 3.0)){
07154         m = x - 2.0;
07155         m2 = m*m;
07156         return -thirteen24 + 0.5*x + m2*(-0.25 - 0.5*m + 0.25*m2);
07157     } else if ((x > 3.0) && (x <= 4.0)){
07158         m = x - 3.0;
07159         m2 = m*m;
07160         return fortyseven24 - 0.5*x + m2*(-0.25 + 0.5*m - one6*m2);
07161     } else if ((x > 4.0) && (x <= 5.0)){
07162         m = x - 4.0;
07163         m2 = m*m;
07164         return seventeen24 - one6*x + m2*(0.25 - one6*m + one24*m2);
07165     } else {
07166         return 0.0;
07167     }
07168 }
07169
07170 VPUBLIC double dbspline4(double x) {
07171
07172     double m, m2;
07173     static double one6 = 1.0/6.0;
07174     static double one3 = 1.0/3.0;
07175     static double two3 = 2.0/3.0;
07176     static double thirteen6 = 13.0/6.0;
07177
07178     if ((x > 0.0) && (x <= 1.0)){
07179         m2 = x*x;
07180         return one6*x*m2;
07181     } else if ((x > 1.0) && (x <= 2.0)){
07182         m = x - 1.0;
07183         m2 = m*m;
07184         return -one3 + 0.5*x + m2*(0.5 - two3*m);
07185     } else if ((x > 2.0) && (x <= 3.0)){
07186         m = x - 2.0;
07187         m2 = m*m;
07188         return 1.5 - 0.5*x + m2*(-1.5 + m);
07189     } else if ((x > 3.0) && (x <= 4.0)){
07190         m = x - 3.0;
07191         m2 = m*m;
07192         return 1.0 - 0.5*x + m2*(1.5 - two3*m);
07193     } else if ((x > 4.0) && (x <= 5.0)){
07194         m = x - 4.0;
07195         m2 = m*m;
07196         return -thirteen6 + 0.5*x + m2*(-0.5 + one6*m);
07197     } else {
07198         return 0.0;
07199     }
07200 }
07201
07202 VPUBLIC double d2bspline4(double x) {
07203
07204     double m, m2;
07205
07206     if ((x > 0.0) && (x <= 1.0)){
07207         return 0.5*x*x;
07208     } else if ((x > 1.0) && (x <= 2.0)){
07209         m = x - 1.0;
07210         m2 = m*m;
07211         return -0.5 + x - 2.0*m2;
07212     } else if ((x > 2.0) && (x <= 3.0)){
07213         m = x - 2.0;
07214         m2 = m*m;
07215         return 5.5 - 3.0*x + 3.0*m2;
07216     } else if ((x > 3.0) && (x <= 4.0)){
07217         m = x - 3.0;
07218         m2 = m*m;

```



```

07219         return -9.5 + 3.0*x - 2.0*m2;
07220     } else if ((x > 4.0) && (x <= 5.0)){
07221         m = x - 4.0;
07222         m2 = m*m;
07223         return 4.5 - x + 0.5*m2;
07224     } else {
07225         return 0.0;
07226     }
07227 }
07228
07229 VPUBLIC double d3bspline4(double x) {
07230
07231     if ((x > 0.0) && (x <= 1.0)) return x;
07232     else if ((x > 1.0) && (x <= 2.0)) return 5.0 - 4.0 * x;
07233     else if ((x > 2.0) && (x <= 3.0)) return -15.0 + 6.0 * x;
07234     else if ((x > 3.0) && (x <= 4.0)) return 15.0 - 4.0 * x;
07235     else if ((x > 4.0) && (x <= 5.0)) return x - 5.0;
07236     else return 0.0;
07237 }
07238 }
07239
07240 VPUBLIC void fillcoPermanentMultipole(Vpmg *thee) {
07241     Valist *alist;
07242     Vpbe *pbe;
07243     Vatom *atom;
07244     /* Conversions */
07245     double zmagic, f;
07246     /* Grid */
07247     double xmin, xmax, ymin, ymax, zmin, zmax;
07248     double xlen, ylen, zlen, position[3], ifloat, jfloat, kfloat;
07249     double hx, hy, hzed, *apos;
07250     /* Multipole */
07251     double charge, *dipole, *quad;
07252     double c, ux, uy, uz, qxx, qyx, qyy, qzx, qzy, qzz, qave;
07253     /* B-spline weights */
07254     double mx, my, mz, dmx, dmy, dmz, d2mx, d2my, d2mz;
07255     double mi, mj, mk;
07256     /* Loop variables */
07257     int i, ii, jj, kk, nx, ny, nz, iatom;
07258     int im2, im1, ip1, ip2, jm2, jm1, jp1, jp2, km2, km1, kp1, kp2;
07259
07260     /* sanity check */
07261     double mir, mjr, mkr, mr2;
07262     double debye, mc, mux, muy, muz, mqxx, mqyx, mqyy, mqzx, mqzy, mqzz;
07263
07264     VASSERT(thee != VNULL);
07265
07266     /* Get PBE info */
07267     pbe = thee->pbe;
07268     alist = pbe->alist;
07269     zmagic = Vpbe_getZmagic(pbe);
07270
07271     /* Mesh info */
07272     nx = thee->pmgp->nx;
07273     ny = thee->pmgp->ny;
07274     nz = thee->pmgp->nz;
07275     hx = thee->pmgp->hx;
07276     hy = thee->pmgp->hy;
07277     hzed = thee->pmgp->hzed;
07278
07279     /* Conversion */
07280     f = zmagic/(hx*hy*hzed);
07281
07282     /* Define the total domain size */
07283     xlen = thee->pmgp->xlen;
07284     ylen = thee->pmgp->ylen;
07285     zlen = thee->pmgp->zlen;
07286
07287     /* Define the min/max dimensions */
07288     xmin = thee->pmgp->xcent - (xlen/2.0);
07289     ymin = thee->pmgp->ycent - (ylen/2.0);
07290     zmin = thee->pmgp->zcent - (zlen/2.0);
07291     xmax = thee->pmgp->xcent + (xlen/2.0);
07292     ymax = thee->pmgp->ycent + (ylen/2.0);
07293     zmax = thee->pmgp->zcent + (zlen/2.0);
07294
07295     /* Fill in the source term (permanent atomic multipoles) */
07296     Vnm_print(0, "fillcoPermanentMultipole: filling in source term.\n");
07297     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
07298
07299

```

```

07300         atom = Valist_getAtom(alist, iatom);
07301         apos = Vatom_getPosition(atom);
07302
07303         c = Vatom_getCharge(atom)*f;
07304
07305     #if defined(WITH_TINKER)
07306         dipole = Vatom_getDipole(atom);
07307         ux = dipole[0]/hx*f;
07308         uy = dipole[1]/hy*f;
07309         uz = dipole[2]/hz*f;
07310         quad = Vatom_getQuadrupole(atom);
07311         qxx = (1.0/3.0)*quad[0]/(hx*hx)*f;
07312         qyx = (2.0/3.0)*quad[3]/(hx*hy)*f;
07313         qyy = (1.0/3.0)*quad[4]/(hy*hy)*f;
07314         qzx = (2.0/3.0)*quad[6]/(hz*hx)*f;
07315         qzy = (2.0/3.0)*quad[7]/(hz*hy)*f;
07316         qzz = (1.0/3.0)*quad[8]/(hz*hz)*f;
07317     #else
07318         ux = 0.0;
07319         uy = 0.0;
07320         uz = 0.0;
07321         qxx = 0.0;
07322         qyx = 0.0;
07323         qyy = 0.0;
07324         qzx = 0.0;
07325         qzy = 0.0;
07326         qzz = 0.0;
07327     #endif /* if defined(WITH_TINKER) */
07328
07329     /* check
07330     mc = 0.0;
07331     mux = 0.0;
07332     muy = 0.0;
07333     muz = 0.0;
07334     mqxx = 0.0;
07335     mqyx = 0.0;
07336     mqyy = 0.0;
07337     mqzx = 0.0;
07338     mqzy = 0.0;
07339     mqzz = 0.0; */
07340
07341     /* Make sure we're on the grid */
07342     if ((apos[0]<=(xmin-2*hx)) || (apos[0]>=(xmax+2*hx)) || \
07343         (apos[1]<=(ymin-2*hy)) || (apos[1]>=(ymax+2*hy)) || \
07344         (apos[2]<=(zmin-2*hz)) || (apos[2]>=(zmax+2*hz))) {
07345         Vnm_print(2, "fillcoPermanentMultipole: Atom # %d at (%4.3f, %4.3f, %4.3f) is off the mesh
07346 (ignoring this atom):\n", iatom, apos[0], apos[1], apos[2]);
07347         Vnm_print(2, "fillcoPermanentMultipole: xmin = %g, xmax = %g\n", xmin, xmax);
07348         Vnm_print(2, "fillcoPermanentMultipole: ymin = %g, ymax = %g\n", ymin, ymax);
07349         Vnm_print(2, "fillcoPermanentMultipole: zmin = %g, zmax = %g\n", zmin, zmax);
07350         fflush(stderr);
07351     } else {
07352         /* Convert the atom position to grid reference frame */
07353         position[0] = apos[0] - xmin;
07354         position[1] = apos[1] - ymin;
07355         position[2] = apos[2] - zmin;
07356
07357         /* Figure out which vertices we're next to */
07358         ifloat = position[0]/hx;
07359         jfloat = position[1]/hy;
07360         kfloat = position[2]/hz;
07361
07362         ip1 = (int)ceil(ifloat);
07363         ip2 = ip1 + 2;
07364         im1 = (int)floor(ifloat);
07365         im2 = im1 - 2;
07366         jp1 = (int)ceil(jfloat);
07367         jp2 = jp1 + 2;
07368         jm1 = (int)floor(jfloat);
07369         jm2 = jm1 - 2;
07370         kp1 = (int)ceil(kfloat);
07371         kp2 = kp1 + 2;
07372         km1 = (int)floor(kfloat);
07373         km2 = km1 - 2;
07374
07375         /* This step shouldn't be necessary, but it saves nasty debugging
07376          * later on if something goes wrong */
07377         ip2 = VMIN2(ip2,nx-1);
07378         ip1 = VMIN2(ip1,nx-1);
07379         im1 = VMAX2(im1,0);

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```

07380         im2 = VMAX2(im2,0);
07381         jp2 = VMIN2(jp2,ny-1);
07382         jp1 = VMIN2(jp1,ny-1);
07383         jm1 = VMAX2(jm1,0);
07384         jm2 = VMAX2(jm2,0);
07385         kp2 = VMIN2(kp2,nz-1);
07386         kp1 = VMIN2(kp1,nz-1);
07387         km1 = VMAX2(km1,0);
07388         km2 = VMAX2(km2,0);
07389
07390         /* Now assign fractions of the charge to the nearby verts */
07391         for (ii=im2; ii<=ip2; ii++) {
07392             mi = VFCHI4(ii,ifloat);
07393             mx = bspline4(mi);
07394             dmx = dbspline4(mi);
07395             d2mx = d2bspline4(mi);
07396             for (jj=jm2; jj<=jp2; jj++) {
07397                 mj = VFCHI4(jj,jfloat);
07398                 my = bspline4(mj);
07399                 dmy = dbspline4(mj);
07400                 d2my = d2bspline4(mj);
07401                 for (kk=km2; kk<=kp2; kk++) {
07402                     mk = VFCHI4(kk,kfloat);
07403                     mz = bspline4(mk);
07404                     dmz = dbspline4(mk);
07405                     d2mz = d2bspline4(mk);
07406                     charge = mx*my*mz*c -
07407                             dmx*my*mz*ux - mx*dmy*mz*uy - mx*my*dmz*uz +
07408                             d2mx*my*mz*qxx +
07409                             dmx*dmy*mz*qyx + mx*d2my*mz*qyy +
07410                             dmx*my*dmz*qzx + mx*dmy*dmz*qzy + mx*my*d2mz*qzz;
07411                     thee->charge[IJK(ii,jj,kk)] += charge;
07412
07413                     /* sanity check - recalculate traceless multipoles
07414                      from the grid charge distribution for this
07415                      site.
07416
07417                     mir = (mi - 2.5) * hx;
07418                     mjr = (mj - 2.5) * hy;
07419                     mkr = (mk - 2.5) * hzed;
07420                     mr2 = mir*mir+mjr*mjr+mkr*mkr;
07421                     mc += charge;
07422                     mux += mir * charge;
07423                     muy += mjr * charge;
07424                     muz += mkr * charge;
07425                     mqxx += (1.5*mir*mir - 0.5*mr2) * charge;
07426                     mqyx += 1.5*mjr*mir * charge;
07427                     mqyy += (1.5*mjr*mjr - 0.5*mr2) * charge;
07428                     mqzx += 1.5*mkr*mir * charge;
07429                     mqzy += 1.5*mkr*mjr * charge;
07430                     mqzz += (1.5*mkr*mkr - 0.5*mr2) * charge;
07431                     */
07432                 }
07433             }
07434         }
07435     } /* endif (on the mesh) */
07436
07437     /* print out the Grid vs. Ideal Point Multipole. */
07438
07439     /*
07440     debye = 4.8033324;
07441     mc = mc/f;
07442     mux = mux/f*debye;
07443     muy = muy/f*debye;
07444     muz = muz/f*debye;
07445     mqxx = mqxx/f*debye;
07446     mqyy = mqyy/f*debye;
07447     mqzz = mqzz/f*debye;
07448     mqyx = mqyx/f*debye;
07449     mqzx = mqzx/f*debye;
07450     mqzy = mqzy/f*debye;
07451
07452     printf(" Grid v. Actual Permanent Multipole for Site %i\n",iatom);
07453     printf(" G: %10.6f\n",mc);
07454     printf(" A: %10.6f\n\n",c/f);
07455     printf(" G: %10.6f %10.6f %10.6f\n",mux,muy,muz);
07456     printf(" A: %10.6f %10.6f %10.6f\n\n",
07457            (ux * hx / f) * debye,
07458            (uy * hy / f) * debye,
07459            (uz * hzed / f) * debye);
07460     printf(" G: %10.6f\n",mqxx);

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```

07461         printf(" A: %10.6f\n",quad[0]*debye);
07462         printf(" G: %10.6f %10.6f\n",mqyx,mqyy);
07463         printf(" A: %10.6f %10.6f\n",quad[3]*debye,quad[4]*debye);
07464         printf(" G: %10.6f %10.6f %10.6f\n",mqzx,mqzy,mqzz);
07465         printf(" A: %10.6f %10.6f %10.6f\n\n",
07466                quad[6]*debye,quad[7]*debye,quad[8]*debye);  */
07467     } /* endfor (each atom) */
07468 }
07469 }
07470
07471 #if defined(WITH_TINKER)
07472
07473 VPUBLIC void fillcoInducedDipole(Vpmg *thee) {
07474
07475     Valist *alist;
07476     Vpbe *pbe;
07477     Vatom *atom;
07478     /* Conversions */
07479     double zmagic, f;
07480     /* Grid */
07481     double xmin, xmax, ymin, ymax, zmin, zmax;
07482     double xlen, ylen, zlen, ifloat, jfloat, kfloat;
07483     double hx, hy, hzed, *apos, position[3];
07484     /* B-spline weights */
07485     double mx, my, mz, dmX, dmy, dmz;
07486     /* Dipole */
07487     double charge, *dipole, ux,uy,uz;
07488     double mi,mj,mk;
07489     /* Loop indeces */
07490     int i, ii, jj, kk, nx, ny, nz, iatom;
07491     int im2, im1, ip1, ip2, jm2, jm1, jp1, jp2, km2, km1, kp1, kp2;
07492
07493     double debye;
07494     double mux,muy,muz;
07495     double mir,mjr,mkr;
07496
07497     VASSERT(thee != VNULL);
07498
07499     /* Get PBE info */
07500     pbe = thee->pbe;
07501     alist = pbe->alist;
07502     zmagic = Vpbe_getZmagic(pbe);
07503
07504     /* Mesh info */
07505     nx = thee->pmgp->nx;
07506     ny = thee->pmgp->ny;
07507     nz = thee->pmgp->nz;
07508     hx = thee->pmgp->hx;
07509     hy = thee->pmgp->hy;
07510     hzed = thee->pmgp->hzed;
07511
07512     /* Conversion */
07513     f = zmagic/(hx*hy*hzed);
07514
07515     /* Define the total domain size */
07516     xlen = thee->pmgp->xlen;
07517     ylen = thee->pmgp->ylen;
07518     zlen = thee->pmgp->zlen;
07519
07520     /* Define the min/max dimensions */
07521     xmin = thee->pmgp->xcent - (xlen/2.0);
07522     ymin = thee->pmgp->ycent - (ylen/2.0);
07523     zmin = thee->pmgp->zcent - (zlen/2.0);
07524     xmax = thee->pmgp->xcent + (xlen/2.0);
07525     ymax = thee->pmgp->ycent + (ylen/2.0);
07526     zmax = thee->pmgp->zcent + (zlen/2.0);
07527
07528     /* Fill in the source term (induced dipoles) */
07529     Vnm_print(0, "fillcoInducedDipole: filling in the source term.\n");
07530     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
07531
07532         atom = Valist_getAtom(alist, iatom);
07533         apos = Vatom_getPosition(atom);
07534
07535         dipole = Vatom_getInducedDipole(atom);
07536         ux = dipole[0]/hx*f;
07537         uy = dipole[1]/hy*f;
07538         uz = dipole[2]/hzed*f;
07539
07540         mux = 0.0;
07541         muy = 0.0;

```

```

07542     muz = 0.0;
07543
07544     /* Make sure we're on the grid */
07545     if ((apos[0]<=(xmin-2*hx)) || (apos[0]>=(xmax+2*hx)) || \
07546         (apos[1]<=(ymin-2*hy)) || (apos[1]>=(ymax+2*hy)) || \
07547         (apos[2]<=(zmin-2*hzed)) || (apos[2]>=(zmax+2*hzed))) {
07548         Vnm_print(2, "fillcoInducedDipole: Atom #%d at (%4.3f, %4.3f, %4.3f) is off the mesh (ignoring
this atom):\n", iatom, apos[0], apos[1], apos[2]);
07549         Vnm_print(2, "fillcoInducedDipole: xmin = %g, xmax = %g\n", xmin, xmax);
07550         Vnm_print(2, "fillcoInducedDipole: ymin = %g, ymax = %g\n", ymin, ymax);
07551         Vnm_print(2, "fillcoInducedDipole: zmin = %g, zmax = %g\n", zmin, zmax);
07552         fflush(stderr);
07553     } else {
07554
07555         /* Convert the atom position to grid reference frame */
07556         position[0] = apos[0] - xmin;
07557         position[1] = apos[1] - ymin;
07558         position[2] = apos[2] - zmin;
07559
07560         /* Figure out which vertices we're next to */
07561         ifloat = position[0]/hx;
07562         jfloat = position[1]/hy;
07563         kfloat = position[2]/hzed;
07564
07565         ip1 = (int)ceil(ifloat);
07566         ip2 = ip1 + 2;
07567         im1 = (int)floor(ifloat);
07568         im2 = im1 - 2;
07569         jp1 = (int)ceil(jfloat);
07570         jp2 = jp1 + 2;
07571         jm1 = (int)floor(jfloat);
07572         jm2 = jm1 - 2;
07573         kp1 = (int)ceil(kfloat);
07574         kp2 = kp1 + 2;
07575         km1 = (int)floor(kfloat);
07576         km2 = km1 - 2;
07577
07578         /* This step shouldn't be necessary, but it saves nasty debugging
07579          * later on if something goes wrong */
07580         ip2 = VMIN2(ip2, nx-1);
07581         ip1 = VMIN2(ip1, nx-1);
07582         im1 = VMAX2(im1, 0);
07583         im2 = VMAX2(im2, 0);
07584         jp2 = VMIN2(jp2, ny-1);
07585         jp1 = VMIN2(jp1, ny-1);
07586         jm1 = VMAX2(jm1, 0);
07587         jm2 = VMAX2(jm2, 0);
07588         kp2 = VMIN2(kp2, nz-1);
07589         kp1 = VMIN2(kp1, nz-1);
07590         km1 = VMAX2(km1, 0);
07591         km2 = VMAX2(km2, 0);
07592
07593         /* Now assign fractions of the dipole to the nearby verts */
07594         for (ii=im2; ii<=ip2; ii++) {
07595             mi = VFCHI4(ii, ifloat);
07596             mx = bspline4(mi);
07597             dm1 = db spline4(mi);
07598             for (jj=jm2; jj<=jp2; jj++) {
07599                 mj = VFCHI4(jj, jfloat);
07600                 my = bspline4(mj);
07601                 dm2 = db spline4(mj);
07602                 for (kk=km2; kk<=kp2; kk++) {
07603                     mk = VFCHI4(kk, kfloat);
07604                     mz = bspline4(mk);
07605                     dm3 = db spline4(mk);
07606                     charge = -dm1*my*mz*ux - mx*dm2*mz*uy - mx*my*dm3*uz;
07607                     thee->charge[IJK(ii, jj, kk)] += charge;
07608
07609                     /*
07610                     mir = (mi - 2.5) * hx;
07611                     mjr = (mj - 2.5) * hy;
07612                     mkr = (mk - 2.5) * hzed;
07613                     mux += mir * charge;
07614                     muy += mjr * charge;
07615                     muz += mkr * charge;
07616                     */
07617                 }
07618             }
07619         }
07620     } /* endif (on the mesh) */
07621

```

```

07622         /* check
07623         debye = 4.8033324;
07624         mux = mux/f*debye;
07625         muy = muy/f*debye;
07626         muz = muz/f*debye;
07627
07628         printf(" Grid v. Actual Induced Dipole for Site %i\n",iatom);
07629         printf(" G: %10.6f %10.6f %10.6f\n",mux,muy,muz);
07630         printf(" A: %10.6f %10.6f %10.6f\n\n",
07631             (ux * hx / f) * debye,
07632             (uy * hy / f) * debye,
07633             (uz * hzed /f) * debye);
07634     */
07635
07636     } /* endfor (each atom) */
07637 }
07638
07639 VPUBLIC void fillcoNLInducedDipole(Vpmg *thee) {
07640     Valist *alist;
07641     Vpbe *pbe;
07642     Vatom *atom;
07643     /* Conversions */
07644     double zmagic, f;
07645     /* Grid */
07646     double xmin, xmax, ymin, ymax, zmin, zmax;
07647     double xlen, ylen, zlen, ifloat, jfloat, kfloat;
07648     double hx, hy, hzed, *apos, position[3];
07649     /* B-spline weights */
07650     double mx, my, mz, dmx, dmy, dmz;
07651     /* Dipole */
07652     double charge, *dipole, ux,uy,uz;
07653     double mi,mj,mk;
07654     /* Loop indeces */
07655     int i, ii, jj, kk, nx, ny, nz, iatom;
07656     int im2, im1, ip1, ip2, jm2, jm1, jpl, jp2, km2, km1, kpl, kp2;
07657
07658     /* sanity check
07659     double debye;
07660     double mux,muy,muz;
07661     double mir,mjr,mkr;
07662     */
07663
07664     VASSERT(thee != VNULL);
07665
07666     /* Get PBE info */
07667     pbe = thee->pbe;
07668     alist = pbe->alist;
07669     zmagic = Vpbe_getZmagic(pbe);
07670
07671     /* Mesh info */
07672     nx = thee->pmgp->nx;
07673     ny = thee->pmgp->ny;
07674     nz = thee->pmgp->nz;
07675     hx = thee->pmgp->hx;
07676     hy = thee->pmgp->hy;
07677     hzed = thee->pmgp->hzed;
07678
07679     /* Conversion */
07680     f = zmagic/(hx*hy*hzed);
07681
07682     /* Define the total domain size */
07683     xlen = thee->pmgp->xlen;
07684     ylen = thee->pmgp->ylen;
07685     zlen = thee->pmgp->zlen;
07686
07687     /* Define the min/max dimensions */
07688     xmin = thee->pmgp->xcent - (xlen/2.0);
07689     ymin = thee->pmgp->ycent - (ylen/2.0);
07690     zmin = thee->pmgp->zcent - (zlen/2.0);
07691     xmax = thee->pmgp->xcent + (xlen/2.0);
07692     ymax = thee->pmgp->ycent + (ylen/2.0);
07693     zmax = thee->pmgp->zcent + (zlen/2.0);
07694
07695     /* Fill in the source term (non-local induced dipoles) */
07696     Vnm_print(0, "fillcoNLInducedDipole: filling in source term.\n");
07697     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
07698
07699         atom = Valist_getAtom(alist, iatom);
07700         apos = Vatom_getPosition(atom);
07701
07702

```

```

07703     dipole = Vatom_getNLInducedDipole(atom);
07704     ux = dipole[0]/hx*f;
07705     uy = dipole[1]/hy*f;
07706     uz = dipole[2]/hzed*f;
07707
07708     /*
07709     mux = 0.0;
07710     muy = 0.0;
07711     muz = 0.0;
07712     */
07713
07714     /* Make sure we're on the grid */
07715     if ((apos[0]<=(xmin-2*hx)) || (apos[0]>=(xmax+2*hx)) || \
07716         (apos[1]<=(ymin-2*hy)) || (apos[1]>=(ymax+2*hy)) || \
07717         (apos[2]<=(zmin-2*hzed)) || (apos[2]>=(zmax+2*hzed))) {
07718         Vnm_print(2, "fillcoNLInducedDipole: Atom #%d at (%4.3f, %4.3f,%4.3f) is off the mesh
(ignoreing this atom):\n", iatom, apos[0], apos[1], apos[2]);
07719         Vnm_print(2, "fillcoNLInducedDipole: xmin = %g, xmax = %g\n", xmin, xmax);
07720         Vnm_print(2, "fillcoNLInducedDipole: ymin = %g, ymax = %g\n", ymin, ymax);
07721         Vnm_print(2, "fillcoNLInducedDipole: zmin = %g, zmax = %g\n", zmin, zmax);
07722         fflush(stderr);
07723     } else {
07724
07725         /* Convert the atom position to grid reference frame */
07726         position[0] = apos[0] - xmin;
07727         position[1] = apos[1] - ymin;
07728         position[2] = apos[2] - zmin;
07729
07730         /* Figure out which vertices we're next to */
07731         ifloat = position[0]/hx;
07732         jfloat = position[1]/hy;
07733         kfloat = position[2]/hzed;
07734
07735         ip1 = (int)ceil(ifloat);
07736         ip2 = ip1 + 2;
07737         im1 = (int)floor(ifloat);
07738         im2 = im1 - 2;
07739         jp1 = (int)ceil(jfloat);
07740         jp2 = jp1 + 2;
07741         jm1 = (int)floor(jfloat);
07742         jm2 = jm1 - 2;
07743         kp1 = (int)ceil(kfloat);
07744         kp2 = kp1 + 2;
07745         km1 = (int)floor(kfloat);
07746         km2 = km1 - 2;
07747
07748         /* This step shouldn't be necessary, but it saves nasty debugging
07749         * later on if something goes wrong */
07750         ip2 = VMIN2(ip2,nx-1);
07751         ip1 = VMIN2(ip1,nx-1);
07752         im1 = VMAX2(im1,0);
07753         im2 = VMAX2(im2,0);
07754         jp2 = VMIN2(jp2,ny-1);
07755         jp1 = VMIN2(jp1,ny-1);
07756         jm1 = VMAX2(jm1,0);
07757         jm2 = VMAX2(jm2,0);
07758         kp2 = VMIN2(kp2,nz-1);
07759         kp1 = VMIN2(kp1,nz-1);
07760         km1 = VMAX2(km1,0);
07761         km2 = VMAX2(km2,0);
07762
07763         /* Now assign fractions of the non local induced dipole
07764         to the nearby verts */
07765         for (ii=im2; ii<=ip2; ii++) {
07766             mi = VFCHI4(ii,ifloat);
07767             mx = bspline4(mi);
07768             dmx = dbspline4(mi);
07769             for (jj=jm2; jj<=jp2; jj++) {
07770                 mj = VFCHI4(jj,jfloat);
07771                 my = bspline4(mj);
07772                 dmy = dbspline4(mj);
07773                 for (kk=km2; kk<=kp2; kk++) {
07774                     mk = VFCHI4(kk,kfloat);
07775                     mz = bspline4(mk);
07776                     dmz = dbspline4(mk);
07777                     charge = -dmx*my*mz*ux - mx*dmy*mz*uy - mx*my*dmz*uz;
07778                     thee->charge[IJK(ii,jj,kk)] += charge;
07779
07780                     /*
07781                     mir = (mi - 2.5) * hx;
07782                     mjr = (mj - 2.5) * hy;

```

```

07783             mkr = (mk - 2.5) * hzed;
07784             mux += mir * charge;
07785             muy += mjr * charge;
07786             muz += mkr * charge;
07787             */
07788         }
07789     }
07790 }
07791 } /* endif (on the mesh) */
07792
07793 /*
07794 debye = 4.8033324;
07795 mux = mux/f*debye;
07796 muy = muy/f*debye;
07797 muz = muz/f*debye;
07798
07799 printf(" Grid v. Actual Non-Local Induced Dipole for Site %i\n",iatom);
07800 printf(" G: %10.6f %10.6f %10.6f\n",mux,muy,muz);
07801 printf(" A: %10.6f %10.6f %10.6f\n\n",
07802        (ux * hx / f) * debye,
07803        (uy * hy / f) * debye,
07804        (uz * hzed /f) * debye); */
07805
07806 } /* endfor (each atom) */
07807 }
07808
07809 VPUBLIC double Vpmg_qfPermanentMultipoleEnergy(Vpmg *thee, int atomID) {
07810
07811     double *u;
07812     Vatom *atom;
07813     /* Grid variables */
07814     int nx, ny, nz;
07815     double xmax, xmin, ymax, ymin, zmax, zmin;
07816     double hx, hy, hzed, ifloat, jfloat, kfloat;
07817     double mi, mj, mk;
07818     double *position;
07819     /* B-spline weights */
07820     double mx, my, mz, dmx, dmy, dmz, d2mx, d2my, d2mz;
07821     /* Loop indeces */
07822     int ip1,ip2,im1,im2,jp1,jp2,jm1,jm2,kp1,kp2,km1,km2;
07823     int i,j,ii,jj,kk;
07824     /* Potential, field, field gradient and multipole components */
07825     double pot, rfe[3], rfde[3][3], energy;
07826     double f, charge, *dipole, *quad;
07827     double qxx, qyx, qyy, qzx, qzy, qzz;
07828
07829
07830     VASSERT(thee != VNULL);
07831     VASSERT(thee->filled);
07832
07833     /* Get the mesh information */
07834     nx = thee->pmgp->nx;
07835     ny = thee->pmgp->ny;
07836     nz = thee->pmgp->nz;
07837     hx = thee->pmgp->hx;
07838     hy = thee->pmgp->hy;
07839     hzed = thee->pmgp->hzed;
07840     xmax = thee->xf[nx-1];
07841     ymax = thee->yf[ny-1];
07842     zmax = thee->zf[nz-1];
07843     xmin = thee->xf[0];
07844     ymin = thee->yf[0];
07845     zmin = thee->zf[0];
07846
07847     u = thee->u;
07848
07849     atom = Valist_getAtom(thee->pbe->alist, atomID);
07850
07851     /* Currently all atoms must be in the same partition. */
07852
07853     VASSERT(atom->partID != 0);
07854
07855     /* Convert the atom position to grid coordinates */
07856
07857     position = Vatom_getPosition(atom);
07858     ifloat = (position[0] - xmin)/hx;
07859     jfloat = (position[1] - ymin)/hy;
07860     kfloat = (position[2] - zmin)/hzed;
07861     ip1 = (int)ceil(ifloat);
07862     ip2 = ip1 + 2;
07863     im1 = (int)floor(ifloat);

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07864     im2 = im1 - 2;
07865     jp1 = (int)ceil(jfloat);
07866     jp2 = jp1 + 2;
07867     jm1 = (int)floor(jfloat);
07868     jm2 = jm1 - 2;
07869     kp1 = (int)ceil(kfloat);
07870     kp2 = kp1 + 2;
07871     km1 = (int)floor(kfloat);
07872     km2 = km1 - 2;
07873
07874     /* This step shouldn't be necessary, but it saves nasty debugging
07875      * later on if something goes wrong */
07876     ip2 = VMIN2(ip2,nx-1);
07877     ip1 = VMIN2(ip1,nx-1);
07878     im1 = VMAX2(im1,0);
07879     im2 = VMAX2(im2,0);
07880     jp2 = VMIN2(jp2,ny-1);
07881     jp1 = VMIN2(jp1,ny-1);
07882     jm1 = VMAX2(jm1,0);
07883     jm2 = VMAX2(jm2,0);
07884     kp2 = VMIN2(kp2,nz-1);
07885     kp1 = VMIN2(kp1,nz-1);
07886     km1 = VMAX2(km1,0);
07887     km2 = VMAX2(km2,0);
07888
07889     /* Initialize observables to zero */
07890     energy = 0.0;
07891     pot = 0.0;
07892     for (i=0;i<3;i++){
07893         rfe[i] = 0.0;
07894         for (j=0;j<3;j++){
07895             rfde[i][j] = 0.0;
07896         }
07897     }
07898
07899     for (ii=im2; ii<=ip2; ii++) {
07900         mi = VFCHI4(ii,ifloat);
07901         mx = bspline4(mi);
07902         dmx = dbspline4(mi);
07903         d2mx = d2bspline4(mi);
07904         for (jj=jm2; jj<=jp2; jj++) {
07905             mj = VFCHI4(jj,jfloat);
07906             my = bspline4(mj);
07907             dmy = dbspline4(mj);
07908             d2my = d2bspline4(mj);
07909             for (kk=km2; kk<=kp2; kk++) {
07910                 mk = VFCHI4(kk,kfloat);
07911                 mz = bspline4(mk);
07912                 dmz = dbspline4(mk);
07913                 d2mz = d2bspline4(mk);
07914                 f = u[IJK(ii,jj,kk)];
07915                 /* potential */
07916                 pot += f*mx*my*mz;
07917                 /* field */
07918                 rfe[0] += f*dmx*my*mz/hx;
07919                 rfe[1] += f*mx*dmy*mz/hy;
07920                 rfe[2] += f*mx*my*dmz/hzed;
07921                 /* field gradient */
07922                 rfde[0][0] += f*d2mx*my*mz/(hx*hx);
07923                 rfde[1][0] += f*dmx*dmy*mz/(hy*hx);
07924                 rfde[1][1] += f*mx*d2my*mz/(hy*hy);
07925                 rfde[2][0] += f*dmx*my*dmz/(hx*hzed);
07926                 rfde[2][1] += f*mx*dmy*dmz/(hy*hzed);
07927                 rfde[2][2] += f*mx*my*d2mz/(hzed*hzed);
07928             }
07929         }
07930     }
07931
07932     charge = Vatom_getCharge(atom);
07933     dipole = Vatom_getDipole(atom);
07934     quad = Vatom_getQuadrupole(atom);
07935     qxx = quad[0]/3.0;
07936     qyx = quad[3]/3.0;
07937     qyy = quad[4]/3.0;
07938     qzx = quad[6]/3.0;
07939     qzy = quad[7]/3.0;
07940     qzz = quad[8]/3.0;
07941
07942     energy = pot * charge
07943             - rfe[0] * dipole[0]
07944             - rfe[1] * dipole[1]

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```

07945         - rfe[2] * dipole[2]
07946         + rfde[0][0]*qxx
07947         + 2.0*rfde[1][0]*qyx + rfde[1][1]*qyy
07948         + 2.0*rfde[2][0]*qzx + 2.0*rfde[2][1]*qzy + rfde[2][2]*qzz;
07949
07950     return energy;
07951 }
07952
07953 VPUBLIC void Vpmg_fieldSpline4(Vpmg *thee, int atomID, double field[3]) {
07954
07955     Vatom *atom;
07956     double *u, f;
07957     /* Grid variables */
07958     int nx, ny, nz;
07959     double xmax, xmin, ymax, ymin, zmax, zmin;
07960     double hx, hy, hzed, ifloat, jfloat, kfloat;
07961     double *apos, position[3];
07962     /* B-Spline weights */
07963     double mx, my, mz, dmz, dmy, dmz;
07964     double mi, mj, mk;
07965     /* Loop indices */
07966     int ip1, ip2, im1, im2, jp1, jp2, jm1, jm2, kp1, kp2, km1, km2;
07967     int i, j, ii, jj, kk;
07968
07969
07970     VASSERT (thee != VNULL);
07971
07972     /* Get the mesh information */
07973     nx = thee->pmgp->nx;
07974     ny = thee->pmgp->ny;
07975     nz = thee->pmgp->nz;
07976     hx = thee->pmgp->hx;
07977     hy = thee->pmgp->hy;
07978     hzed = thee->pmgp->hzed;
07979     xmax = thee->xf[nx-1];
07980     ymax = thee->yf[ny-1];
07981     zmax = thee->zf[nz-1];
07982     xmin = thee->xf[0];
07983     ymin = thee->yf[0];
07984     zmin = thee->zf[0];
07985
07986     u = thee->u;
07987
07988     atom = Valist_getAtom(thee->pbe->alist, atomID);
07989
07990     /* Currently all atoms must be in the same partition. */
07991
07992     VASSERT (atom->partID != 0);
07993
07994     /* Convert the atom position to grid coordinates */
07995
07996     apos = Vatom_getPosition(atom);
07997     position[0] = apos[0] - xmin;
07998     position[1] = apos[1] - ymin;
07999     position[2] = apos[2] - zmin;
08000     ifloat = position[0]/hx;
08001     jfloat = position[1]/hy;
08002     kfloat = position[2]/hzed;
08003     ip1 = (int)ceil(ifloat);
08004     ip2 = ip1 + 2;
08005     im1 = (int)floor(ifloat);
08006     im2 = im1 - 2;
08007     jp1 = (int)ceil(jfloat);
08008     jp2 = jp1 + 2;
08009     jm1 = (int)floor(jfloat);
08010     jm2 = jm1 - 2;
08011     kp1 = (int)ceil(kfloat);
08012     kp2 = kp1 + 2;
08013     km1 = (int)floor(kfloat);
08014     km2 = km1 - 2;
08015
08016     /* This step shouldn't be necessary, but it saves nasty debugging
08017      * later on if something goes wrong */
08018     ip2 = VMIN2(ip2, nx-1);
08019     ip1 = VMIN2(ip1, nx-1);
08020     im1 = VMAX2(im1, 0);
08021     im2 = VMAX2(im2, 0);
08022     jp2 = VMIN2(jp2, ny-1);
08023     jp1 = VMIN2(jp1, ny-1);
08024     jm1 = VMAX2(jm1, 0);
08025     jm2 = VMAX2(jm2, 0);

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```

08026     kp2 = VMIN2(kp2,nz-1);
08027     kp1 = VMIN2(kp1,nz-1);
08028     km1 = VMAX2(km1,0);
08029     km2 = VMAX2(km2,0);
08030
08031     for (i=0;i<3;i++){
08032         field[i] = 0.0;
08033     }
08034
08035     for (ii=im2; ii<=ip2; ii++) {
08036         mi = VFCHI4(ii,ifloat);
08037         mx = bspline4(mi);
08038         dmx = dbspline4(mi);
08039         for (jj=jm2; jj<=jp2; jj++) {
08040             mj = VFCHI4(jj,jfloat);
08041             my = bspline4(mj);
08042             dmy = dbspline4(mj);
08043             for (kk=km2; kk<=kp2; kk++) {
08044                 mk = VFCHI4(kk,kfloat);
08045                 mz = bspline4(mk);
08046                 dmz = dbspline4(mk);
08047                 f = u[IJK(ii,jj,kk)];
08048
08049                 field[0] += f*dmx*my*mz/hx;
08050                 field[1] += f*mx*dmy*mz/hy;
08051                 field[2] += f*mx*my*dmz/hzed;
08052             }
08053         }
08054     }
08055 }
08056
08057 VPUBLIC void Vpmg_qfPermanentMultipoleForce(Vpmg *thee, int atomID,
08058                                             double force[3], double torque[3]) {
08059
08060     Vatom *atom;
08061     double f, *u, *apos, position[3];
08062
08063     /* Grid variables */
08064     int nx,ny,nz;
08065     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax;
08066     double hx, hy, hzed, ifloat, jfloat, kfloat;
08067
08068     /* B-spline weights */
08069     double mx, my, mz, dmx, dmy, dmz, d2mx, d2my, d2mz, d3mx, d3my, d3mz;
08070     double mi, mj, mk;
08071
08072     /* Loop indeces */
08073     int i, j, k, ii, jj, kk;
08074     int im2, im1, ip1, ip2, jm2, jm1, jp1, jp2, km2, km1, kp1, kp2;
08075
08076     /* Potential, field, field gradient and 2nd field gradient */
08077     double pot, e[3], de[3][3], d2e[3][3][3];
08078
08079     /* Permanent multipole components */
08080     double *dipole, *quad;
08081     double c, ux, uy, uz, qxx, qxy, qxz, qyx, qyy, qyz, qzx, qzy, qzz;
08082
08083     VASSERT(thee != VNULL);
08084     VASSERT(thee->filled);
08085
08086     atom = Valist_getAtom(thee->pbe->alist, atomID);
08087
08088     /* Currently all atoms must be in the same partition. */
08089
08090     VASSERT(atom->partID != 0);
08091
08092     apos = Vatom_getPosition(atom);
08093
08094     c = Vatom_getCharge(atom);
08095     dipole = Vatom_getDipole(atom);
08096     ux = dipole[0];
08097     uy = dipole[1];
08098     uz = dipole[2];
08099     quad = Vatom_getQuadrupole(atom);
08100     qxx = quad[0]/3.0;
08101     qxy = quad[1]/3.0;
08102     qxz = quad[2]/3.0;
08103     qyx = quad[3]/3.0;
08104     qyy = quad[4]/3.0;
08105     qyz = quad[5]/3.0;
08106     qzx = quad[6]/3.0;

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```

08107     qzy = quad[7]/3.0;
08108     qzz = quad[8]/3.0;
08109
08110     /* Initialize observables */
08111     pot = 0.0;
08112     for (i=0; i<3; i++){
08113         e[i] = 0.0;
08114         for (j=0; j<3; j++){
08115             de[i][j] = 0.0;
08116             for (k=0; k<3; k++){
08117                 d2e[i][j][k] = 0.0;
08118             }
08119         }
08120     }
08121
08122     /* Mesh info */
08123     nx = thee->pmgp->nx;
08124     ny = thee->pmgp->ny;
08125     nz = thee->pmgp->nz;
08126     hx = thee->pmgp->hx;
08127     hy = thee->pmgp->hy;
08128     hzed = thee->pmgp->hzed;
08129     xlen = thee->pmgp->xlen;
08130     ylen = thee->pmgp->ylen;
08131     zlen = thee->pmgp->zlen;
08132     xmin = thee->pmgp->xmin;
08133     ymin = thee->pmgp->ymin;
08134     zmin = thee->pmgp->zmin;
08135     xmax = thee->pmgp->xmax;
08136     ymax = thee->pmgp->ymax;
08137     zmax = thee->pmgp->zmax;
08138     u = thee->u;
08139
08140     /* Make sure we're on the grid */
08141     if ((apos[0]<=(xmin+2*hx)) || (apos[0]>=(xmax-2*hx)) \
08142         || (apos[1]<=(ymin+2*hy)) || (apos[1]>=(ymax-2*hy)) \
08143         || (apos[2]<=(zmin+2*hzed)) || (apos[2]>=(zmax-2*hzed))) {
08144         Vnm_print(2, "qfPermanentMultipoleForce: Atom off the mesh (ignoring) %6.3f %6.3f %6.3f\n",
08145             apos[0], apos[1], apos[2]);
08146         fflush(stderr);
08147     } else {
08148         /* Convert the atom position to grid coordinates */
08149         position[0] = apos[0] - xmin;
08150         position[1] = apos[1] - ymin;
08151         position[2] = apos[2] - zmin;
08152         ifloat = position[0]/hx;
08153         jfloat = position[1]/hy;
08154         kfloat = position[2]/hzed;
08155         ip1 = (int)ceil(ifloat);
08156         ip2 = ip1 + 2;
08157         im1 = (int)floor(ifloat);
08158         im2 = im1 - 2;
08159         jp1 = (int)ceil(jfloat);
08160         jp2 = jp1 + 2;
08161         jm1 = (int)floor(jfloat);
08162         jm2 = jm1 - 2;
08163         kp1 = (int)ceil(kfloat);
08164         kp2 = kp1 + 2;
08165         km1 = (int)floor(kfloat);
08166         km2 = km1 - 2;
08167
08168         /* This step shouldn't be necessary, but it saves nasty debugging
08169          * later on if something goes wrong */
08170         ip2 = VMIN2(ip2, nx-1);
08171         ip1 = VMIN2(ip1, nx-1);
08172         im1 = VMAX2(im1, 0);
08173         im2 = VMAX2(im2, 0);
08174         jp2 = VMIN2(jp2, ny-1);
08175         jp1 = VMIN2(jp1, ny-1);
08176         jm1 = VMAX2(jm1, 0);
08177         jm2 = VMAX2(jm2, 0);
08178         kp2 = VMIN2(kp2, nz-1);
08179         kp1 = VMIN2(kp1, nz-1);
08180         km1 = VMAX2(km1, 0);
08181         km2 = VMAX2(km2, 0);
08182
08183         for (ii=im2; ii<=ip2; ii++) {
08184             mi = VFCHI4(ii, ifloat);
08185             mx = bspline4(mi);
08186             dmx = dbspline4(mi);

```

```

08187     d2mx = d2bspline4(mi);
08188     d3mx = d3bspline4(mi);
08189     for (jj=jm2; jj<=jp2; jj++) {
08190         mj = VFCHI4(jj,jfloat);
08191         my = bspline4(mj);
08192         dmy = dbspline4(mj);
08193         d2my = d2bspline4(mj);
08194         d3my = d3bspline4(mj);
08195         for (kk=km2; kk<=kp2; kk++) {
08196             mk = VFCHI4(kk,kfloat);
08197             mz = bspline4(mk);
08198             dmz = dbspline4(mk);
08199             d2mz = d2bspline4(mk);
08200             d3mz = d3bspline4(mk);
08201             f = u[IJK(ii,jj,kk)];
08202             /* Potential */
08203             pot += f*mx*my*mz;
08204             /* Field */
08205             e[0] += f*dmx*my*mz/hx;
08206             e[1] += f*mx*dmy*mz/hy;
08207             e[2] += f*mx*my*dmz/hzed;
08208             /* Field gradient */
08209             de[0][0] += f*d2mx*my*mz/(hx*hx);
08210             de[1][0] += f*dmx*dmy*mz/(hy*hx);
08211             de[1][1] += f*mx*d2my*mz/(hy*hy);
08212             de[2][0] += f*dmx*my*dmz/(hx*hzed);
08213             de[2][1] += f*mx*dmy*dmz/(hy*hzed);
08214             de[2][2] += f*mx*my*d2mz/(hzed*hzed);
08215             /* 2nd Field Gradient
08216             VxVxVa */
08217             d2e[0][0][0] += f*d3mx*my*mz/(hx*hx*hx);
08218             d2e[0][0][1] += f*d2mx*dmy*mz/(hx*hy*hx);
08219             d2e[0][0][2] += f*d2mx*my*dmz/(hx*hx*hzed);
08220             /* VyVxVa */
08221             d2e[1][0][0] += f*d2mx*dmy*mz/(hx*hx*hy);
08222             d2e[1][0][1] += f*dmx*d2my*mz/(hx*hy*hy);
08223             d2e[1][0][2] += f*dmx*dmy*dmz/(hx*hy*hzed);
08224             /* VyVyVa */
08225             d2e[1][1][0] += f*dmx*d2my*mz/(hx*hy*hy);
08226             d2e[1][1][1] += f*mx*d3my*mz/(hy*hy*hy);
08227             d2e[1][1][2] += f*mx*d2my*dmz/(hy*hy*hzed);
08228             /* VzVxVa */
08229             d2e[2][0][0] += f*d2mx*my*dmz/(hx*hx*hzed);
08230             d2e[2][0][1] += f*dmx*dmy*dmz/(hx*hy*hzed);
08231             d2e[2][0][2] += f*dmx*my*d2mz/(hx*hzed*hzed);
08232             /* VzVyVa */
08233             d2e[2][1][0] += f*dmx*dmy*dmz/(hx*hy*hzed);
08234             d2e[2][1][1] += f*mx*d2my*dmz/(hy*hy*hzed);
08235             d2e[2][1][2] += f*mx*dmy*d2mz/(hy*hzed*hzed);
08236             /* VzVzVa */
08237             d2e[2][2][0] += f*dmx*my*d2mz/(hx*hzed*hzed);
08238             d2e[2][2][1] += f*mx*dmy*d2mz/(hy*hzed*hzed);
08239             d2e[2][2][2] += f*mx*my*d3mz/(hzed*hzed*hzed);
08240         }
08241     }
08242 }
08243 }
08244
08245 /* Monopole Force */
08246 force[0] = e[0]*c;
08247 force[1] = e[1]*c;
08248 force[2] = e[2]*c;
08249
08250 /* Dipole Force */
08251 force[0] -= de[0][0]*ux+de[1][0]*uy+de[2][0]*uz;
08252 force[1] -= de[1][0]*ux+de[1][1]*uy+de[2][1]*uz;
08253 force[2] -= de[2][0]*ux+de[2][1]*uy+de[2][2]*uz;
08254
08255 /* Quadrupole Force */
08256 force[0] += d2e[0][0][0]*qxx
08257           + d2e[1][0][0]*qyx*2.0+d2e[1][1][0]*qyy
08258           + d2e[2][0][0]*qzx*2.0+d2e[2][1][0]*qzy*2.0+d2e[2][2][0]*qzz;
08259 force[1] += d2e[0][0][1]*qxx
08260           + d2e[1][0][1]*qyx*2.0+d2e[1][1][1]*qyy
08261           + d2e[2][0][1]*qzx*2.0+d2e[2][1][1]*qzy*2.0+d2e[2][2][1]*qzz;
08262 force[2] += d2e[0][0][2]*qxx
08263           + d2e[1][0][2]*qyx*2.0+d2e[1][1][2]*qyy
08264           + d2e[2][0][2]*qzx*2.0+d2e[2][1][2]*qzy*2.0+d2e[2][2][2]*qzz;
08265
08266 /* Dipole Torque */
08267 torque[0] = uy * e[2] - uz * e[1];

```

```

08268 torque[1] = uz * e[0] - ux * e[2];
08269 torque[2] = ux * e[1] - uy * e[0];
08270 /* Quadrupole Torque */
08271 de[0][1] = de[1][0];
08272 de[0][2] = de[2][0];
08273 de[1][2] = de[2][1];
08274 torque[0] -= 2.0*(qyx*de[0][2] + qyy*de[1][2] + qyz*de[2][2]
08275               - qzx*de[0][1] - qzy*de[1][1] - qzz*de[2][1]);
08276 torque[1] -= 2.0*(qzx*de[0][0] + qzy*de[1][0] + qzz*de[2][0]
08277               - qxx*de[0][2] - qxy*de[1][2] - qxz*de[2][2]);
08278 torque[2] -= 2.0*(qxx*de[0][1] + qxy*de[1][1] + qxz*de[2][1]
08279               - qyx*de[0][0] - qyy*de[1][0] - qyz*de[2][0]);
08280
08281
08282 /* printf(" qPhi Force %f %f %f\n", force[0], force[1], force[2]);
08283          printf(" qPhi Torque %f %f %f\n", torque[0], torque[1], torque[2]); */
08284 }
08285
08286 VPUBLIC void Vpmg_ibPermanentMultipoleForce(Vpmg *thee, int atomID,
08287                                           double force[3]) {
08288
08289     Valist *alist;
08290     Vacc *acc;
08291     Vpbe *pbe;
08292     Vatom *atom;
08293     Vsurf_Meth srfm;
08294
08295     /* Grid variables */
08296     double *apos, position[3], arad, irad, zkappa2, hx, hy, hzed;
08297     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax, rtot2;
08298     double rtot, dx, dx2, dy, dy2, dz, dz2, gpos[3], tgrad[3], fmag;
08299     double izmagic;
08300     int i, j, k, nx, ny, nz, imin, imax, jmin, jmax, kmin, kmax;
08301
08302     VASSERT(thee != VNULL);
08303
08304     /* Nonlinear PBE is not implemented for AMOEBA */
08305     VASSERT(!thee->pmgp->nonlin);
08306
08307     acc = thee->pbe->acc;
08308     srfm = thee->surfMeth;
08309     atom = Valist_getAtom(thee->pbe->alist, atomID);
08310
08311     /* Currently all atoms must be in the same partition. */
08312
08313     VASSERT(atom->partID != 0);
08314     apos = Vatom_getPosition(atom);
08315     arad = Vatom_getRadius(atom);
08316
08317     /* Reset force */
08318     force[0] = 0.0;
08319     force[1] = 0.0;
08320     force[2] = 0.0;
08321
08322     /* Get PBE info */
08323     pbe = thee->pbe;
08324     acc = pbe->acc;
08325     alist = pbe->alist;
08326     irad = Vpbe_getMaxIonRadius(pbe);
08327     zkappa2 = Vpbe_getZkappa2(pbe);
08328     izmagic = 1.0/Vpbe_getZmagic(pbe);
08329
08330     /* Should be a check for this further up. */
08331     VASSERT(zkappa2 > VPMGSMALL);
08332
08333     /* Mesh info */
08334     nx = thee->pmgp->nx;
08335     ny = thee->pmgp->ny;
08336     nz = thee->pmgp->nz;
08337     hx = thee->pmgp->hx;
08338     hy = thee->pmgp->hy;
08339     hzed = thee->pmgp->hzed;
08340     xlen = thee->pmgp->xlen;
08341     ylen = thee->pmgp->ylen;
08342     zlen = thee->pmgp->zlen;
08343     xmin = thee->pmgp->xmin;
08344     ymin = thee->pmgp->ymin;
08345     zmin = thee->pmgp->zmin;
08346     xmax = thee->pmgp->xmax;
08347     ymax = thee->pmgp->ymax;
08348     zmax = thee->pmgp->zmax;

```

```

08349
08350     /* Make sure we're on the grid */
08351     if ((apos[0]<=xmin) || (apos[0]>=xmax) || \
08352         (apos[1]<=ymin) || (apos[1]>=ymax) || \
08353         (apos[2]<=zmin) || (apos[2]>=zmax)) {
08354         Vnm_print(2, "ibPermanentMultipoleForce: Atom %d at (%4.3f, %4.3f, %4.3f) is off the mesh
(ignore):\n", atomID, apos[0], apos[1], apos[2]);
08355         Vnm_print(2, "ibPermanentMultipoleForce: xmin = %g, xmax = %g\n", xmin, xmax);
08356         Vnm_print(2, "ibPermanentMultipoleForce: ymin = %g, ymax = %g\n", ymin, ymax);
08357         Vnm_print(2, "ibPermanentMultipoleForce: zmin = %g, zmax = %g\n", zmin, zmax);
08358         fflush(stderr);
08359     } else {
08360
08361         /* Convert the atom position to grid reference frame */
08362         position[0] = apos[0] - xmin;
08363         position[1] = apos[1] - ymin;
08364         position[2] = apos[2] - zmin;
08365
08366         /* Integrate over points within this atom's (inflated) radius */
08367         rtot = (irad + arad + thee->splineWin);
08368         rtot2 = VSQR(rtot);
08369         dx = rtot + 0.5*hx;
08370         imin = VMAX2(0, (int)ceil((position[0] - dx)/hx));
08371         imax = VMIN2(nx-1, (int)floor((position[0] + dx)/hx));
08372         for (i=imin; i<=imax; i++) {
08373             dx2 = VSQR(position[0] - hx*i);
08374             if (rtot2 > dx2) dy = VSQR(rtot2 - dx2) + 0.5*hy;
08375             else dy = 0.5*hy;
08376             jmin = VMAX2(0, (int)ceil((position[1] - dy)/hy));
08377             jmax = VMIN2(ny-1, (int)floor((position[1] + dy)/hy));
08378             for (j=jmin; j<=jmax; j++) {
08379                 dy2 = VSQR(position[1] - hy*j);
08380                 if (rtot2 > (dx2+dy2)) dz = VSQR(rtot2-dx2-dy2)+0.5*hzed;
08381                 else dz = 0.5*hzed;
08382                 kmin = VMAX2(0, (int)ceil((position[2] - dz)/hzed));
08383                 kmax = VMIN2(nz-1, (int)floor((position[2] + dz)/hzed));
08384                 for (k=kmin; k<=kmax; k++) {
08385                     dz2 = VSQR(k*hzed - position[2]);
08386                     /* See if grid point is inside ivdw radius and set ccf
08387                      * accordingly (do spline assignment here) */
08388                     if ((dz2 + dy2 + dx2) <= rtot2) {
08389                         gpos[0] = i*hx + xmin;
08390                         gpos[1] = j*hy + ymin;
08391                         gpos[2] = k*hzed + zmin;
08392                         Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, irad, atom, tgrad);
08393                         fmag = VSQR(three->u[IJK(i,j,k)])*thee->kappa[IJK(i,j,k)];
08394                         force[0] += (zkappa2*fmag*tgrad[0]);
08395                         force[1] += (zkappa2*fmag*tgrad[1]);
08396                         force[2] += (zkappa2*fmag*tgrad[2]);
08397                     }
08398                 } /* k loop */
08399             } /* j loop */
08400         } /* i loop */
08401     }
08402
08403     force[0] = force[0] * 0.5 * hx * hy * hzed * izmagic;
08404     force[1] = force[1] * 0.5 * hx * hy * hzed * izmagic;
08405     force[2] = force[2] * 0.5 * hx * hy * hzed * izmagic;
08406
08407 }
08408
08409 VPUBLIC void Vpmg_dbPermanentMultipoleForce(Vpmg *thee, int atomID,
08410                                             double force[3]) {
08411
08412     Vacc *acc;
08413     Vpbe *pbe;
08414     Vatom *atom;
08415     Vsurf_Meth srfm;
08416
08417     double *apos, position[3], arad, hx, hy, hzed, izmagic, deps, depsi;
08418     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax, rtot2, epsp;
08419     double rtot, dx, gpos[3], tgrad[3], dbFmag, epsw, kT;
08420     double *u, Hxijk, Hyijk, Hzijk, Hximljk, Hyijmlk, Hzijkm1;
08421     double dHxijk[3], dHyijk[3], dHzijk[3], dHximljk[3], dHyijmlk[3];
08422     double dHzijkml[3];
08423     int i, j, k, l, nx, ny, nz, imin, imax, jmin, jmax, kmin, kmax;
08424
08425     VASSERT(thee != VNULL);
08426
08427     acc = thee->pbe->acc;
08428     srfm = thee->surfMeth;

```

```

08429     atom = Valist_getAtom(thee->pbe->alist, atomID);
08430
08431     /* Currently all atoms must be in the same partition. */
08432
08433     VASSERT(atom->partID != 0);
08434     arad = Vatom_getRadius(atom);
08435     apos = Vatom_getPosition(atom);
08436
08437     /* Reset force */
08438     force[0] = 0.0;
08439     force[1] = 0.0;
08440     force[2] = 0.0;
08441
08442     /* Get PBE info */
08443     pbe = thee->pbe;
08444     acc = pbe->acc;
08445     epsp = Vpbe_getSoluteDiel(pbe);
08446     epsw = Vpbe_getSolventDiel(pbe);
08447     kT = Vpbe_getTemperature(pbe) * (1e-3) * Vunit_Na * Vunit_kb;
08448     izmagic = 1.0 / Vpbe_getZmagic(pbe);
08449
08450
08451     deps = (epsw - epsp);
08452     depsi = 1.0 / deps;
08453
08454     VASSERT(VABS(deps) > VPMGSMALL);
08455
08456     /* Mesh info */
08457     nx = thee->pmgp->nx;
08458     ny = thee->pmgp->ny;
08459     nz = thee->pmgp->nz;
08460     hx = thee->pmgp->hx;
08461     hy = thee->pmgp->hy;
08462     hzed = thee->pmgp->hzed;
08463     xlen = thee->pmgp->xlen;
08464     ylen = thee->pmgp->ylen;
08465     zlen = thee->pmgp->zlen;
08466     xmin = thee->pmgp->xmin;
08467     ymin = thee->pmgp->ymin;
08468     zmin = thee->pmgp->zmin;
08469     xmax = thee->pmgp->xmax;
08470     ymax = thee->pmgp->ymax;
08471     zmax = thee->pmgp->zmax;
08472     u = thee->u;
08473
08474     /* Make sure we're on the grid */
08475     if ((apos[0] <= xmin) || (apos[0] >= xmax) || \
08476         (apos[1] <= ymin) || (apos[1] >= ymax) || \
08477         (apos[2] <= zmin) || (apos[2] >= zmax)) {
08478         Vnm_print(2, "dbPermanentMultipoleForce: Atom at (%4.3f, %4.3f, %4.3f) is off the mesh
08479         (ignoring):\n", apos[0], apos[1], apos[2]);
08480         Vnm_print(2, "dbPermanentMultipoleForce: xmin = %g, xmax = %g\n", xmin, xmax);
08481         Vnm_print(2, "dbPermanentMultipoleForce: ymin = %g, ymax = %g\n", ymin, ymax);
08482         Vnm_print(2, "dbPermanentMultipoleForce: zmin = %g, zmax = %g\n", zmin, zmax);
08483         fflush(stderr);
08484     } else {
08485
08486         /* Convert the atom position to grid reference frame */
08487         position[0] = apos[0] - xmin;
08488         position[1] = apos[1] - ymin;
08489         position[2] = apos[2] - zmin;
08490
08491         /* Integrate over points within this atom's (inflated) radius */
08492         rtot = (arad + thee->splineWin);
08493         rtot2 = VSQR(rtot);
08494         dx = rtot/hx;
08495         imin = (int)floor((position[0]-rtot)/hx);
08496         if (imin < 1) {
08497             Vnm_print(2, "dbPermanentMultipoleForce: Atom off grid!\n");
08498             return;
08499         }
08500         imax = (int)ceil((position[0]+rtot)/hx);
08501         if (imax > (nx-2)) {
08502             Vnm_print(2, "dbPermanentMultipoleForce: Atom off grid!\n");
08503             return;
08504         }
08505         jmin = (int)floor((position[1]-rtot)/hy);
08506         if (jmin < 1) {
08507             Vnm_print(2, "dbPermanentMultipoleForce: Atom off grid!\n");
08508             return;
08509         }
08510     }

```



```

08509     jmax = (int)ceil((position[1]+rtot)/hy);
08510     if (jmax > (ny-2)) {
08511         Vnm_print(2, "dbPermanentMultipoleForce: Atom off grid!\n");
08512         return;
08513     }
08514     kmin = (int)floor((position[2]-rtot)/hzd);
08515     if (kmin < 1) {
08516         Vnm_print(2, "dbPermanentMultipoleForce: Atom off grid!\n");
08517         return;
08518     }
08519     kmax = (int)ceil((position[2]+rtot)/hzd);
08520     if (kmax > (nz-2)) {
08521         Vnm_print(2, "dbPermanentMultipoleForce: Atom off grid!\n");
08522         return;
08523     }
08524     for (i=imin; i<=imax; i++) {
08525         for (j=jmin; j<=jmax; j++) {
08526             for (k=kmin; k<=kmax; k++) {
08527                 /* i,j,k */
08528                 gpos[0] = (i+0.5)*hx + xmin;
08529                 gpos[1] = j*hy + ymin;
08530                 gpos[2] = k*hzd + zmin;
08531                 Hxijk = (thee->epsx[IJK(i,j,k)] - epsp)*depsi;
08532                 Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
08533                     atom, dHxijk);
08534                 for (l=0; l<3; l++) dHxijk[l] *= Hxijk;
08535                 gpos[0] = i*hx + xmin;
08536                 gpos[1] = (j+0.5)*hy + ymin;
08537                 gpos[2] = k*hzd + zmin;
08538                 Hyijk = (thee->epsy[IJK(i,j,k)] - epsp)*depsi;
08539                 Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
08540                     atom, dHyijk);
08541                 for (l=0; l<3; l++) dHyijk[l] *= Hyijk;
08542                 gpos[0] = i*hx + xmin;
08543                 gpos[1] = j*hy + ymin;
08544                 gpos[2] = (k+0.5)*hzd + zmin;
08545                 Hzijk = (thee->epsz[IJK(i,j,k)] - epsp)*depsi;
08546                 Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
08547                     atom, dHzijk);
08548                 for (l=0; l<3; l++) dHzijk[l] *= Hzijk;
08549                 /* i-1,j,k */
08550                 gpos[0] = (i-0.5)*hx + xmin;
08551                 gpos[1] = j*hy + ymin;
08552                 gpos[2] = k*hzd + zmin;
08553                 Hximljk = (thee->epsx[IJK(i-1,j,k)] - epsp)*depsi;
08554                 Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
08555                     atom, dHximljk);
08556                 for (l=0; l<3; l++) dHximljk[l] *= Hximljk;
08557                 /* i,j-1,k */
08558                 gpos[0] = i*hx + xmin;
08559                 gpos[1] = (j-0.5)*hy + ymin;
08560                 gpos[2] = k*hzd + zmin;
08561                 Hyijmlk = (thee->epsy[IJK(i,j-1,k)] - epsp)*depsi;
08562                 Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
08563                     atom, dHyijmlk);
08564                 for (l=0; l<3; l++) dHyijmlk[l] *= Hyijmlk;
08565                 /* i,j,k-1 */
08566                 gpos[0] = i*hx + xmin;
08567                 gpos[1] = j*hy + ymin;
08568                 gpos[2] = (k-0.5)*hzd + zmin;
08569                 Hzijkml = (thee->epsz[IJK(i,j,k-1)] - epsp)*depsi;
08570                 Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
08571                     atom, dHzijkml);
08572                 for (l=0; l<3; l++) dHzijkml[l] *= Hzijkml;
08573                 dbFmag = u[IJK(i,j,k)];
08574                 tgrad[0] =
08575                     (dHxijk[0] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)])
08576                     + dHximljk[0] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) /VSQR(hx)
08577                     + (dHyijk[0] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)])
08578                     + dHyijmlk[0] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) /VSQR(hy)
08579                     + (dHzijk[0] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)])
08580                     + dHzijkml[0] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) /VSQR(hzd);
08581                 tgrad[1] =
08582                     (dHxijk[1] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)])
08583                     + dHximljk[1] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) /VSQR(hx)
08584                     + (dHyijk[1] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)])
08585                     + dHyijmlk[1] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) /VSQR(hy)
08586                     + (dHzijk[1] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)])
08587                     + dHzijkml[1] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) /VSQR(hzd);
08588                 tgrad[2] =
08589                     (dHxijk[2] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)])

```

```

08590         + dHximljk[2]*(u[IJK(i-1,j,k)]-u[IJK(i,j,k)]) /VSQR(hx)
08591         + (dHyijk[2] *(u[IJK(i,j+1,k)]-u[IJK(i,j,k)]))
08592         + dHyijm1k[2]*(u[IJK(i,j-1,k)]-u[IJK(i,j,k)]) /VSQR(hy)
08593         + (dHzijjk[2] *(u[IJK(i,j,k+1)]-u[IJK(i,j,k)]))
08594         + dHzijkm1[2]*(u[IJK(i,j,k-1)]-u[IJK(i,j,k)]) /VSQR(hzed);
08595         force[0] += (dbFmag*tgrad[0]);
08596         force[1] += (dbFmag*tgrad[1]);
08597         force[2] += (dbFmag*tgrad[2]);
08598     } /* k loop */
08599 } /* j loop */
08600 } /* i loop */
08601 force[0] = -force[0]*hx*hy*hzed*deps*0.5*izmagic;
08602 force[1] = -force[1]*hx*hy*hzed*deps*0.5*izmagic;
08603 force[2] = -force[2]*hx*hy*hzed*deps*0.5*izmagic;
08604 }
08605 }
08606
08607 VPUBLIC void Vpmg_qfDirectPolForce(Vpmg *thee, Vgrid* perm, Vgrid *induced,
08608                                     int atomID, double force[3], double torque[3]) {
08609
08610     Vatom *atom;
08611     Vpbe *pbe;
08612     double f, fp, *u, *up, *apos, position[3];
08613
08614     /* Grid variables */
08615     int nx,ny,nz;
08616     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax;
08617     double hx, hy, hzed, ifloat, jfloat, kfloat;
08618
08619     /* B-spline weights */
08620     double mx, my, mz, dmz, dmy, dmz, d2mx, d2my, d2mz, d3mx, d3my, d3mz;
08621     double mi, mj, mk;
08622
08623     /* Loop indeces */
08624     int i, j, k, ii, jj, kk;
08625     int im2, im1, ip1, ip2, jm2, jm1, jp1, jp2, km2, km1, kp1, kp2;
08626
08627     /* Permanent potential, field, field gradient and 2nd field gradient */
08628     double pot, e[3], de[3][3], d2e[3][3][3];
08629     /* Induced dipole field */
08630     double dep[3][3];
08631
08632     /* Permanent multipole components */
08633     double *dipole, *quad;
08634     double c, ux, uy, uz, qxx, qxy, qxz, qyx, qyy, qyz, qzx, qzy, qzz;
08635     double uix, uiy, uiz;
08636
08637     VASSERT(thee != VNULL);
08638     VASSERT(induced != VNULL); /* the potential due to permanent multipoles */
08639     VASSERT(induced != VNULL); /* the potential due to local induced dipoles */
08640     VASSERT(thee->pbe != VNULL);
08641     VASSERT(thee->pbe->alist != VNULL);
08642
08643     atom = Valist_getAtom(thee->pbe->alist, atomID);
08644     VASSERT(atom->partID != 0); /* all atoms must be in the same partition */
08645     apos = Vatom_getPosition(atom);
08646
08647     c = Vatom_getCharge(atom);
08648     dipole = Vatom_getDipole(atom);
08649     ux = dipole[0];
08650     uy = dipole[1];
08651     uz = dipole[2];
08652     quad = Vatom_getQuadrupole(atom);
08653     qxx = quad[0]/3.0;
08654     qxy = quad[1]/3.0;
08655     qxz = quad[2]/3.0;
08656     qyx = quad[3]/3.0;
08657     qyy = quad[4]/3.0;
08658     qyz = quad[5]/3.0;
08659     qzx = quad[6]/3.0;
08660     qzy = quad[7]/3.0;
08661     qzz = quad[8]/3.0;
08662
08663     dipole = Vatom_getInducedDipole(atom);
08664     uix = dipole[0];
08665     uiy = dipole[1];
08666     uiz = dipole[2];
08667
08668     /* Reset Field Gradients */
08669     pot = 0.0;
08670     for (i=0;i<3;i++){

```

```

08671     e[i] = 0.0;
08672     for (j=0; j<3; j++){
08673         de[i][j] = 0.0;
08674         dep[i][j] = 0.0;
08675         for (k=0; k<3; k++){
08676             d2e[i][j][k] = 0.0;
08677         }
08678     }
08679 }
08680
08681 /* Mesh info */
08682 nx = thee->pmgp->nx;
08683 ny = thee->pmgp->ny;
08684 nz = thee->pmgp->nz;
08685 hx = thee->pmgp->hx;
08686 hy = thee->pmgp->hy;
08687 hzed = thee->pmgp->hzed;
08688 xlen = thee->pmgp->xlen;
08689 ylen = thee->pmgp->ylen;
08690 zlen = thee->pmgp->zlen;
08691 xmin = thee->pmgp->xmin;
08692 ymin = thee->pmgp->ymin;
08693 zmin = thee->pmgp->zmin;
08694 xmax = thee->pmgp->xmax;
08695 ymax = thee->pmgp->ymax;
08696 zmax = thee->pmgp->zmax;
08697 u = induced->data;
08698 up = perm->data;
08699
08700 /* Make sure we're on the grid */
08701 if ((apos[0]<=(xmin+2*hx)) || (apos[0]>=(xmax-2*hx)) \
08702     || (apos[1]<=(ymin+2*hy)) || (apos[1]>=(ymax-2*hy)) \
08703     || (apos[2]<=(zmin+2*hzed)) || (apos[2]>=(zmax-2*hzed))) {
08704     Vnm_print(2, "qfDirectPolForce: Atom off the mesh (ignoring) %6.3f %6.3f %6.3f\n", apos[0],
08705 apos[1], apos[2]);
08706     fflush(stderr);
08707 } else {
08708
08709     /* Convert the atom position to grid coordinates */
08710     position[0] = apos[0] - xmin;
08711     position[1] = apos[1] - ymin;
08712     position[2] = apos[2] - zmin;
08713     ifloat = position[0]/hx;
08714     jfloat = position[1]/hy;
08715     kfloat = position[2]/hzed;
08716     ip1 = (int)ceil(ifloat);
08717     ip2 = ip1 + 2;
08718     im1 = (int)floor(ifloat);
08719     im2 = im1 - 2;
08720     jp1 = (int)ceil(jfloat);
08721     jp2 = jp1 + 2;
08722     jm1 = (int)floor(jfloat);
08723     jm2 = jm1 - 2;
08724     kp1 = (int)ceil(kfloat);
08725     kp2 = kp1 + 2;
08726     km1 = (int)floor(kfloat);
08727     km2 = km1 - 2;
08728
08729     /* This step shouldn't be necessary, but it saves nasty debugging
08730      * later on if something goes wrong */
08731     ip2 = VMIN2(ip2, nx-1);
08732     ip1 = VMIN2(ip1, nx-1);
08733     im1 = VMAX2(im1, 0);
08734     im2 = VMAX2(im2, 0);
08735     jp2 = VMIN2(jp2, ny-1);
08736     jp1 = VMIN2(jp1, ny-1);
08737     jm1 = VMAX2(jm1, 0);
08738     jm2 = VMAX2(jm2, 0);
08739     kp2 = VMIN2(kp2, nz-1);
08740     kp1 = VMIN2(kp1, nz-1);
08741     km1 = VMAX2(km1, 0);
08742     km2 = VMAX2(km2, 0);
08743
08744     for (ii=im2; ii<=ip2; ii++) {
08745         mi = VFCHI4(ii, ifloat);
08746         mx = bspline4(mi);
08747         dmx = dbspline4(mi);
08748         d2mx = d2bspline4(mi);
08749         d3mx = d3bspline4(mi);
08750         for (jj=jm2; jj<=jp2; jj++) {

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08751         mj = VFCHI4(jj,jfloat);
08752         my = bspline4(mj);
08753         dmy = dbspline4(mj);
08754         d2my = d2bspline4(mj);
08755         d3my = d3bspline4(mj);
08756         for (kk=km2; kk<=kp2; kk++) {
08757             mk = VFCHI4(kk,kfloat);
08758             mz = bspline4(mk);
08759             dmz = dbspline4(mk);
08760             d2mz = d2bspline4(mk);
08761             d3mz = d3bspline4(mk);
08762             f = u[IJK(ii,jj,kk)];
08763             fp = up[IJK(ii,jj,kk)];
08764             /* The potential */
08765             pot += f*mx*my*mz;
08766             /* The field */
08767             e[0] += f*dmx*my*mz/hx;
08768             e[1] += f*mx*dmy*mz/hy;
08769             e[2] += f*mx*my*dmz/hzed;
08770             /* The gradient of the field */
08771             de[0][0] += f*d2mx*my*mz/(hx*hx);
08772             de[1][0] += f*dmx*dmy*mz/(hy*hx);
08773             de[1][1] += f*mx*d2my*mz/(hy*hy);
08774             de[2][0] += f*dmx*my*dmz/(hx*hzed);
08775             de[2][1] += f*mx*dmy*dmz/(hy*hzed);
08776             de[2][2] += f*mx*my*d2mz/(hzed*hzed);
08777             /* The gradient of the (permanent) field */
08778             dep[0][0] += fp*d2mx*my*mz/(hx*hx);
08779             dep[1][0] += fp*dmx*dmy*mz/(hy*hx);
08780             dep[1][1] += fp*mx*d2my*mz/(hy*hy);
08781             dep[2][0] += fp*dmx*my*dmz/(hx*hzed);
08782             dep[2][1] += fp*mx*dmy*dmz/(hy*hzed);
08783             dep[2][2] += fp*mx*my*d2mz/(hzed*hzed);
08784             /* The 2nd gradient of the field
08785             VxVxVa */
08786             d2e[0][0][0] += f*d3mx*my*mz/(hx*hx*hx);
08787             d2e[0][0][1] += f*d2mx*dmy*mz/(hx*hy*hx);
08788             d2e[0][0][2] += f*d2mx*my*dmz/(hx*hx*hzed);
08789             /* VyVxVa */
08790             d2e[1][0][0] += f*d2mx*dmy*mz/(hx*hx*hy);
08791             d2e[1][0][1] += f*dmx*d2my*mz/(hx*hy*hy);
08792             d2e[1][0][2] += f*dmx*dmy*dmz/(hx*hy*hzed);
08793             /* VyVyVa */
08794             d2e[1][1][0] += f*dmx*d2my*mz/(hx*hy*hy);
08795             d2e[1][1][1] += f*mx*d3my*mz/(hy*hy*hy);
08796             d2e[1][1][2] += f*mx*d2my*dmz/(hy*hy*hzed);
08797             /* VzVxVa */
08798             d2e[2][0][0] += f*d2mx*my*dmz/(hx*hx*hzed);
08799             d2e[2][0][1] += f*dmx*dmy*dmz/(hx*hy*hzed);
08800             d2e[2][0][2] += f*dmx*my*d2mz/(hx*hzed*hzed);
08801             /* VzVyVa */
08802             d2e[2][1][0] += f*dmx*dmy*dmz/(hx*hy*hzed);
08803             d2e[2][1][1] += f*mx*d2my*dmz/(hy*hy*hzed);
08804             d2e[2][1][2] += f*mx*dmy*d2mz/(hy*hzed*hzed);
08805             /* VzVzVa */
08806             d2e[2][2][0] += f*dmx*my*d2mz/(hx*hzed*hzed);
08807             d2e[2][2][1] += f*mx*dmy*d2mz/(hy*hzed*hzed);
08808             d2e[2][2][2] += f*mx*my*d3mz/(hzed*hzed*hzed);
08809         }
08810     }
08811 }
08812
08813
08814 /* force on permanent multipole due to induced reaction field */
08815
08816 /* Monopole Force */
08817 force[0] = e[0]*c;
08818 force[1] = e[1]*c;
08819 force[2] = e[2]*c;
08820
08821 /* Dipole Force */
08822 force[0] -= de[0][0]*ux+de[1][0]*uy+de[2][0]*uz;
08823 force[1] -= de[1][0]*ux+de[1][1]*uy+de[2][1]*uz;
08824 force[2] -= de[2][0]*ux+de[2][1]*uy+de[2][2]*uz;
08825
08826 /* Quadrupole Force */
08827 force[0] += d2e[0][0][0]*qxx
08828           + d2e[1][0][0]*qyx*2.0+d2e[1][1][0]*qyy
08829           + d2e[2][0][0]*qzx*2.0+d2e[2][1][0]*qzy*2.0+d2e[2][2][0]*qzz;
08830 force[1] += d2e[0][0][1]*qxx
08831           + d2e[1][0][1]*qyx*2.0+d2e[1][1][1]*qyy

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08832         + d2e[2][0][1]*qzx*2.0+d2e[2][1][1]*qzy*2.0+d2e[2][2][1]*qzz;
08833     force[2] += d2e[0][0][2]*qxx
08834         + d2e[1][0][2]*qyx*2.0+d2e[1][1][2]*qyy
08835         + d2e[2][0][2]*qzx*2.0+d2e[2][1][2]*qzy*2.0+d2e[2][2][2]*qzz;
08836
08837     /* torque on permanent mulitpole due to induced reaction field */
08838
08839     /* Dipole Torque */
08840     torque[0] = uy * e[2] - uz * e[1];
08841     torque[1] = uz * e[0] - ux * e[2];
08842     torque[2] = ux * e[1] - uy * e[0];
08843
08844     /* Quadrupole Torque */
08845     /* Tx = -2.0*(Sum_a (Qya*dEaz) + Sum_b (Qzb*dEby))
08846        Ty = -2.0*(Sum_a (Qza*dEax) + Sum_b (Qxb*dEbz))
08847        Tz = -2.0*(Sum_a (Qxa*dEay) + Sum_b (Qyb*dEbx)) */
08848     de[0][1] = de[1][0];
08849     de[0][2] = de[2][0];
08850     de[1][2] = de[2][1];
08851     torque[0] -= 2.0*(qyx*de[0][2] + qyy*de[1][2] + qyz*de[2][2]
08852         - qzx*de[0][1] - qzy*de[1][1] - qzz*de[2][1]);
08853     torque[1] -= 2.0*(qzx*de[0][0] + qzy*de[1][0] + qzz*de[2][0]
08854         - qxx*de[0][2] - qxy*de[1][2] - qxz*de[2][2]);
08855     torque[2] -= 2.0*(qxx*de[0][1] + qxy*de[1][1] + qxz*de[2][1]
08856         - qyx*de[0][0] - qyy*de[1][0] - qyz*de[2][0]);
08857
08858     /* force on induced dipole due to permanent reaction field */
08859
08860     force[0] -= dep[0][0]*uix+dep[1][0]*uiy+dep[2][0]*uiz;
08861     force[1] -= dep[1][0]*uix+dep[1][1]*uiy+dep[2][1]*uiz;
08862     force[2] -= dep[2][0]*uix+dep[2][1]*uiy+dep[2][2]*uiz;
08863
08864     force[0] = 0.5 * force[0];
08865     force[1] = 0.5 * force[1];
08866     force[2] = 0.5 * force[2];
08867     torque[0] = 0.5 * torque[0];
08868     torque[1] = 0.5 * torque[1];
08869     torque[2] = 0.5 * torque[2];
08870
08871     /* printf(" qPhi Force %f %f %f\n", force[0], force[1], force[2]);
08872        printf(" qPhi Torque %f %f %f\n", torque[0], torque[1], torque[2]); */
08873 }
08874
08875 VPUBLIC void Vpmg_qfNLDirectPolForce(Vpmg *thee, Vgrid *perm, Vgrid *nlInduced,
08876                                     int atomID, double force[3], double torque[3]) {
08877
08878     Vatom *atom;
08879     double *apos, *dipole, *quad, position[3], hx, hy, hzed;
08880     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax;
08881     double pot, e[3], de[3][3], dep[3][3], d2e[3][3][3];
08882     double mx, my, mz, dmx, dmy, dmz, mi, mj, mk;
08883     double d2mx, d2my, d2mz, d3mx, d3my, d3mz;
08884     double *u, *up, charge, ifloat, jfloat, kfloat;
08885     double f, fp, c, ux, uy, uz, qxx, qxy, qxz, qyx, qyy, qyz, qzx, qzy, qzz;
08886     double uix, uiy, uiz;
08887     int i,j,k,nx, ny, nz, im2, im1, ip1, ip2, jm2, jm1, jp1, jp2, km2, km1;
08888     int kp1, kp2, ii, jj, kk;
08889
08890     VASSERT(thee != VNULL);
08891     VASSERT(perm != VNULL); /* potential due to permanent multipoles. */
08892     VASSERT(nlInduced != VNULL); /* potential due to non-local induced dipoles */
08893     VASSERT(!thee->pmpg->nonlin); /* Nonlinear PBE is not implemented for AMOEBA */
08894
08895     atom = Valist_getAtom(thee->pbe->alist, atomID);
08896     VASSERT(atom->partID != 0); /* Currently all atoms must be in the same partition. */
08897     apos = Vatom_getPosition(atom);
08898
08899     c = Vatom_getCharge(atom);
08900     dipole = Vatom_getDipole(atom);
08901     ux = dipole[0];
08902     uy = dipole[1];
08903     uz = dipole[2];
08904     quad = Vatom_getQuadrupole(atom);
08905     qxx = quad[0]/3.0;
08906     qxy = quad[1]/3.0;
08907     qxz = quad[2]/3.0;
08908     qyx = quad[3]/3.0;
08909     qyy = quad[4]/3.0;
08910     qyz = quad[5]/3.0;
08911     qzx = quad[6]/3.0;
08912     qzy = quad[7]/3.0;

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08913     qzz = quad[8]/3.0;
08914
08915     dipole = Vatom_getNLInducedDipole(atom);
08916     uix = dipole[0];
08917     uiy = dipole[1];
08918     uiz = dipole[2];
08919
08920     /* Reset Field Gradients */
08921     pot = 0.0;
08922     for (i=0;i<3;i++){
08923         e[i] = 0.0;
08924         for (j=0;j<3;j++){
08925             de[i][j] = 0.0;
08926             dep[i][j] = 0.0;
08927             for (k=0;k<3;k++){
08928                 d2e[i][j][k] = 0.0;
08929             }
08930         }
08931     }
08932
08933     /* Mesh info */
08934     nx = thee->pmgp->nx;
08935     ny = thee->pmgp->ny;
08936     nz = thee->pmgp->nz;
08937     hx = thee->pmgp->hx;
08938     hy = thee->pmgp->hy;
08939     hzed = thee->pmgp->hzed;
08940     xlen = thee->pmgp->xlen;
08941     ylen = thee->pmgp->ylen;
08942     zlen = thee->pmgp->zlen;
08943     xmin = thee->pmgp->xmin;
08944     ymin = thee->pmgp->ymin;
08945     zmin = thee->pmgp->zmin;
08946     xmax = thee->pmgp->xmax;
08947     ymax = thee->pmgp->ymax;
08948     zmax = thee->pmgp->zmax;
08949     u = nlInduced->data;
08950     up = perm->data;
08951
08952
08953     /* Make sure we're on the grid */
08954     if ((apos[0]<=(xmin+2*hx)) || (apos[0]>=(xmax-2*hx)) \
08955         || (apos[1]<=(ymin+2*hy)) || (apos[1]>=(ymax-2*hy)) \
08956         || (apos[2]<=(zmin+2*hzed)) || (apos[2]>=(zmax-2*hzed))) {
08957         Vnm_print(2, "qfNLDirectMultipoleForce: Atom off the mesh (ignoring) %6.3f %6.3f %6.3f\n",
08958             apos[0], apos[1], apos[2]);
08959     } else {
08960         /* Convert the atom position to grid coordinates */
08961         position[0] = apos[0] - xmin;
08962         position[1] = apos[1] - ymin;
08963         position[2] = apos[2] - zmin;
08964         ifloat = position[0]/hx;
08965         jfloat = position[1]/hy;
08966         kfloat = position[2]/hzed;
08967         ip1 = (int)ceil(ifloat);
08968         ip2 = ip1 + 2;
08969         im1 = (int)floor(ifloat);
08970         im2 = im1 - 2;
08971         jp1 = (int)ceil(jfloat);
08972         jp2 = jp1 + 2;
08973         jm1 = (int)floor(jfloat);
08974         jm2 = jm1 - 2;
08975         kp1 = (int)ceil(kfloat);
08976         kp2 = kp1 + 2;
08977         km1 = (int)floor(kfloat);
08978         km2 = km1 - 2;
08979
08980         /* This step shouldn't be necessary, but it saves nasty debugging
08981          * later on if something goes wrong */
08982         ip2 = VMIN2(ip2,nx-1);
08983         ip1 = VMIN2(ip1,nx-1);
08984         im1 = VMAX2(im1,0);
08985         im2 = VMAX2(im2,0);
08986         jp2 = VMIN2(jp2,ny-1);
08987         jp1 = VMIN2(jp1,ny-1);
08988         jm1 = VMAX2(jm1,0);
08989         jm2 = VMAX2(jm2,0);
08990         kp2 = VMIN2(kp2,nz-1);
08991         kp1 = VMIN2(kp1,nz-1);
08992         km1 = VMAX2(km1,0);

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```

08993     km2 = VMAX2(km2,0);
08994
08995     for (ii=im2; ii<=ip2; ii++) {
08996         mi = VFCHI4(ii,ifloat);
08997         mx = bspline4(mi);
08998         dmx = dbspline4(mi);
08999         d2mx = d2bspline4(mi);
09000         d3mx = d3bspline4(mi);
09001         for (jj=jm2; jj<=jp2; jj++) {
09002             mj = VFCHI4(jj,jfloat);
09003             my = bspline4(mj);
09004             dmy = dbspline4(mj);
09005             d2my = d2bspline4(mj);
09006             d3my = d3bspline4(mj);
09007             for (kk=km2; kk<=kp2; kk++) {
09008                 mk = VFCHI4(kk,kfloat);
09009                 mz = bspline4(mk);
09010                 dmz = dbspline4(mk);
09011                 d2mz = d2bspline4(mk);
09012                 d3mz = d3bspline4(mk);
09013                 f = u[IJK(ii,jj,kk)];
09014                 fp = up[IJK(ii,jj,kk)];
09015                 /* The potential */
09016                 pot += f*mx*my*mz;
09017                 /* The field */
09018                 e[0] += f*dmx*my*mz/hx;
09019                 e[1] += f*mx*dmy*mz/hy;
09020                 e[2] += f*mx*my*dmz/hzed;
09021                 /* The gradient of the field */
09022                 de[0][0] += f*d2mx*my*mz/(hx*hx);
09023                 de[1][0] += f*dmx*dmy*mz/(hy*hx);
09024                 de[1][1] += f*mx*d2my*mz/(hy*hy);
09025                 de[2][0] += f*dmx*my*dmz/(hx*hzed);
09026                 de[2][1] += f*mx*dmy*dmz/(hy*hzed);
09027                 de[2][2] += f*mx*my*d2mz/(hzed*hzed);
09028                 /* The gradient of the (permanent) field */
09029                 dep[0][0] += fp*d2mx*my*mz/(hx*hx);
09030                 dep[1][0] += fp*dmx*dmy*mz/(hy*hx);
09031                 dep[1][1] += fp*mx*d2my*mz/(hy*hy);
09032                 dep[2][0] += fp*dmx*my*dmz/(hx*hzed);
09033                 dep[2][1] += fp*mx*dmy*dmz/(hy*hzed);
09034                 dep[2][2] += fp*mx*my*d2mz/(hzed*hzed);
09035                 /* The 2nd gradient of the field */
09036                 /* VxVxVa */
09037                 d2e[0][0][0] += f*d3mx*my*mz/(hx*hx*hx);
09038                 d2e[0][0][1] += f*d2mx*dmy*mz/(hx*hy*hx);
09039                 d2e[0][0][2] += f*d2mx*my*dmz/(hx*hx*hzed);
09040                 /* VyVxVa */
09041                 d2e[1][0][0] += f*d2mx*dmy*mz/(hx*hx*hy);
09042                 d2e[1][0][1] += f*dmx*d2my*mz/(hx*hy*hy);
09043                 d2e[1][0][2] += f*dmx*dmy*dmz/(hx*hy*hzed);
09044                 /* VyVyVa */
09045                 d2e[1][1][0] += f*dmx*d2my*mz/(hx*hy*hy);
09046                 d2e[1][1][1] += f*mx*d3my*mz/(hy*hy*hy);
09047                 d2e[1][1][2] += f*mx*d2my*dmz/(hy*hy*hzed);
09048                 /* VzVxVa */
09049                 d2e[2][0][0] += f*d2mx*my*dmz/(hx*hx*hzed);
09050                 d2e[2][0][1] += f*dmx*dmy*dmz/(hx*hy*hzed);
09051                 d2e[2][0][2] += f*dmx*my*d2mz/(hx*hzed*hzed);
09052                 /* VzVyVa */
09053                 d2e[2][1][0] += f*dmx*dmy*dmz/(hx*hy*hzed);
09054                 d2e[2][1][1] += f*mx*d2my*dmz/(hy*hy*hzed);
09055                 d2e[2][1][2] += f*mx*dmy*d2mz/(hy*hzed*hzed);
09056                 /* VzVzVa */
09057                 d2e[2][2][0] += f*dmx*my*d2mz/(hx*hzed*hzed);
09058                 d2e[2][2][1] += f*mx*dmy*d2mz/(hy*hzed*hzed);
09059                 d2e[2][2][2] += f*mx*my*d3mz/(hzed*hzed*hzed);
09060             }
09061         }
09062     }
09063 }
09064
09065 /* force on permanent multipole due to non-local induced reaction field */
09066
09067 /* Monopole Force */
09068 force[0] = e[0]*c;
09069 force[1] = e[1]*c;
09070 force[2] = e[2]*c;
09071
09072 /* Dipole Force */
09073 force[0] -= de[0][0]*ux+de[1][0]*uy+de[2][0]*uz;

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09074     force[1] -= de[1][0]*ux+de[1][1]*uy+de[2][1]*uz;
09075     force[2] -= de[2][0]*ux+de[2][1]*uy+de[2][2]*uz;
09076
09077     /* Quadrupole Force */
09078     force[0] += d2e[0][0][0]*qxx
09079               + d2e[1][0][0]*qyx*2.0+d2e[1][1][0]*qyy
09080               + d2e[2][0][0]*qzx*2.0+d2e[2][1][0]*qzy*2.0+d2e[2][2][0]*qzz;
09081     force[1] += d2e[0][0][1]*qxx
09082               + d2e[1][0][1]*qyx*2.0+d2e[1][1][1]*qyy
09083               + d2e[2][0][1]*qzx*2.0+d2e[2][1][1]*qzy*2.0+d2e[2][2][1]*qzz;
09084     force[2] += d2e[0][0][2]*qxx
09085               + d2e[1][0][2]*qyx*2.0+d2e[1][1][2]*qyy
09086               + d2e[2][0][2]*qzx*2.0+d2e[2][1][2]*qzy*2.0+d2e[2][2][2]*qzz;
09087
09088     /* torque on permanent multipole due to non-local induced reaction field */
09089
09090     /* Dipole Torque */
09091     torque[0] = uy * e[2] - uz * e[1];
09092     torque[1] = uz * e[0] - ux * e[2];
09093     torque[2] = ux * e[1] - uy * e[0];
09094
09095     /* Quadrupole Torque */
09096     /* Tx = -2.0*(Sum_a (Qya*dEaz) + Sum_b (Qzb*dEby))
09097        Ty = -2.0*(Sum_a (Qza*dEax) + Sum_b (Qxb*dEbx))
09098        Tz = -2.0*(Sum_a (Qxa*dEay) + Sum_b (Qyb*dEbx)) */
09099     de[0][1] = de[1][0];
09100     de[0][2] = de[2][0];
09101     de[1][2] = de[2][1];
09102     torque[0] -= 2.0*(qyx*de[0][2] + qyy*de[1][2] + qyz*de[2][2]
09103                   - qzx*de[0][1] - qzy*de[1][1] - qzz*de[2][1]);
09104     torque[1] -= 2.0*(qzx*de[0][0] + qzy*de[1][0] + qzz*de[2][0]
09105                   - qxx*de[0][2] - qxy*de[1][2] - qxz*de[2][2]);
09106     torque[2] -= 2.0*(qxx*de[0][1] + qxy*de[1][1] + qxz*de[2][1]
09107                   - qyx*de[0][0] - qyy*de[1][0] - qyz*de[2][0]);
09108
09109     /* force on non-local induced dipole due to permanent reaction field */
09110
09111     force[0] -= dep[0][0]*uix+dep[1][0]*uiy+dep[2][0]*uiz;
09112     force[1] -= dep[1][0]*uix+dep[1][1]*uiy+dep[2][1]*uiz;
09113     force[2] -= dep[2][0]*uix+dep[2][1]*uiy+dep[2][2]*uiz;
09114
09115     force[0] = 0.5 * force[0];
09116     force[1] = 0.5 * force[1];
09117     force[2] = 0.5 * force[2];
09118     torque[0] = 0.5 * torque[0];
09119     torque[1] = 0.5 * torque[1];
09120     torque[2] = 0.5 * torque[2];
09121
09122     /* printf(" qPhi Force %f %f %f\n", force[0], force[1], force[2]);
09123        printf(" qPhi Torque %f %f %f\n", torque[0], torque[1], torque[2]); */
09124 }
09125
09126 VPUBLIC void Vpmg_ibDirectPolForce(Vpmg *thee, Vgrid *perm, Vgrid *induced,
09127                                   int atomID, double force[3]) {
09128
09129     Vatom *atom;
09130     Valist *alist;
09131     Vacc *acc;
09132     Vpbe *pbe;
09133     Vsurf_Meth srfm;
09134
09135     double *apos, position[3], arad, irad, zkappa2, hx, hy, hzed;
09136     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax, rtot2;
09137     double rtot, dx, dx2, dy, dy2, dz, dz2, gpos[3], tgrad[3], fmag;
09138     double izmagic;
09139     int i, j, k, nx, ny, nz, imin, imax, jmin, jmax, kmin, kmax;
09140
09141     VASSERT(thee != VNULL);
09142     VASSERT(perm != VNULL); /* potential due to permanent multipoles.*/
09143     VASSERT(induced != VNULL); /* potential due to induced dipoles. */
09144     VASSERT(!thee->pmgp->nonlin); /* Nonlinear PBE is not implemented for AMOEBA */
09145
09146     acc = thee->pbe->acc;
09147     srfm = thee->surfMeth;
09148     atom = Valist_getAtom(thee->pbe->alist, atomID);
09149     VASSERT(atom->partID != 0); /* Currently all atoms must be in the same partition. */
09150     apos = Vatom_getPosition(atom);
09151     arad = Vatom_getRadius(atom);
09152
09153     /* Reset force */
09154     force[0] = 0.0;

```



```

09155     force[1] = 0.0;
09156     force[2] = 0.0;
09157
09158     /* Get PBE info */
09159     pbe = thee->pbe;
09160     acc = pbe->acc;
09161     alist = pbe->alist;
09162     irad = Vpbe_getMaxIonRadius(pbe);
09163     zkappa2 = Vpbe_getZkappa2(pbe);
09164     izmagic = 1.0/Vpbe_getZmagic(pbe);
09165
09166     VASSERT(zkappa2 > VPMGSMALL); /* It is ok to run AMOEBA with no ions, but this is checked for higher
up in the driver. */
09167
09168     /* Mesh info */
09169     nx = induced->nx;
09170     ny = induced->ny;
09171     nz = induced->nz;
09172     hx = induced->hx;
09173     hy = induced->hy;
09174     hzed = induced->hzed;
09175     xmin = induced->xmin;
09176     ymin = induced->ymin;
09177     zmin = induced->zmin;
09178     xmax = induced->xmax;
09179     ymax = induced->ymax;
09180     zmax = induced->zmax;
09181     xlen = xmax-xmin;
09182     ylen = ymax-ymin;
09183     zlen = zmax-zmin;
09184
09185     /* Make sure we're on the grid */
09186     if ((apos[0]<=xmin) || (apos[0]>=xmax) || \
09187         (apos[1]<=ymin) || (apos[1]>=ymax) || \
09188         (apos[2]<=zmin) || (apos[2]>=zmax)) {
09189         Vnm_print(2, "Vpmg_ibForce: Atom at (%4.3f, %4.3f, %4.3f) is off the mesh (ignoring):\n",
09190             apos[0], apos[1], apos[2]);
09191         Vnm_print(2, "Vpmg_ibForce:      xmin = %g, xmax = %g\n", xmin, xmax);
09192         Vnm_print(2, "Vpmg_ibForce:      ymin = %g, ymax = %g\n", ymin, ymax);
09193         Vnm_print(2, "Vpmg_ibForce:      zmin = %g, zmax = %g\n", zmin, zmax);
09194         fflush(stderr);
09195     } else {
09196
09197         /* Convert the atom position to grid reference frame */
09198         position[0] = apos[0] - xmin;
09199         position[1] = apos[1] - ymin;
09200         position[2] = apos[2] - zmin;
09201
09202         /* Integrate over points within this atom's (inflated) radius */
09203         rtot = (irad + arad + thee->splineWin);
09204         rtot2 = VSQR(rtot);
09205         dx = rtot + 0.5*hx;
09206         imin = VMAX2(0, (int)ceil((position[0] - dx)/hx));
09207         imax = VMIN2(nx-1, (int)floor((position[0] + dx)/hx));
09208         for (i=imin; i<=imax; i++) {
09209             dx2 = VSQR(position[0] - hx*i);
09210             if (rtot2 > dx2) dy = VSQR(rtot2 - dx2) + 0.5*hy;
09211             else dy = 0.5*hy;
09212             jmin = VMAX2(0, (int)ceil((position[1] - dy)/hy));
09213             jmax = VMIN2(ny-1, (int)floor((position[1] + dy)/hy));
09214             for (j=jmin; j<=jmax; j++) {
09215                 dy2 = VSQR(position[1] - hy*j);
09216                 if (rtot2 > (dx2+dy2)) dz = VSQR(rtot2-dx2-dy2)+0.5*hzed;
09217                 else dz = 0.5*hzed;
09218                 kmin = VMAX2(0, (int)ceil((position[2] - dz)/hzed));
09219                 kmax = VMIN2(nz-1, (int)floor((position[2] + dz)/hzed));
09220                 for (k=kmin; k<=kmax; k++) {
09221                     dz2 = VSQR(k*hzed - position[2]);
09222                     /* See if grid point is inside ivdw radius and set ccf
09223                        * accordingly (do spline assignment here) */
09224                     if ((dz2 + dy2 + dx2) <= rtot2) {
09225                         gpos[0] = i*hx + xmin;
09226                         gpos[1] = j*hy + ymin;
09227                         gpos[2] = k*hzed + zmin;
09228                         Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, irad,
09229                             atom, tgrad);
09230                         fmag = induced->data[IJK(i,j,k)];
09231                         fmag *= perm->data[IJK(i,j,k)];
09232                         fmag *= thee->kappa[IJK(i,j,k)];
09233                         force[0] += (zkappa2*fmag*tgrad[0]);
09234                         force[1] += (zkappa2*fmag*tgrad[1]);

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09235         force[2] += (zkappa2*fmag*tgrad[2]);
09236     }
09237     } /* k loop */
09238     } /* j loop */
09239     } /* i loop */
09240 }
09241
09242 force[0] = force[0] * 0.5 * hx * hy * hzed * izmagic;
09243 force[1] = force[1] * 0.5 * hx * hy * hzed * izmagic;
09244 force[2] = force[2] * 0.5 * hx * hy * hzed * izmagic;
09245
09246 }
09247
09248 VPUBLIC void Vpmg_ibNLDirectPolForce(Vpmg *thee, Vgrid *perm, Vgrid *nlInduced,
09249                                     int atomID, double force[3]) {
09250     Vpmg_ibDirectPolForce(thee, perm, nlInduced, atomID, force);
09251 }
09252
09253 VPUBLIC void Vpmg_dbDirectPolForce(Vpmg *thee, Vgrid *perm, Vgrid *induced,
09254                                   int atomID, double force[3]) {
09255     Vatom *atom;
09256     Vacc *acc;
09257     Vpbe *pbe;
09258     Vsurf_Meth srfm;
09259
09260     double *apos, position[3], arad, hx, hy, hzed, izmagic, depsi, depsi;
09261     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax, rtot2, epsp;
09262     double rtot, dx, gpos[3], tgrad[3], dbFmag, epsw, kT;
09263     double *u, *up, Hxijk, Hyijk, Hzijk, Hximljk, Hyijmlk, Hzijkm1;
09264     double dHxijk[3], dHyijk[3], dHzijk[3], dHximljk[3], dHyijmlk[3];
09265     double dHzijkm1[3];
09266     int i, j, k, l, nx, ny, nz, imin, imax, jmin, jmax, kmin, kmax;
09267
09268     VASSERT(thee != VNULL);
09269     VASSERT(perm != VNULL); /* permanent multipole PMG solution. */
09270     VASSERT(induced != VNULL); /* potential due to induced dipoles. */
09271
09272     acc = thee->pbe->acc;
09273     atom = Valist_getAtom(thee->pbe->alist, atomID);
09274     VASSERT (atom->partID != 0); /* Currently all atoms must be in the same partition. */
09275     apos = Vatom_getPosition(atom);
09276     arad = Vatom_getRadius(atom);
09277
09278     /* Reset force */
09279     force[0] = 0.0;
09280     force[1] = 0.0;
09281     force[2] = 0.0;
09282
09283     /* Get PBE info */
09284     pbe = thee->pbe;
09285     acc = pbe->acc;
09286     srfm = thee->surfMeth;
09287     epsp = Vpbe_getSoluteDiel(pbe);
09288     epsw = Vpbe_getSolventDiel(pbe);
09289     kT = Vpbe_getTemperature(pbe)*(1e-3)*Vunit_Na*Vunit_kb;
09290     izmagic = 1.0/Vpbe_getZmagic(pbe);
09291
09292     depsi = (epsw - epsp);
09293     depsi = 1.0/depsi;
09294     VASSERT(VABS(depsi) > VPMGSMALL);
09295
09296     /* Mesh info */
09297     nx = thee->pmgp->nx;
09298     ny = thee->pmgp->ny;
09299     nz = thee->pmgp->nz;
09300     hx = thee->pmgp->hx;
09301     hy = thee->pmgp->hy;
09302     hzed = thee->pmgp->hzed;
09303     xlen = thee->pmgp->xlen;
09304     ylen = thee->pmgp->ylen;
09305     zlen = thee->pmgp->zlen;
09306     xmin = thee->pmgp->xmin;
09307     ymin = thee->pmgp->ymin;
09308     zmin = thee->pmgp->zmin;
09309     xmax = thee->pmgp->xmax;
09310     ymax = thee->pmgp->ymax;
09311     zmax = thee->pmgp->zmax;
09312
09313     /* If the permanent and induced potentials are flipped the
09314        results are exactly the same. */
09315     u = induced->data;

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```

09316     up = perm->data;
09317
09318     /* Make sure we're on the grid */
09319     if ((apos[0]<=xmin) || (apos[0]>=xmax) || \
09320         (apos[1]<=ymin) || (apos[1]>=ymax) || \
09321         (apos[2]<=zmin) || (apos[2]>=zmax)) {
09322         Vnm_print(2, "Vpmg_dbDirectPolForce: Atom at (%4.3f, %4.3f, %4.3f) is off the mesh
09323         (ignoring):\n", apos[0], apos[1], apos[2]);
09324         Vnm_print(2, "Vpmg_dbDirectPolForce:      xmin = %g, xmax = %g\n", xmin, xmax);
09325         Vnm_print(2, "Vpmg_dbDirectPolForce:      ymin = %g, ymax = %g\n", ymin, ymax);
09326         Vnm_print(2, "Vpmg_dbDirectPolForce:      zmin = %g, zmax = %g\n", zmin, zmax);
09327         fflush(stderr);
09328     } else {
09329         /* Convert the atom position to grid reference frame */
09330         position[0] = apos[0] - xmin;
09331         position[1] = apos[1] - ymin;
09332         position[2] = apos[2] - zmin;
09333
09334         /* Integrate over points within this atom's (inflated) radius */
09335         rtot = (arad + thee->splineWin);
09336         rtot2 = VSQR(rtot);
09337         dx = rtot/hx;
09338         imin = (int)floor((position[0]-rtot)/hx);
09339         if (imin < 1) {
09340             Vnm_print(2, "Vpmg_dbDirectPolForce: Atom %d off grid!\n", atomID);
09341             return;
09342         }
09343         imax = (int)ceil((position[0]+rtot)/hx);
09344         if (imax > (nx-2)) {
09345             Vnm_print(2, "Vpmg_dbDirectPolForce: Atom %d off grid!\n", atomID);
09346             return;
09347         }
09348         jmin = (int)floor((position[1]-rtot)/hy);
09349         if (jmin < 1) {
09350             Vnm_print(2, "Vpmg_dbDirectPolForce: Atom %d off grid!\n", atomID);
09351             return;
09352         }
09353         jmax = (int)ceil((position[1]+rtot)/hy);
09354         if (jmax > (ny-2)) {
09355             Vnm_print(2, "Vpmg_dbDirectPolForce: Atom %d off grid!\n", atomID);
09356             return;
09357         }
09358         kmin = (int)floor((position[2]-rtot)/hz);
09359         if (kmin < 1) {
09360             Vnm_print(2, "Vpmg_dbDirectPolForce: Atom %d off grid!\n", atomID);
09361             return;
09362         }
09363         kmax = (int)ceil((position[2]+rtot)/hz);
09364         if (kmax > (nz-2)) {
09365             Vnm_print(2, "Vpmg_dbDirectPolForce: Atom %d off grid!\n", atomID);
09366             return;
09367         }
09368         for (i=imin; i<=imax; i++) {
09369             for (j=jmin; j<=jmax; j++) {
09370                 for (k=kmin; k<=kmax; k++) {
09371                     /* i,j,k */
09372                     gpos[0] = (i+0.5)*hx + xmin;
09373                     gpos[1] = j*hy + ymin;
09374                     gpos[2] = k*hz + zmin;
09375                     Hxijk = (thee->epsx[IJK(i,j,k)] - epsp)*depsi;
09376                     Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
09377                                     atom, dHxijk);
09378                     for (l=0; l<3; l++) dHxijk[l] *= Hxijk;
09379                     gpos[0] = i*hx + xmin;
09380                     gpos[1] = (j+0.5)*hy + ymin;
09381                     gpos[2] = k*hz + zmin;
09382                     Hyijk = (thee->epsy[IJK(i,j,k)] - epsp)*depsi;
09383                     Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
09384                                     atom, dHyijk);
09385                     for (l=0; l<3; l++) dHyijk[l] *= Hyijk;
09386                     gpos[0] = i*hx + xmin;
09387                     gpos[1] = j*hy + ymin;
09388                     gpos[2] = (k+0.5)*hz + zmin;
09389                     Hzijk = (thee->epsz[IJK(i,j,k)] - epsp)*depsi;
09390                     Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
09391                                     atom, dHzijk);
09392                     for (l=0; l<3; l++) dHzijk[l] *= Hzijk;
09393                     /* i-1,j,k */
09394                     gpos[0] = (i-0.5)*hx + xmin;
09395                     gpos[1] = j*hy + ymin;

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```

09396         gpos[2] = k*hzed + zmin;
09397         Hximljk = (thee->epsx[IJK(i-1,j,k)] - epsp)*depsi;
09398         Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
09399             atom, dHximljk);
09400         for (l=0; l<3; l++) dHximljk[l] *= Hximljk;
09401         /* i,j-1,k */
09402         gpos[0] = i*hx + xmin;
09403         gpos[1] = (j-0.5)*hy + ymin;
09404         gpos[2] = k*hzed + zmin;
09405         Hyijmlk = (thee->epsy[IJK(i,j-1,k)] - epsp)*depsi;
09406         Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
09407             atom, dHyijmlk);
09408         for (l=0; l<3; l++) dHyijmlk[l] *= Hyijmlk;
09409         /* i,j,k-1 */
09410         gpos[0] = i*hx + xmin;
09411         gpos[1] = j*hy + ymin;
09412         gpos[2] = (k-0.5)*hzed + zmin;
09413         Hzijkm1 = (thee->epsz[IJK(i,j,k-1)] - epsp)*depsi;
09414         Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
09415             atom, dHzijkm1);
09416         for (l=0; l<3; l++) dHzijkm1[l] *= Hzijkm1;
09417
09418         dbFmag = up[IJK(i,j,k)];
09419         tgrad[0] =
09420             (dHxijk[0] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)])
09421             + dHximljk[0] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) / VSQR(hx)
09422             + (dHyijk[0] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)])
09423             + dHyijmlk[0] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) / VSQR(hy)
09424             + (dHzijkm1[0] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)])
09425             + dHzijkm1[0] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) / VSQR(hzed);
09426         tgrad[1] =
09427             (dHxijk[1] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)])
09428             + dHximljk[1] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) / VSQR(hx)
09429             + (dHyijk[1] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)])
09430             + dHyijmlk[1] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) / VSQR(hy)
09431             + (dHzijkm1[1] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)])
09432             + dHzijkm1[1] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) / VSQR(hzed);
09433         tgrad[2] =
09434             (dHxijk[2] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)])
09435             + dHximljk[2] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) / VSQR(hx)
09436             + (dHyijk[2] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)])
09437             + dHyijmlk[2] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) / VSQR(hy)
09438             + (dHzijkm1[2] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)])
09439             + dHzijkm1[2] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) / VSQR(hzed);
09440         force[0] += (dbFmag*tgrad[0]);
09441         force[1] += (dbFmag*tgrad[1]);
09442         force[2] += (dbFmag*tgrad[2]);
09443
09444         } /* k loop */
09445     } /* j loop */
09446 } /* i loop */
09447
09448     force[0] = -force[0]*hx*hy*hzed*deps*0.5*izmagic;
09449     force[1] = -force[1]*hx*hy*hzed*deps*0.5*izmagic;
09450     force[2] = -force[2]*hx*hy*hzed*deps*0.5*izmagic;
09451 }
09452 }
09453 }
09454
09455 VPUBLIC void Vpmg_dbNLDirectPolForce(Vpmg *thee, Vgrid *perm, Vgrid *nlInduced,
09456     int atomID, double force[3]) {
09457     Vpmg_dbDirectPolForce(thee, perm, nlInduced, atomID, force);
09458 }
09459
09460 VPUBLIC void Vpmg_qfMutualPolForce(Vpmg *thee, Vgrid *induced,
09461     Vgrid *nlincluded, int atomID, double force[3]) {
09462
09463     Vatom *atom;
09464     double *apos, *dipole, position[3], hx, hy, hzed;
09465     double *u, *unl;
09466     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax;
09467     double de[3][3], denl[3][3];
09468     double mx, my, mz, dmx, dmy, dmz, d2mx, d2my, d2mz, mi, mj, mk;
09469     double ifloat, jfloat, kfloat;
09470     double f, fnl, uix, uiy, uiz, uixnl, uiynl, uiznl;
09471     int i,j,k,nx, ny, nz, im2, im1, ip1, ip2, jm2, jm1, jp1, jp2, km2, km1;
09472     int kp1, kp2, ii, jj, kk;
09473
09474     VASSERT(thee != VNULL); /* PMG object with PBE info. */
09475     VASSERT(induced != VNULL); /* potential due to induced dipoles. */
09476     VASSERT(nlincluded != VNULL); /* potential due to non-local induced dipoles. */

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09477     atom = Valist_getAtom(three->pbe->alist, atomID);
09478     VASSERT(atom->partID != 0); /* all atoms must be in the same partition. */
09479     apos = Vatom_getPosition(atom);
09480     dipole = Vatom_getInducedDipole(atom);
09481     uix = dipole[0];
09482     uiy = dipole[1];
09483     uiz = dipole[2];
09484     dipole = Vatom_getNLInducedDipole(atom);
09485     uixnl = dipole[0];
09486     uiynl = dipole[1];
09487     uiznl = dipole[2];
09488     u = induced->data;
09489     unl = nlinduced->data;
09490
09491     for (i=0; i<3; i++){
09492         for (j=0; j<3; j++){
09493             de[i][j] = 0.0;
09494             denl[i][j] = 0.0;
09495         }
09496     }
09497
09498     /* Mesh info */
09499     nx = induced->nx;
09500     ny = induced->ny;
09501     nz = induced->nz;
09502     hx = induced->hx;
09503     hy = induced->hy;
09504     hzed = induced->hzed;
09505     xmin = induced->xmin;
09506     ymin = induced->ymin;
09507     zmin = induced->zmin;
09508     xmax = induced->xmax;
09509     ymax = induced->ymax;
09510     zmax = induced->zmax;
09511     xlen = xmax-xmin;
09512     ylen = ymax-ymin;
09513     zlen = zmax-zmin;
09514
09515     /* If we aren't in the current position, then we're done */
09516     if (atom->partID == 0) return;
09517
09518     /* Make sure we're on the grid */
09519     if ((apos[0]<=(xmin+2*hx)) || (apos[0]>=(xmax-2*hx)) \
09520         || (apos[1]<=(ymin+2*hy)) || (apos[1]>=(ymax-2*hy)) \
09521         || (apos[2]<=(zmin+2*hzed)) || (apos[2]>=(zmax-2*hzed))) {
09522         Vnm_print(2, "qfMutualPolForce: Atom off the mesh (ignoring) %6.3f %6.3f %6.3f\n", apos[0],
09523             apos[1], apos[2]);
09524         fflush(stderr);
09525     } else {
09526         /* Convert the atom position to grid coordinates */
09527         position[0] = apos[0] - xmin;
09528         position[1] = apos[1] - ymin;
09529         position[2] = apos[2] - zmin;
09530         ifloat = position[0]/hx;
09531         jfloat = position[1]/hy;
09532         kfloat = position[2]/hzed;
09533         ip1 = (int)ceil(ifloat);
09534         ip2 = ip1 + 2;
09535         im1 = (int)floor(ifloat);
09536         im2 = im1 - 2;
09537         jp1 = (int)ceil(jfloat);
09538         jp2 = jp1 + 2;
09539         jm1 = (int)floor(jfloat);
09540         jm2 = jm1 - 2;
09541         kp1 = (int)ceil(kfloat);
09542         kp2 = kp1 + 2;
09543         km1 = (int)floor(kfloat);
09544         km2 = km1 - 2;
09545
09546         /* This step shouldn't be necessary, but it saves nasty debugging
09547          * later on if something goes wrong */
09548         ip2 = VMIN2(ip2, nx-1);
09549         ip1 = VMIN2(ip1, nx-1);
09550         im1 = VMAX2(im1, 0);
09551         im2 = VMAX2(im2, 0);
09552         jp2 = VMIN2(jp2, ny-1);
09553         jp1 = VMIN2(jp1, ny-1);
09554         jm1 = VMAX2(jm1, 0);
09555         jm2 = VMAX2(jm2, 0);
09556         kp2 = VMIN2(kp2, nz-1);

```

```

09557     kp1 = VMIN2(kp1,nz-1);
09558     km1 = VMAX2(km1,0);
09559     km2 = VMAX2(km2,0);
09560
09561     for (ii=im2; ii<=ip2; ii++) {
09562         mi = VFCHI4(ii,ifloat);
09563         mx = bspline4(mi);
09564         dmx = dbspline4(mi);
09565         d2mx = d2bspline4(mi);
09566         for (jj=jm2; jj<=jp2; jj++) {
09567             mj = VFCHI4(jj,jfloat);
09568             my = bspline4(mj);
09569             dmy = dbspline4(mj);
09570             d2my = d2bspline4(mj);
09571             for (kk=km2; kk<=kp2; kk++) {
09572                 mk = VFCHI4(kk,kfloat);
09573                 mz = bspline4(mk);
09574                 dmz = dbspline4(mk);
09575                 d2mz = d2bspline4(mk);
09576                 f = u[IJK(ii,jj,kk)];
09577                 fnl = unl[IJK(ii,jj,kk)];
09578
09579                 /* The gradient of the reaction field
09580                  due to induced dipoles */
09581                 de[0][0] += f*d2mx*my*mz/(hx*hx);
09582                 de[1][0] += f*dmx*dmy*mz/(hy*hx);
09583                 de[1][1] += f*mx*d2my*mz/(hy*hy);
09584                 de[2][0] += f*dmx*my*dmz/(hx*hzed);
09585                 de[2][1] += f*mx*dmy*dmz/(hy*hzed);
09586                 de[2][2] += f*mx*my*d2mz/(hzed*hzed);
09587
09588                 /* The gradient of the reaction field
09589                  due to non-local induced dipoles */
09590                 denl[0][0] += fnl*d2mx*my*mz/(hx*hx);
09591                 denl[1][0] += fnl*dmx*dmy*mz/(hy*hx);
09592                 denl[1][1] += fnl*mx*d2my*mz/(hy*hy);
09593                 denl[2][0] += fnl*dmx*my*dmz/(hx*hzed);
09594                 denl[2][1] += fnl*mx*dmy*dmz/(hy*hzed);
09595                 denl[2][2] += fnl*mx*my*d2mz/(hzed*hzed);
09596             }
09597         }
09598     }
09599 }
09600
09601 /* mutual polarization force */
09602 force[0] = -(de[0][0]*uixnl + de[1][0]*uiynl + de[2][0]*uiznl);
09603 force[1] = -(de[1][0]*uixnl + de[1][1]*uiynl + de[2][1]*uiznl);
09604 force[2] = -(de[2][0]*uixnl + de[2][1]*uiynl + de[2][2]*uiznl);
09605 force[0] -= denl[0][0]*uix + denl[1][0]*uiy + denl[2][0]*uiz;
09606 force[1] -= denl[1][0]*uix + denl[1][1]*uiy + denl[2][1]*uiz;
09607 force[2] -= denl[2][0]*uix + denl[2][1]*uiy + denl[2][2]*uiz;
09608
09609 force[0] = 0.5 * force[0];
09610 force[1] = 0.5 * force[1];
09611 force[2] = 0.5 * force[2];
09612
09613 }
09614
09615 VPUBLIC void Vpmg_ibMutualPolForce(Vpmg *thee, Vgrid *induced, Vgrid *nlininduced,
09616                                   int atomID, double force[3]) {
09617
09618     Vatom *atom;
09619     Valist *alist;
09620     Vacc *acc;
09621     Vpbe *pbe;
09622     Vsurf_Meth srfm;
09623
09624     double *apos, position[3], arad, irad, zkappa2, hx, hy, hzed;
09625     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax, rtot2;
09626     double rtot, dx, dx2, dy, dy2, dz, dz2, gpos[3], tgrad[3], fmag;
09627     double izmagic;
09628     int i, j, k, nx, ny, nz, imin, imax, jmin, jmax, kmin, kmax;
09629
09630     VASSERT(thee != VNULL); /* We need a PMG object with PBE info. */
09631     VASSERT(induced != VNULL); /* We need the potential due to induced dipoles. */
09632     VASSERT(nlininduced != VNULL); /* We need the potential due to non-local induced dipoles. */
09633     VASSERT(!thee->pmgp->nonlin); /* Nonlinear PBE is not implemented for AMOEBA */
09634
09635     atom = Valist_getAtom(thee->pbe->alist, atomID);
09636     VASSERT (atom->partID != 0); /* Currently all atoms must be in the same partition. */
09637

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09638     acc = thee->pbe->acc;
09639     srfrm = thee->surfMeth;
09640     apos = Vatom_getPosition(atom);
09641     arad = Vatom_getRadius(atom);
09642
09643     /* Reset force */
09644     force[0] = 0.0;
09645     force[1] = 0.0;
09646     force[2] = 0.0;
09647
09648     /* If we aren't in the current position, then we're done */
09649     if (atom->partID == 0) return;
09650
09651     /* Get PBE info */
09652     pbe = thee->pbe;
09653     acc = pbe->acc;
09654     alist = pbe->alist;
09655     irad = Vpbe_getMaxIonRadius(pbe);
09656     zkappa2 = Vpbe_getZkappa2(pbe);
09657     izmagic = 1.0/Vpbe_getZmagic(pbe);
09658
09659     VASSERT (zkappa2 > VPMGSMALL); /* Should be a check for this further up.*/
09660
09661     /* Mesh info */
09662     nx = induced->nx;
09663     ny = induced->ny;
09664     nz = induced->nz;
09665     hx = induced->hx;
09666     hy = induced->hy;
09667     hzed = induced->hz;
09668     xmin = induced->xmin;
09669     ymin = induced->ymin;
09670     zmin = induced->zmin;
09671     xmax = induced->xmax;
09672     ymax = induced->ymax;
09673     zmax = induced->zmax;
09674     xlen = xmax-xmin;
09675     ylen = ymax-ymin;
09676     zlen = zmax-zmin;
09677
09678     /* Make sure we're on the grid */
09679     if ((apos[0]<=xmin) || (apos[0]>=xmax) || \
09680         (apos[1]<=ymin) || (apos[1]>=ymax) || \
09681         (apos[2]<=zmin) || (apos[2]>=zmax)) {
09682         Vnm_print(2, "Vpmg_ibMutalPolForce: Atom at (%4.3f, %4.3f, %4.3f) is off the mesh (ignoring):\n",
09683             apos[0], apos[1], apos[2]);
09684         Vnm_print(2, "Vpmg_ibMutalPolForce:      xmin = %g, xmax = %g\n", xmin, xmax);
09685         Vnm_print(2, "Vpmg_ibMutalPolForce:      ymin = %g, ymax = %g\n", ymin, ymax);
09686         Vnm_print(2, "Vpmg_ibMutalPolForce:      zmin = %g, zmax = %g\n", zmin, zmax);
09687         fflush(stderr);
09688     } else {
09689         /* Convert the atom position to grid reference frame */
09690         position[0] = apos[0] - xmin;
09691         position[1] = apos[1] - ymin;
09692         position[2] = apos[2] - zmin;
09693
09694         /* Integrate over points within this atom's (inflated) radius */
09695         rtot = (irad + arad + thee->splineWin);
09696         rtot2 = VSQR(rtot);
09697         dx = rtot + 0.5*hx;
09698         imin = VMAX2(0, (int)ceil((position[0] - dx)/hx));
09699         imax = VMIN2(nx-1, (int)floor((position[0] + dx)/hx));
09700         for (i=imin; i<=imax; i++) {
09701             dx2 = VSQR(position[0] - hx*i);
09702             if (rtot2 > dx2) dy = VSQR(rtot2 - dx2) + 0.5*hy;
09703             else dy = 0.5*hy;
09704             jmin = VMAX2(0, (int)ceil((position[1] - dy)/hy));
09705             jmax = VMIN2(ny-1, (int)floor((position[1] + dy)/hy));
09706             for (j=jmin; j<=jmax; j++) {
09707                 dy2 = VSQR(position[1] - hy*j);
09708                 if (rtot2 > (dx2+dy2)) dz = VSQR(rtot2-dx2-dy2)+0.5*hz;
09709                 else dz = 0.5*hz;
09710                 kmin = VMAX2(0, (int)ceil((position[2] - dz)/hz));
09711                 kmax = VMIN2(nz-1, (int)floor((position[2] + dz)/hz));
09712                 for (k=kmin; k<=kmax; k++) {
09713                     dz2 = VSQR(k*hz - position[2]);
09714                     /* See if grid point is inside ivdw radius and set ccf
09715                      * accordingly (do spline assignment here) */
09716                     if ((dz2 + dy2 + dx2) <= rtot2) {
09717                         gpos[0] = i*hx + xmin;

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09718         gpos[1] = j*hy + ymin;
09719         gpos[2] = k*hzed + zmin;
09720         Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, irad,
09721             atom, tgrad);
09722         fmag = induced->data[IJK(i,j,k)];
09723         fmag *= nlinduced->data[IJK(i,j,k)];
09724         fmag *= thee->kappa[IJK(i,j,k)];
09725         force[0] += (zkappa2*fmag*tgrad[0]);
09726         force[1] += (zkappa2*fmag*tgrad[1]);
09727         force[2] += (zkappa2*fmag*tgrad[2]);
09728     }
09729     } /* k loop */
09730     } /* j loop */
09731     } /* i loop */
09732 }
09733
09734 force[0] = force[0] * 0.5 * hx * hy * hzed * izmagic;
09735 force[1] = force[1] * 0.5 * hx * hy * hzed * izmagic;
09736 force[2] = force[2] * 0.5 * hx * hy * hzed * izmagic;
09737 }
09738
09739 VPUBLIC void Vpmg_dbMutualPolForce(Vpmg *thee, Vgrid *induced,
09740     Vgrid *nlinduced, int atomID,
09741     double force[3]) {
09742
09743     Vatom *atom;
09744     Vacc *acc;
09745     Vpbe *pbe;
09746     Vsurf_Meth srfm;
09747
09748     double *apos, position[3], arad, hx, hy, hzed, izmagic, deps, depsi;
09749     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax, rtot2, epsp;
09750     double rtot, dx, gpos[3], tgrad[3], dbFmag, epsw, kT;
09751     double *u, *unl, Hxijk, Hyijk, Hzijk, Hximljk, Hyijmlk, Hzijkml;
09752     double dHxijk[3], dHyijk[3], dHzijk[3], dHximljk[3], dHyijmlk[3];
09753     double dHzijkml[3];
09754     int i, j, k, l, nx, ny, nz, imin, imax, jmin, jmax, kmin, kmax;
09755
09756     VASSERT(thee != VNULL); /* PMG object with PBE info. */
09757     VASSERT(induced != VNULL); /* potential due to induced dipoles.*/
09758     VASSERT(nlinduced != VNULL); /* potential due to non-local induced dipoles.*/
09759
09760     acc = thee->pbe->acc;
09761     srfm = thee->surfMeth;
09762     atom = Valist_getAtom(thee->pbe->alist, atomID);
09763     VASSERT (atom->partID != 0); /* all atoms must be in the same partition.*/
09764     apos = Vatom_getPosition(atom);
09765     arad = Vatom_getRadius(atom);
09766
09767     /* Reset force */
09768     force[0] = 0.0;
09769     force[1] = 0.0;
09770     force[2] = 0.0;
09771
09772     /* Get PBE info */
09773     pbe = thee->pbe;
09774     acc = pbe->acc;
09775     epsp = Vpbe_getSoluteDiel(pbe);
09776     epsw = Vpbe_getSolventDiel(pbe);
09777     kT = Vpbe_getTemperature(pbe)*(1e-3)*Vunit_Na*Vunit_kb;
09778     izmagic = 1.0/Vpbe_getZmagic(pbe);
09779
09780     deps = (epsw - epsp);
09781     depsi = 1.0/deps;
09782     VASSERT(VABS(deps) > VPMGSMALL);
09783
09784     /* Mesh info */
09785     nx = thee->pmgp->nx;
09786     ny = thee->pmgp->ny;
09787     nz = thee->pmgp->nz;
09788     hx = thee->pmgp->hx;
09789     hy = thee->pmgp->hy;
09790     hzed = thee->pmgp->hzed;
09791     xlen = thee->pmgp->xlen;
09792     ylen = thee->pmgp->ylen;
09793     zlen = thee->pmgp->zlen;
09794     xmin = thee->pmgp->xmin;
09795     ymin = thee->pmgp->ymin;
09796     zmin = thee->pmgp->zmin;
09797     xmax = thee->pmgp->xmax;
09798     ymax = thee->pmgp->ymax;

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09799     zmax = thee->pmpg->zmax;
09800     u = induced->data;
09801     unl = nlinduced->data;
09802
09803     /* Make sure we're on the grid */
09804     if ((apos[0]<=xmin) || (apos[0]>=xmax) || \
09805         (apos[1]<=ymin) || (apos[1]>=ymax) || \
09806         (apos[2]<=zmin) || (apos[2]>=zmax)) {
09807         Vnm_print(2, "Vpmg_dbMutualPolForce: Atom at (%4.3f, %4.3f, %4.3f) is off the mesh
(ignore):\n", apos[0], apos[1], apos[2]);
09808         Vnm_print(2, "Vpmg_dbMutualPolForce:      xmin = %g, xmax = %g\n", xmin, xmax);
09809         Vnm_print(2, "Vpmg_dbMutualPolForce:      ymin = %g, ymax = %g\n", ymin, ymax);
09810         Vnm_print(2, "Vpmg_dbMutualPolForce:      zmin = %g, zmax = %g\n", zmin, zmax);
09811         fflush(stderr);
09812     } else {
09813
09814         /* Convert the atom position to grid reference frame */
09815         position[0] = apos[0] - xmin;
09816         position[1] = apos[1] - ymin;
09817         position[2] = apos[2] - zmin;
09818
09819         /* Integrate over points within this atom's (inflated) radius */
09820         rtot = (arad + thee->splineWin);
09821         rtot2 = VSQR(rtot);
09822         dx = rtot/hx;
09823         imin = (int)floor((position[0]-rtot)/hx);
09824         if (imin < 1) {
09825             Vnm_print(2, "Vpmg_dbMutualPolForce: Atom %d off grid!\n", atomID);
09826             return;
09827         }
09828         imax = (int)ceil((position[0]+rtot)/hx);
09829         if (imax > (nx-2)) {
09830             Vnm_print(2, "Vpmg_dbMutualPolForce: Atom %d off grid!\n", atomID);
09831             return;
09832         }
09833         jmin = (int)floor((position[1]-rtot)/hy);
09834         if (jmin < 1) {
09835             Vnm_print(2, "Vpmg_dbMutualPolForce: Atom %d off grid!\n", atomID);
09836             return;
09837         }
09838         jmax = (int)ceil((position[1]+rtot)/hy);
09839         if (jmax > (ny-2)) {
09840             Vnm_print(2, "Vpmg_dbMutualPolForce: Atom %d off grid!\n", atomID);
09841             return;
09842         }
09843         kmin = (int)floor((position[2]-rtot)/hz);
09844         if (kmin < 1) {
09845             Vnm_print(2, "Vpmg_dbMutualPolForce: Atom %d off grid!\n", atomID);
09846             return;
09847         }
09848         kmax = (int)ceil((position[2]+rtot)/hz);
09849         if (kmax > (nz-2)) {
09850             Vnm_print(2, "Vpmg_dbMutualPolForce: Atom %d off grid!\n", atomID);
09851             return;
09852         }
09853         for (i=imin; i<=imax; i++) {
09854             for (j=jmin; j<=jmax; j++) {
09855                 for (k=kmin; k<=kmax; k++) {
09856                     /* i,j,k */
09857                     gpos[0] = (i+0.5)*hx + xmin;
09858                     gpos[1] = j*hy + ymin;
09859                     gpos[2] = k*hz + zmin;
09860                     Hxijk = (thee->epsx[IJK(i,j,k)] - epsp)*depsi;
09861                     Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
atom, dHxijk);
09862                     for (l=0; l<3; l++) dHxijk[l] *= Hxijk;
09863                     gpos[0] = i*hx + xmin;
09864                     gpos[1] = (j+0.5)*hy + ymin;
09865                     gpos[2] = k*hz + zmin;
09866                     Hyijk = (thee->epsy[IJK(i,j,k)] - epsp)*depsi;
09867                     Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
atom, dHyijk);
09868                     for (l=0; l<3; l++) dHyijk[l] *= Hyijk;
09869                     gpos[0] = i*hx + xmin;
09870                     gpos[1] = j*hy + ymin;
09871                     gpos[2] = (k+0.5)*hz + zmin;
09872                     Hzijk = (thee->epsz[IJK(i,j,k)] - epsp)*depsi;
09873                     Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
atom, dHzijk);
09874                     for (l=0; l<3; l++) dHzijk[l] *= Hzijk;
09875                     /* i-1,j,k */

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09879         gpos[0] = (i-0.5)*hx + xmin;
09880         gpos[1] = j*hy + ymin;
09881         gpos[2] = k*hzed + zmin;
09882         Hximljk = (thee->epsx[IJK(i-1,j,k)] - epsp)*depsi;
09883         Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
09884             atom, dHximljk);
09885         for (l=0; l<3; l++) dHximljk[l] *= Hximljk;
09886         /* i,j-1,k */
09887         gpos[0] = i*hx + xmin;
09888         gpos[1] = (j-0.5)*hy + ymin;
09889         gpos[2] = k*hzed + zmin;
09890         Hyijmlk = (thee->epsy[IJK(i,j-1,k)] - epsp)*depsi;
09891         Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
09892             atom, dHyijmlk);
09893         for (l=0; l<3; l++) dHyijmlk[l] *= Hyijmlk;
09894         /* i,j,k-1 */
09895         gpos[0] = i*hx + xmin;
09896         gpos[1] = j*hy + ymin;
09897         gpos[2] = (k-0.5)*hzed + zmin;
09898         Hzijkml = (thee->epsz[IJK(i,j,k-1)] - epsp)*depsi;
09899         Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
09900             atom, dHzijkml);
09901         for (l=0; l<3; l++) dHzijkml[l] *= Hzijkml;
09902         dbFmag = unl[IJK(i,j,k)];
09903         tgrad[0] =
09904             (dHxijk[0] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)])
09905             + dHximljk[0] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) /VSQR(hx)
09906             + (dHyijk[0] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)])
09907             + dHyijmlk[0] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) /VSQR(hy)
09908             + (dHziijk[0] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)])
09909             + dHzijkml[0] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) /VSQR(hzed);
09910         tgrad[1] =
09911             (dHxijk[1] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)])
09912             + dHximljk[1] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) /VSQR(hx)
09913             + (dHyijk[1] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)])
09914             + dHyijmlk[1] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) /VSQR(hy)
09915             + (dHziijk[1] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)])
09916             + dHzijkml[1] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) /VSQR(hzed);
09917         tgrad[2] =
09918             (dHxijk[2] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)])
09919             + dHximljk[2] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) /VSQR(hx)
09920             + (dHyijk[2] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)])
09921             + dHyijmlk[2] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) /VSQR(hy)
09922             + (dHziijk[2] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)])
09923             + dHzijkml[2] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) /VSQR(hzed);
09924         force[0] += (dbFmag*tgrad[0]);
09925         force[1] += (dbFmag*tgrad[1]);
09926         force[2] += (dbFmag*tgrad[2]);
09927     } /* k loop */
09928 } /* j loop */
09929 } /* i loop */
09930
09931     force[0] = -force[0]*hx*hy*hzed*deps*0.5*izmagic;
09932     force[1] = -force[1]*hx*hy*hzed*deps*0.5*izmagic;
09933     force[2] = -force[2]*hx*hy*hzed*deps*0.5*izmagic;
09934 }
09935 }
09936
09937 #endif /* if defined(WITH_TINKER) */
09938
09939 VPRIVATE void fillCoefSpline4(Vpmg *thee) {
09940
09941     Valist *alist;
09942     Vpbe *pbe;
09943     Vatom *atom;
09944     double xmin, xmax, ymin, ymax, zmin, zmax, ionmask, ionstr, dist2;
09945     double xlen, ylen, zlen, position[3], itot, stot, ictot, ictot2, sctot;
09946     double irad, dx, dy, dz, epsw, epsp, w2i;
09947     double hx, hy, hzed, *apos, arad, sctot2;
09948     double dx2, dy2, dz2, stot2, itot2, rtot, rtot2, splineWin;
09949     double dist, value, denom, sm, sm2, sm3, sm4, sm5, sm6, sm7;
09950     double e, e2, e3, e4, e5, e6, e7;
09951     double b, b2, b3, b4, b5, b6, b7;
09952     double c0, c1, c2, c3, c4, c5, c6, c7;
09953     double ic0, ic1, ic2, ic3, ic4, ic5, ic6, ic7;
09954     int i, j, k, nx, ny, nz, iatom;
09955     int imin, imax, jmin, jmax, kmin, kmax;
09956
09957     VASSERT(thee != VNULL);
09958     splineWin = thee->splineWin;
09959

```

```

09960      /* Get PBE info */
09961      pbe = thee->pbe;
09962      alist = pbe->alist;
09963      irad = Vpbe_getMaxIonRadius(pbe);
09964      ionstr = Vpbe_getBulkIonicStrength(pbe);
09965      epsw = Vpbe_getSolventDiel(pbe);
09966      epsp = Vpbe_getSoluteDiel(pbe);
09967
09968      /* Mesh info */
09969      nx = thee->pmgp->nx;
09970      ny = thee->pmgp->ny;
09971      nz = thee->pmgp->nz;
09972      hx = thee->pmgp->hx;
09973      hy = thee->pmgp->hy;
09974      hzed = thee->pmgp->hzed;
09975
09976      /* Define the total domain size */
09977      xlen = thee->pmgp->xlen;
09978      ylen = thee->pmgp->ylen;
09979      zlen = thee->pmgp->zlen;
09980
09981      /* Define the min/max dimensions */
09982      xmin = thee->pmgp->xcent - (xlen/2.0);
09983      ymin = thee->pmgp->ycent - (ylen/2.0);
09984      zmin = thee->pmgp->zcent - (zlen/2.0);
09985      xmax = thee->pmgp->xcent + (xlen/2.0);
09986      ymax = thee->pmgp->ycent + (ylen/2.0);
09987      zmax = thee->pmgp->zcent + (zlen/2.0);
09988
09989      /* This is a floating point parameter related to the non-zero nature of the
09990      * bulk ionic strength. If the ionic strength is greater than zero; this
09991      * parameter is set to 1.0 and later scaled by the appropriate pre-factors.
09992      * Otherwise, this parameter is set to 0.0 */
09993      if (ionstr > VPMGSMALL) ionmask = 1.0;
09994      else ionmask = 0.0;
09995
09996      /* Reset the kappa, epsx, epsy, and epsz arrays */
09997      for (i=0; i<(nx*ny*nz); i++) {
09998          thee->kappa[i] = 1.0;
09999          thee->epsx[i] = 1.0;
10000          thee->epsy[i] = 1.0;
10001          thee->epsz[i] = 1.0;
10002      }
10003
10004      /* Loop through the atoms and do assign the dielectric */
10005      for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
10006
10007          atom = Valist_getAtom(alist, iatom);
10008          apos = Vatom_getPosition(atom);
10009          arad = Vatom_getRadius(atom);
10010
10011          b = arad - splineWin;
10012          e = arad + splineWin;
10013          e2 = e * e;
10014          e3 = e2 * e;
10015          e4 = e3 * e;
10016          e5 = e4 * e;
10017          e6 = e5 * e;
10018          e7 = e6 * e;
10019          b2 = b * b;
10020          b3 = b2 * b;
10021          b4 = b3 * b;
10022          b5 = b4 * b;
10023          b6 = b5 * b;
10024          b7 = b6 * b;
10025          denom = e7 - 7.0*b*e6 + 21.0*b2*e5 - 35.0*e4*b3
10026                  + 35.0*e3*b4 - 21.0*b5*e2 + 7.0*e*b6 - b7;
10027          c0 = b4*(35.0*e3 - 21.0*b*e2 + 7*e*b2 - b3)/denom;
10028          c1 = -140.0*b3*e3/denom;
10029          c2 = 210.0*e2*b2*(e + b)/denom;
10030          c3 = -140.0*e*b*(e2 + 3.0*b*e + b2)/denom;
10031          c4 = 35.0*(e3 + 9.0*b*e2 + + 9.0*e*b2 + b3)/denom;
10032          c5 = -84.0*(e2 + 3.0*b*e + b2)/denom;
10033          c6 = 70.0*(e + b)/denom;
10034          c7 = -20.0/denom;
10035
10036          b = irad + arad - splineWin;
10037          e = irad + arad + splineWin;
10038          e2 = e * e;
10039          e3 = e2 * e;
10040          e4 = e3 * e;

```

```

10041     e5 = e4 * e;
10042     e6 = e5 * e;
10043     e7 = e6 * e;
10044     b2 = b * b;
10045     b3 = b2 * b;
10046     b4 = b3 * b;
10047     b5 = b4 * b;
10048     b6 = b5 * b;
10049     b7 = b6 * b;
10050     denom = e7 - 7.0*b*e6 + 21.0*b2*e5 - 35.0*e4*b3
10051             + 35.0*e3*b4 - 21.0*b5*e2 + 7.0*e*b6 - b7;
10052     ic0 = b4*(35.0*e3 - 21.0*b*e2 + 7*e*b2 - b3)/denom;
10053     ic1 = -140.0*b3*e3/denom;
10054     ic2 = 210.0*e2*b2*(e + b)/denom;
10055     ic3 = -140.0*e*b*(e2 + 3.0*b*e + b2)/denom;
10056     ic4 = 35.0*(e3 + 9.0*b*e2 + 9.0*e*b2 + b3)/denom;
10057     ic5 = -84.0*(e2 + 3.0*b*e + b2)/denom;
10058     ic6 = 70.0*(e + b)/denom;
10059     ic7 = -20.0/denom;
10060
10061     /* Make sure we're on the grid */
10062     if ((apos[0]<=xmin) || (apos[0]>=xmax) || \
10063         (apos[1]<=ymin) || (apos[1]>=ymax) || \
10064         (apos[2]<=zmin) || (apos[2]>=zmax)) {
10065         if ((three->pmgp->bcfl != BCFL_FOCUS) &&
10066             (three->pmgp->bcfl != BCFL_MAP)) {
10067             Vnm_print(2, "Vpmg_fillco: Atom #d at (%4.3f, %4.3f, \
10068 %4.3f) is off the mesh (ignoring):\n",
10069                     iatom, apos[0], apos[1], apos[2]);
10070             Vnm_print(2, "Vpmg_fillco:   xmin = %g, xmax = %g\n",
10071                     xmin, xmax);
10072             Vnm_print(2, "Vpmg_fillco:   ymin = %g, ymax = %g\n",
10073                     ymin, ymax);
10074             Vnm_print(2, "Vpmg_fillco:   zmin = %g, zmax = %g\n",
10075                     zmin, zmax);
10076         }
10077         fflush(stderr);
10078
10079     } else if (arad > VPMGSMALL) { /* if we're on the mesh */
10080
10081         /* Convert the atom position to grid reference frame */
10082         position[0] = apos[0] - xmin;
10083         position[1] = apos[1] - ymin;
10084         position[2] = apos[2] - zmin;
10085
10086         /* MARK ION ACCESSIBILITY AND DIELECTRIC VALUES FOR LATER
10087          * ASSIGNMENT (Steps #1-3) */
10088         itot = irad + arad + splineWin;
10089         itot2 = VSQR(itot);
10090         ictot = VMAX2(0, (irad + arad - splineWin));
10091         ictot2 = VSQR(ictot);
10092         stot = arad + splineWin;
10093         stot2 = VSQR(stot);
10094         sctot = VMAX2(0, (arad - splineWin));
10095         sctot2 = VSQR(sctot);
10096
10097         /* We'll search over grid points which are in the greater of
10098          * these two radii */
10099         rtot = VMAX2(itot, stot);
10100         rtot2 = VMAX2(itot2, stot2);
10101         dx = rtot + 0.5*hx;
10102         dy = rtot + 0.5*hy;
10103         dz = rtot + 0.5*hzed;
10104         imin = VMAX2(0, (int)floor((position[0] - dx)/hx));
10105         imax = VMIN2(nx-1, (int)ceil((position[0] + dx)/hx));
10106         jmin = VMAX2(0, (int)floor((position[1] - dy)/hy));
10107         jmax = VMIN2(ny-1, (int)ceil((position[1] + dy)/hy));
10108         kmin = VMAX2(0, (int)floor((position[2] - dz)/hzed));
10109         kmax = VMIN2(nz-1, (int)ceil((position[2] + dz)/hzed));
10110         for (i=imin; i<=imax; i++) {
10111             dx2 = VSQR(position[0] - hx*i);
10112             for (j=jmin; j<=jmax; j++) {
10113                 dy2 = VSQR(position[1] - hy*j);
10114                 for (k=kmin; k<=kmax; k++) {
10115                     dz2 = VSQR(position[2] - k*hzed);
10116
10117                     /* ASSIGN CCF */
10118                     if (three->kappa[IJK(i,j,k)] > VPMGSMALL) {
10119                         dist2 = dz2 + dy2 + dx2;
10120                         if (dist2 >= itot2) {
10121                             ;

```

```

10122     }
10123     if (dist2 <= ictot2) {
10124         thee->kappa[IJK(i,j,k)] = 0.0;
10125     }
10126     if ((dist2 < itot2) && (dist2 > ictot2)) {
10127         dist = VSQRT(dist2);
10128         sm = dist;
10129         sm2 = dist2;
10130         sm3 = sm2 * sm;
10131         sm4 = sm3 * sm;
10132         sm5 = sm4 * sm;
10133         sm6 = sm5 * sm;
10134         sm7 = sm6 * sm;
10135         value = ic0 + ic1*sm + ic2*sm2 + ic3*sm3
10136             + ic4*sm4 + ic5*sm5 + ic6*sm6 + ic7*sm7;
10137         if (value > 1.0) {
10138             value = 1.0;
10139         } else if (value < 0.0){
10140             value = 0.0;
10141         }
10142         thee->kappa[IJK(i,j,k)] *= value;
10143     }
10144 }
10145
10146 /* ASSIGN A1CF */
10147 if (thee->epsx[IJK(i,j,k)] > VPMGSMALL) {
10148     dist2 = dz2+dy2+VSQR(position[0]-(i+0.5)*hx);
10149     if (dist2 >= stot2) {
10150         thee->epsx[IJK(i,j,k)] *= 1.0;
10151     }
10152     if (dist2 <= sctot2) {
10153         thee->epsx[IJK(i,j,k)] = 0.0;
10154     }
10155     if ((dist2 > sctot2) && (dist2 < stot2)) {
10156         dist = VSQRT(dist2);
10157         sm = dist;
10158         sm2 = VSQR(sm);
10159         sm3 = sm2 * sm;
10160         sm4 = sm3 * sm;
10161         sm5 = sm4 * sm;
10162         sm6 = sm5 * sm;
10163         sm7 = sm6 * sm;
10164         value = c0 + c1*sm + c2*sm2 + c3*sm3
10165             + c4*sm4 + c5*sm5 + c6*sm6 + c7*sm7;
10166         if (value > 1.0) {
10167             value = 1.0;
10168         } else if (value < 0.0){
10169             value = 0.0;
10170         }
10171         thee->epsx[IJK(i,j,k)] *= value;
10172     }
10173 }
10174
10175 /* ASSIGN A2CF */
10176 if (thee->epsy[IJK(i,j,k)] > VPMGSMALL) {
10177     dist2 = dz2+dx2+VSQR(position[1]-(j+0.5)*hy);
10178     if (dist2 >= stot2) {
10179         thee->epsy[IJK(i,j,k)] *= 1.0;
10180     }
10181     if (dist2 <= sctot2) {
10182         thee->epsy[IJK(i,j,k)] = 0.0;
10183     }
10184     if ((dist2 > sctot2) && (dist2 < stot2)) {
10185         dist = VSQRT(dist2);
10186         sm = dist;
10187         sm2 = VSQR(sm);
10188         sm3 = sm2 * sm;
10189         sm4 = sm3 * sm;
10190         sm5 = sm4 * sm;
10191         sm6 = sm5 * sm;
10192         sm7 = sm6 * sm;
10193         value = c0 + c1*sm + c2*sm2 + c3*sm3
10194             + c4*sm4 + c5*sm5 + c6*sm6 + c7*sm7;
10195         if (value > 1.0) {
10196             value = 1.0;
10197         } else if (value < 0.0){
10198             value = 0.0;
10199         }
10200         thee->epsy[IJK(i,j,k)] *= value;
10201     }
10202 }

```

```

10203
10204         /* ASSIGN A3CF */
10205         if (thee->epsz[IJK(i,j,k)] > VPMGSMALL) {
10206             dist2 = dy2+dx2+VSQR(position[2]-(k+0.5)*hzd);
10207             if (dist2 >= stot2) {
10208                 thee->epsz[IJK(i,j,k)] *= 1.0;
10209             }
10210             if (dist2 <= sctot2) {
10211                 thee->epsz[IJK(i,j,k)] = 0.0;
10212             }
10213             if ((dist2 > sctot2) && (dist2 < stot2)) {
10214                 dist = VSQRT(dist2);
10215                 sm = dist;
10216                 sm2 = dist2;
10217                 sm3 = sm2 * sm;
10218                 sm4 = sm3 * sm;
10219                 sm5 = sm4 * sm;
10220                 sm6 = sm5 * sm;
10221                 sm7 = sm6 * sm;
10222                 value = c0 + c1*sm + c2*sm2 + c3*sm3
10223                     + c4*sm4 + c5*sm5 + c6*sm6 + c7*sm7;
10224                 if (value > 1.0) {
10225                     value = 1.0;
10226                 } else if (value < 0.0) {
10227                     value = 0.0;
10228                 }
10229                 thee->epsz[IJK(i,j,k)] *= value;
10230             }
10231         }
10232     } /* k loop */
10233 } /* j loop */
10234 } /* i loop */
10235 } /* endif (on the mesh) */
10236 } /* endfor (over all atoms) */
10237
10238 Vnm_print(0, "Vpmg_fillco: filling coefficient arrays\n");
10239 /* Interpret markings and fill the coefficient arrays */
10240 for (k=0; k<nz; k++) {
10241     for (j=0; j<ny; j++) {
10242         for (i=0; i<nx; i++) {
10243             thee->kappa[IJK(i,j,k)] = ionmask*thee->kappa[IJK(i,j,k)];
10244             thee->epsx[IJK(i,j,k)] = (epsw-epsp)*thee->epsx[IJK(i,j,k)]
10245                 + epsp;
10246             thee->epsy[IJK(i,j,k)] = (epsw-epsp)*thee->epsy[IJK(i,j,k)]
10247                 + epsp;
10248             thee->epsz[IJK(i,j,k)] = (epsw-epsp)*thee->epsz[IJK(i,j,k)]
10249                 + epsp;
10250         } /* i loop */
10251     } /* j loop */
10252 } /* k loop */
10253
10254 }
10255
10256 VPUBLIC void fillcoPermanentInduced(Vpmg *thee) {
10257
10258     Valist *alist;
10259     Vpbe *pbe;
10260     Vatom *atom;
10261     /* Conversions */
10262     double zmagic, f;
10263     /* Grid */
10264     double xmin, xmax, ymin, ymax, zmin, zmax;
10265     double xlen, ylen, zlen, position[3], ifloat, jfloat, kfloat;
10266     double hx, hy, hzed, *apos;
10267     /* Multipole */
10268     double charge, *dipole, *quad;
10269     double c, ux, uy, uz, qxx, qyx, qyy, qzx, qzy, qzz, qave;
10270     /* B-spline weights */
10271     double mx, my, mz, dmx, dmy, dmz, d2mx, d2my, d2mz;
10272     double mi, mj, mk;
10273     /* Loop variables */
10274     int i, ii, jj, kk, nx, ny, nz, iatom;
10275     int im2, im1, ip1, ip2, jm2, jm1, jp1, jp2, km2, km1, kp1, kp2;
10276
10277     VASSERT(thee != VNULL);
10278
10279     /* Get PBE info */

```

```

10284     pbe = thee->pbe;
10285     alist = pbe->alist;
10286     zmagic = Vpbe_getZmagic(pbe);
10287
10288     /* Mesh info */
10289     nx = thee->pmgp->nx;
10290     ny = thee->pmgp->ny;
10291     nz = thee->pmgp->nz;
10292     hx = thee->pmgp->hx;
10293     hy = thee->pmgp->hy;
10294     hzed = thee->pmgp->hzed;
10295
10296     /* Conversion */
10297     f = zmagic/(hx*hy*hzed);
10298
10299     /* Define the total domain size */
10300     xlen = thee->pmgp->xlen;
10301     ylen = thee->pmgp->ylen;
10302     zlen = thee->pmgp->zlen;
10303
10304     /* Define the min/max dimensions */
10305     xmin = thee->pmgp->xcent - (xlen/2.0);
10306     ymin = thee->pmgp->ycent - (ylen/2.0);
10307     zmin = thee->pmgp->zcent - (zlen/2.0);
10308     xmax = thee->pmgp->xcent + (xlen/2.0);
10309     ymax = thee->pmgp->ycent + (ylen/2.0);
10310     zmax = thee->pmgp->zcent + (zlen/2.0);
10311
10312     /* Fill in the source term (permanent atomic multipoles
10313        and induced dipoles) */
10314     Vnm_print(0, "fillcoPermanentInduced: filling in source term.\n");
10315     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
10316
10317         atom = Valist_getAtom(alist, iatom);
10318         apos = Vatom_getPosition(atom);
10319
10320         c = Vatom_getCharge(atom)*f;
10321
10322     #if defined(WITH_TINKER)
10323         dipole = Vatom_getDipole(atom);
10324         ux = dipole[0]/hx*f;
10325         uy = dipole[1]/hy*f;
10326         uz = dipole[2]/hzed*f;
10327         dipole = Vatom_getInducedDipole(atom);
10328         ux = ux + dipole[0]/hx*f;
10329         uy = uy + dipole[1]/hy*f;
10330         uz = uz + dipole[2]/hzed*f;
10331         quad = Vatom_getQuadrupole(atom);
10332         qxx = (1.0/3.0)*quad[0]/(hx*hx)*f;
10333         qyx = (2.0/3.0)*quad[3]/(hx*hy)*f;
10334         qyy = (1.0/3.0)*quad[4]/(hy*hy)*f;
10335         qzx = (2.0/3.0)*quad[6]/(hzed*hx)*f;
10336         qzy = (2.0/3.0)*quad[7]/(hzed*hy)*f;
10337         qzz = (1.0/3.0)*quad[8]/(hzed*hzed)*f;
10338     #else
10339         ux = 0.0;
10340         uy = 0.0;
10341         uz = 0.0;
10342         qxx = 0.0;
10343         qyx = 0.0;
10344         qyy = 0.0;
10345         qzx = 0.0;
10346         qzy = 0.0;
10347         qzz = 0.0;
10348     #endif /* if defined(WITH_TINKER) */
10349
10350     /* Make sure we're on the grid */
10351     if ((apos[0]<=(xmin-2*hx)) || (apos[0]>=(xmax+2*hx)) || \
10352         (apos[1]<=(ymin-2*hy)) || (apos[1]>=(ymax+2*hy)) || \
10353         (apos[2]<=(zmin-2*hzed)) || (apos[2]>=(zmax+2*hzed))) {
10354         Vnm_print(2, "fillcoPermanentMultipole: Atom #\n");
10355         Vnm_print(2, "fillcoPermanentMultipole: xmin = %g, xmax = %g\n", xmin, xmax);
10356         Vnm_print(2, "fillcoPermanentMultipole: ymin = %g, ymax = %g\n", ymin, ymax);
10357         Vnm_print(2, "fillcoPermanentMultipole: zmin = %g, zmax = %g\n", zmin, zmax);
10358         fflush(stderr);
10359     } else {
10360
10361         /* Convert the atom position to grid reference frame */
10362         position[0] = apos[0] - xmin;
10363         position[1] = apos[1] - ymin;

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```

10364         position[2] = apos[2] - zmin;
10365
10366         /* Figure out which vertices we're next to */
10367         ifloat = position[0]/hx;
10368         jfloat = position[1]/hy;
10369         kfloat = position[2]/hzd;
10370
10371         ip1 = (int)ceil(ifloat);
10372         ip2 = ip1 + 2;
10373         im1 = (int)floor(ifloat);
10374         im2 = im1 - 2;
10375         jp1 = (int)ceil(jfloat);
10376         jp2 = jp1 + 2;
10377         jm1 = (int)floor(jfloat);
10378         jm2 = jm1 - 2;
10379         kp1 = (int)ceil(kfloat);
10380         kp2 = kp1 + 2;
10381         km1 = (int)floor(kfloat);
10382         km2 = km1 - 2;
10383
10384         /* This step shouldn't be necessary, but it saves nasty debugging
10385          * later on if something goes wrong */
10386         ip2 = VMIN2(ip2,nx-1);
10387         ip1 = VMIN2(ip1,nx-1);
10388         im1 = VMAX2(im1,0);
10389         im2 = VMAX2(im2,0);
10390         jp2 = VMIN2(jp2,ny-1);
10391         jp1 = VMIN2(jp1,ny-1);
10392         jm1 = VMAX2(jm1,0);
10393         jm2 = VMAX2(jm2,0);
10394         kp2 = VMIN2(kp2,nz-1);
10395         kp1 = VMIN2(kp1,nz-1);
10396         km1 = VMAX2(km1,0);
10397         km2 = VMAX2(km2,0);
10398
10399         /* Now assign fractions of the charge to the nearby verts */
10400         for (ii=im2; ii<=ip2; ii++) {
10401             mi = VFCHI4(ii,ifloat);
10402             mx = bspline4(mi);
10403             dm1 = d2bspline4(mi);
10404             d2mx = d2bspline4(mi);
10405             for (jj=jm2; jj<=jp2; jj++) {
10406                 mj = VFCHI4(jj,jfloat);
10407                 my = bspline4(mj);
10408                 dmy = d2bspline4(mj);
10409                 d2my = d2bspline4(mj);
10410                 for (kk=km2; kk<=kp2; kk++) {
10411                     mk = VFCHI4(kk,kfloat);
10412                     mz = bspline4(mk);
10413                     dmz = d2bspline4(mk);
10414                     d2mz = d2bspline4(mk);
10415                     charge = mx*my*mz*c -
10416                             dm1*my*mz*ux - mx*dmy*mz*uy - mx*my*dmz*uz +
10417                             d2mx*my*mz*qxx +
10418                             dm1*dmy*mz*qyx + mx*d2my*mz*qyy +
10419                             dm1*my*dmz*qzx + mx*dmy*dmz*qzy + mx*my*d2mz*qzz;
10420                     thee->charge[IJK(ii,jj,kk)] += charge;
10421                 }
10422             }
10423         }
10424     }
10425 } /* endif (on the mesh) */
10426
10427 } /* endfor (each atom) */
10428 }
10429
10430 VPRIVATE void fillCoefSpline3(Vpmg *thee) {
10431     Valist *alist;
10432     Vpbe *pbe;
10433     Vatom *atom;
10434     double xmin, xmax, ymin, ymax, zmin, zmax, ionmask, ionstr, dist2;
10435     double xlen, ylen, zlen, position[3], itot, stot, ictot, ictot2, sctot;
10436     double irad, dx, dy, dz, epsw, epsp, w2i;
10437     double hx, hy, hzed, *apos, arad, sctot2;
10438     double dx2, dy2, dz2, stot2, itot2, rtot, rtot2, splineWin;
10439     double dist, value, denom, sm, sm2, sm3, sm4, sm5;
10440     double e, e2, e3, e4, e5;
10441     double b, b2, b3, b4, b5;
10442     double c0, c1, c2, c3, c4, c5;
10443     double ic0, ic1, ic2, ic3, ic4, ic5;

```



```

10445     int i, j, k, nx, ny, nz, iatom;
10446     int imin, imax, jmin, jmax, kmin, kmax;
10447
10448     VASSERT(thee != VNULL);
10449     splineWin = thee->splineWin;
10450
10451     /* Get PBE info */
10452     pbe = thee->pbe;
10453     alist = pbe->alist;
10454     irad = Vpbe_getMaxIonRadius(pbe);
10455     ionstr = Vpbe_getBulkIonicStrength(pbe);
10456     epsw = Vpbe_getSolventDiel(pbe);
10457     epsp = Vpbe_getSoluteDiel(pbe);
10458
10459     /* Mesh info */
10460     nx = thee->pmgp->nx;
10461     ny = thee->pmgp->ny;
10462     nz = thee->pmgp->nz;
10463     hx = thee->pmgp->hx;
10464     hy = thee->pmgp->hy;
10465     hzed = thee->pmgp->hzed;
10466
10467     /* Define the total domain size */
10468     xlen = thee->pmgp->xlen;
10469     ylen = thee->pmgp->ylen;
10470     zlen = thee->pmgp->zlen;
10471
10472     /* Define the min/max dimensions */
10473     xmin = thee->pmgp->xcent - (xlen/2.0);
10474     ymin = thee->pmgp->ycent - (ylen/2.0);
10475     zmin = thee->pmgp->zcent - (zlen/2.0);
10476     xmax = thee->pmgp->xcent + (xlen/2.0);
10477     ymax = thee->pmgp->ycent + (ylen/2.0);
10478     zmax = thee->pmgp->zcent + (zlen/2.0);
10479
10480     /* This is a floating point parameter related to the non-zero nature of the
10481      * bulk ionic strength. If the ionic strength is greater than zero; this
10482      * parameter is set to 1.0 and later scaled by the appropriate pre-factors.
10483      * Otherwise, this parameter is set to 0.0 */
10484     if (ionstr > VPMGSMALL) ionmask = 1.0;
10485     else ionmask = 0.0;
10486
10487     /* Reset the kappa, epsx, epsy, and epsz arrays */
10488     for (i=0; i<(nx*ny*nz); i++) {
10489         thee->kappa[i] = 1.0;
10490         thee->epsx[i] = 1.0;
10491         thee->epsy[i] = 1.0;
10492         thee->epsz[i] = 1.0;
10493     }
10494
10495     /* Loop through the atoms and do assign the dielectric */
10496     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
10497
10498         atom = Valist_getAtom(alist, iatom);
10499         apos = Vatom_getPosition(atom);
10500         arad = Vatom_getRadius(atom);
10501
10502         b = arad - splineWin;
10503         e = arad + splineWin;
10504         e2 = e * e;
10505         e3 = e2 * e;
10506         e4 = e3 * e;
10507         e5 = e4 * e;
10508         b2 = b * b;
10509         b3 = b2 * b;
10510         b4 = b3 * b;
10511         b5 = b4 * b;
10512         denom = pow((e - b), 5.0);
10513         c0 = -10.0*e2*b3 + 5.0*e*b4 - b5;
10514         c1 = 30.0*e2*b2;
10515         c2 = -30.0*(e2*b + e*b2);
10516         c3 = 10.0*(e2 + 4.0*e*b + b2);
10517         c4 = -15.0*(e + b);
10518         c5 = 6;
10519         c0 = c0/denom;
10520         c1 = c1/denom;
10521         c2 = c2/denom;
10522         c3 = c3/denom;
10523         c4 = c4/denom;
10524         c5 = c5/denom;
10525

```

```

10526     b = irad + arad - splineWin;
10527     e = irad + arad + splineWin;
10528     e2 = e * e;
10529     e3 = e2 * e;
10530     e4 = e3 * e;
10531     e5 = e4 * e;
10532     b2 = b * b;
10533     b3 = b2 * b;
10534     b4 = b3 * b;
10535     b5 = b4 * b;
10536     denom = pow((e - b), 5.0);
10537     ic0 = -10.0*e2*b3 + 5.0*e*b4 - b5;
10538     ic1 = 30.0*e2*b2;
10539     ic2 = -30.0*(e2*b + e*b2);
10540     ic3 = 10.0*(e2 + 4.0*e*b + b2);
10541     ic4 = -15.0*(e + b);
10542     ic5 = 6;
10543     ic0 = c0/denom;
10544     ic1 = c1/denom;
10545     ic2 = c2/denom;
10546     ic3 = c3/denom;
10547     ic4 = c4/denom;
10548     ic5 = c5/denom;
10549
10550     /* Make sure we're on the grid */
10551     if ((apos[0]<=xmin) || (apos[0]>=xmax) || \
10552         (apos[1]<=ymin) || (apos[1]>=ymax) || \
10553         (apos[2]<=zmin) || (apos[2]>=zmax)) {
10554         if ((thee->pmgp->bcfl != BCFL_FOCUS) &&
10555             (thee->pmgp->bcfl != BCFL_MAP)) {
10556             Vnm_print(2, "Vpmg_fillco: Atom #d at (%4.3f, %4.3f, \
10557 %4.3f) is off the mesh (ignoring):\n",
10558                 iatom, apos[0], apos[1], apos[2]);
10559             Vnm_print(2, "Vpmg_fillco:   xmin = %g, xmax = %g\n",
10560                 xmin, xmax);
10561             Vnm_print(2, "Vpmg_fillco:   ymin = %g, ymax = %g\n",
10562                 ymin, ymax);
10563             Vnm_print(2, "Vpmg_fillco:   zmin = %g, zmax = %g\n",
10564                 zmin, zmax);
10565         }
10566         fflush(stderr);
10567     } else if (arad > VPMGSMALL) { /* if we're on the mesh */
10568
10569         /* Convert the atom position to grid reference frame */
10570         position[0] = apos[0] - xmin;
10571         position[1] = apos[1] - ymin;
10572         position[2] = apos[2] - zmin;
10573
10574
10575         /* MARK ION ACCESSIBILITY AND DIELECTRIC VALUES FOR LATER
10576          * ASSIGNMENT (Steps #1-3) */
10577         itot = irad + arad + splineWin;
10578         itot2 = VSQR(itot);
10579         ictot = VMAX2(0, (irad + arad - splineWin));
10580         ictot2 = VSQR(ictot);
10581         stot = arad + splineWin;
10582         stot2 = VSQR(stot);
10583         sctot = VMAX2(0, (arad - splineWin));
10584         sctot2 = VSQR(sctot);
10585
10586         /* We'll search over grid points which are in the greater of
10587          * these two radii */
10588         rtot = VMAX2(itot, stot);
10589         rtot2 = VMAX2(itot2, stot2);
10590         dx = rtot + 0.5*hx;
10591         dy = rtot + 0.5*hy;
10592         dz = rtot + 0.5*hzed;
10593         imin = VMAX2(0, (int)floor((position[0] - dx)/hx));
10594         imax = VMIN2(nx-1, (int)ceil((position[0] + dx)/hx));
10595         jmin = VMAX2(0, (int)floor((position[1] - dy)/hy));
10596         jmax = VMIN2(ny-1, (int)ceil((position[1] + dy)/hy));
10597         kmin = VMAX2(0, (int)floor((position[2] - dz)/hzed));
10598         kmax = VMIN2(nz-1, (int)ceil((position[2] + dz)/hzed));
10599         for (i=imin; i<=imax; i++) {
10600             dx2 = VSQR(position[0] - hx*i);
10601             for (j=jmin; j<=jmax; j++) {
10602                 dy2 = VSQR(position[1] - hy*j);
10603                 for (k=kmin; k<=kmax; k++) {
10604                     dz2 = VSQR(position[2] - k*hzed);
10605
10606                     /* ASSIGN CCF */

```

```

10607         if (thee->kappa[IJK(i,j,k)] > VPMGSMALL) {
10608             dist2 = dz2 + dy2 + dx2;
10609             if (dist2 >= itot2) {
10610                 ;
10611             }
10612             if (dist2 <= ictot2) {
10613                 thee->kappa[IJK(i,j,k)] = 0.0;
10614             }
10615             if ((dist2 < itot2) && (dist2 > ictot2)) {
10616                 dist = VSQRT(dist2);
10617                 sm = dist;
10618                 sm2 = dist2;
10619                 sm3 = sm2 * sm;
10620                 sm4 = sm3 * sm;
10621                 sm5 = sm4 * sm;
10622                 value = ic0 + ic1*sm + ic2*sm2 + ic3*sm3
10623                     + ic4*sm4 + ic5*sm5;
10624                 if (value > 1.0) {
10625                     value = 1.0;
10626                 } else if (value < 0.0){
10627                     value = 0.0;
10628                 }
10629                 thee->kappa[IJK(i,j,k)] *= value;
10630             }
10631         }
10632     }
10633     /* ASSIGN A1CF */
10634     if (thee->epsx[IJK(i,j,k)] > VPMGSMALL) {
10635         dist2 = dz2+dy2+VSQR(position[0]-(i+0.5)*hx);
10636         if (dist2 >= stot2) {
10637             thee->epsx[IJK(i,j,k)] *= 1.0;
10638         }
10639         if (dist2 <= sctot2) {
10640             thee->epsx[IJK(i,j,k)] = 0.0;
10641         }
10642         if ((dist2 > sctot2) && (dist2 < stot2)) {
10643             dist = VSQRT(dist2);
10644             sm = dist;
10645             sm2 = VSQR(sm);
10646             sm3 = sm2 * sm;
10647             sm4 = sm3 * sm;
10648             sm5 = sm4 * sm;
10649             value = c0 + c1*sm + c2*sm2 + c3*sm3
10650                 + c4*sm4 + c5*sm5;
10651             if (value > 1.0) {
10652                 value = 1.0;
10653             } else if (value < 0.0){
10654                 value = 0.0;
10655             }
10656             thee->epsx[IJK(i,j,k)] *= value;
10657         }
10658     }
10659     /* ASSIGN A2CF */
10660     if (thee->epsy[IJK(i,j,k)] > VPMGSMALL) {
10661         dist2 = dz2+dx2+VSQR(position[1]-(j+0.5)*hy);
10662         if (dist2 >= stot2) {
10663             thee->epsy[IJK(i,j,k)] *= 1.0;
10664         }
10665         if (dist2 <= sctot2) {
10666             thee->epsy[IJK(i,j,k)] = 0.0;
10667         }
10668         if ((dist2 > sctot2) && (dist2 < stot2)) {
10669             dist = VSQRT(dist2);
10670             sm = dist;
10671             sm2 = VSQR(sm);
10672             sm3 = sm2 * sm;
10673             sm4 = sm3 * sm;
10674             sm5 = sm4 * sm;
10675             value = c0 + c1*sm + c2*sm2 + c3*sm3
10676                 + c4*sm4 + c5*sm5;
10677             if (value > 1.0) {
10678                 value = 1.0;
10679             } else if (value < 0.0){
10680                 value = 0.0;
10681             }
10682             thee->epsy[IJK(i,j,k)] *= value;
10683         }
10684     }
10685 }
10686
10687     /* ASSIGN A3CF */

```

```

10688         if (thee->epsz[IJK(i,j,k)] > VPMGSMALL) {
10689             dist2 = dy2+dx2+VSQR(position[2]-(k+0.5)*hzd);
10690             if (dist2 >= stot2) {
10691                 thee->epsz[IJK(i,j,k)] *= 1.0;
10692             }
10693             if (dist2 <= sctot2) {
10694                 thee->epsz[IJK(i,j,k)] = 0.0;
10695             }
10696             if ((dist2 > sctot2) && (dist2 < stot2)) {
10697                 dist = VSQR(dist2);
10698                 sm = dist;
10699                 sm2 = dist2;
10700                 sm3 = sm2 * sm;
10701                 sm4 = sm3 * sm;
10702                 sm5 = sm4 * sm;
10703                 value = c0 + c1*sm + c2*sm2 + c3*sm3
10704                     + c4*sm4 + c5*sm5;
10705                 if (value > 1.0) {
10706                     value = 1.0;
10707                 } else if (value < 0.0) {
10708                     value = 0.0;
10709                 }
10710                 thee->epsz[IJK(i,j,k)] *= value;
10711             }
10712         }
10713     }
10714 } /* k loop */
10715 } /* j loop */
10716 } /* i loop */
10717 } /* endif (on the mesh) */
10718 } /* endfor (over all atoms) */
10719
10720 Vnm_print(0, "Vpmg_fillco: filling coefficient arrays\n");
10721 /* Interpret markings and fill the coefficient arrays */
10722 for (k=0; k<nz; k++) {
10723     for (j=0; j<ny; j++) {
10724         for (i=0; i<nx; i++) {
10725             thee->kappa[IJK(i,j,k)] = ionmask*thee->kappa[IJK(i,j,k)];
10726             thee->epsx[IJK(i,j,k)] = (epsw-epsp)*thee->epsx[IJK(i,j,k)]
10727                 + epsp;
10728             thee->epsy[IJK(i,j,k)] = (epsw-epsp)*thee->epsy[IJK(i,j,k)]
10729                 + epsp;
10730             thee->epsz[IJK(i,j,k)] = (epsw-epsp)*thee->epsz[IJK(i,j,k)]
10731                 + epsp;
10732         } /* i loop */
10733     } /* j loop */
10734 } /* k loop */
10735
10736 }
10737
10738
10739
10740
10741 VPRIVATE void bcolcomp(int *iparm, double *rparm, int *iwork, double *rwork,
10742     double *values, int *rowind, int *colptr, int *flag) {
10743     int nrow, ncol, nnzero, i;
10744     int nxc, nyc, nzc, nf, nc, narr, narrc, n_rpc;
10745     int n_iz, n_ipc, iretot, iintot;
10746     int nrwk, niwk, nx, ny, nz, nlev, ierror, maxlev, mxlv;
10747     int mgcoar, mgdisc, mgsolv;
10748     int k_iz;
10749     int k_ipc, k_rpc, k_ac, k_cc, k_fc, k_pc;
10750
10751     WARN_UNTESTED;
10752
10753     // Decode some parameters
10754     nrwk = VAT(iparm, 1);
10755     niwk = VAT(iparm, 2);
10756     nx = VAT(iparm, 3);
10757     ny = VAT(iparm, 4);
10758     nz = VAT(iparm, 5);
10759     nlev = VAT(iparm, 6);
10760
10761     // Some checks on input
10762     mxlv = Vmaxlev(nx, ny, nz);
10763
10764     // Basic grid sizes, etc.
10765     mgcoar = VAT(iparm, 18);
10766     mgdisc = VAT(iparm, 19);
10767     mgsolv = VAT(iparm, 21);
10768     Vmgsz(&mgcoar, &mgdisc, &mgsolv,

```

```

10769         &nx, &ny, &nz,
10770         &nlev,
10771         &nxc, &ny, &nzc,
10772         &nf, &nc,
10773         &narr, &narrc,
10774         &n_rpc, &n_iz, &n_ipc,
10775         &ioretot, &iintot);
10776
10777     // Split up the integer work array
10778     k_iz = 1;
10779     k_ipc = k_iz + n_iz;
10780
10781     // Split up the real work array
10782     k_rpc = 1;
10783     k_cc = k_rpc + n_rpc;
10784     k_fc = k_cc + narr;
10785     k_pc = k_fc + narr;
10786     k_ac = k_pc + 27*narrc;
10787
10788     bcolcomp2(iparm, rparam,
10789              &nx, &ny, &nz, RAT(iwork, k_iz),
10790              RAT(iwork, k_ipc), RAT(rwork, k_rpc),
10791              RAT(rwork, k_ac), RAT(rwork, k_cc),
10792              values, rowind, colptr, flag);
10793 }
10794
10795 VPRIVATE void bcolcomp2(int *iparm, double *rparam,
10796                          int *nx, int *ny, int *nz,
10797                          int *iz, int *ipc, double *rpc,
10798                          double *ac, double *cc, double *values,
10799                          int *rowind, int *colptr, int *flag) {
10800
10801     int nlev = 1;
10802     int lev = VAT(iparm, 6);
10803
10804     MAT2(iz, 50, nlev);
10805
10806     WARN_UNTESTED;
10807
10808     /*
10809     * Build the multigrid data structure in iz
10810     * THIS MAY HAVE BEEN DONE ALREADY, BUT IT'S OK TO DO IT AGAIN,
10811     * RIGHT?
10812     * call buildstr (nx,ny,nz,nlev,iz)
10813     *
10814     * We're interested in the finest level
10815     */
10816     bcolcomp3(nx, ny, nz,
10817              RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
10818              RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
10819              values, rowind, colptr, flag);
10820 }
10821
10822 /*****
10823 * Routine: bcolcomp3
10824 * Purpose: Build a column-compressed matrix in Harwell-Boeing format
10825 * Args:    flag 0 ==> Use Poisson operator only
10826 *          1 ==> Use linearization of full operator around current
10827 *          solution
10828 * Author:   Nathan Baker (mostly ripped off from Harwell-Boeing format
10829 *          documentation)
10830 *****/
10831 VPRIVATE void bcolcomp3(int *nx, int *ny, int *nz,
10832                          int *ipc, double *rpc,
10833                          double *ac, double *cc,
10834                          double *values, int *rowind, int *colptr, int *flag) {
10835
10836     MAT2(ac, *nx * *ny * *nz, 1);
10837
10838     WARN_UNTESTED;
10839
10840     bcolcomp4(nx, ny, nz,
10841              ipc, rpc,
10842              RAT2(ac, 1, 1), cc,
10843              RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
10844              values, rowind, colptr, flag);
10845 }
10846
10847
10848
10849 /*****

```

```

10850 * Routine: bcolcomp4
10851 * Purpose: Build a column-compressed matrix in Harwell-Boeing format
10852 * Args:    flag 0 ==> Use Poisson operator only
10853 *          1 ==> Use linearization of full operator around current
10854 *          solution
10855 * Author:   Nathan Baker (mostly ripped off from Harwell-Boeing format
10856 *          documentation)
10857 *****/
10858 VPRIVATE void bcolcomp4(int *nx, int *ny, int *nz,
10859                          int *ipc, double *rpc,
10860                          double *oC, double *cc, double *oE, double *oN, double *uC,
10861                          double *values, int *rowind, int *colptr, int *flag) {
10862
10863     int nxm2, nym2, nzm2;
10864     int ii, jj, kk, ll;
10865     int i, j, k, l;
10866     int inonz, irow, nn, nrow, ncol, nonz, irow, n;
10867
10868     int doit;
10869
10870     MAT3(oE, *nx, *ny, *nz);
10871     MAT3(oN, *nx, *ny, *nz);
10872     MAT3(uC, *nx, *ny, *nz);
10873     MAT3(cc, *nx, *ny, *nz);
10874     MAT3(oC, *nx, *ny, *nz);
10875
10876     WARN_UNTESTED;
10877
10878     // Get some column, row, and nonzero information
10879     n = *nx * *ny * *nz;
10880     nxm2 = *nx - 2;
10881     nym2 = *ny - 2;
10882     nzm2 = *nz - 2;
10883     nn = nxm2 * nym2 * nzm2;
10884     ncol = nn;
10885     nrow = nn;
10886     nonz = 7 * nn - 2 * nxm2 * nym2 - 2 * nxm2 - 2;
10887
10888     // Intialize some pointers
10889     inonz = 1;
10890
10891     /*
10892     * Run over the dimensions of the matrix (non-zero only in the interior
10893     * of the mesh
10894     */
10895     for (k=2; k<=*nz-1; k++) {
10896         // Offset the index to the output grid index
10897         kk = k - 1;
10898
10899         for (j=2; j<=*ny-1; j++) {
10900             // Offset the index to the output grid index
10901             jj = j - 1;
10902
10903             for (i=2; i<=*nx-1; i++) {
10904                 // Offset the index to the output grid index
10905                 ii = i - 1;
10906
10907                 // Get the output (i,j,k) row number in natural ordering
10908                 ll = (kk - 1) * nxm2 * nym2 + (jj - 1) * nxm2 + (ii - 1) + 1;
10909                 l = (k - 1) * *nx * *ny + (j - 1) * *nx + (i - 1) + 1;
10910
10911                 // Store where this column starts
10912                 VAT(colptr,ll) = inonz;
10913
10914                 // SUB-DIAGONAL 3
10915                 irow = ll - nxm2 * nym2;
10916                 irow = 1 - *nx * *ny;
10917
10918                 doit = (irow >= 1) && (irow <= nn);
10919                 doit = doit && (irow >= 1) && (irow <= n);
10920
10921                 if (doit) {
10922                     VAT(values, inonz) = -VAT3(uC, i, j, k-1);
10923                     VAT(rowind, inonz) = irow;
10924                     inonz++;
10925                 }
10926
10927
10928
10929                 // SUB-DIAGONAL 2
10930                 irow = ll - nxm2;

```

```

10931         irow = 1 - *nx;
10932
10933         doit = (irow >= 1) && (irow <= nn);
10934         doit = doit && (irow >= 1) && (irow <= n);
10935
10936         if (doit) {
10937             VAT(values, inonz) = -VAT3(oN, i, j-1, k);
10938             VAT(rowind, inonz) = irow;
10939             inonz++;
10940         }
10941
10942
10943         // SUB-DIAGONAL 1
10944         irow = 11 - 1;
10945         irow = 1 - 1;
10946
10947
10948         doit = (irow >= 1) && (irow <= nn);
10949         doit = doit && (irow <= 1) && (irow <= n);
10950         if (doit) {
10951             VAT(values, inonz) = -VAT3(oE, i-1, j, k);
10952             VAT(rowind, inonz) = irow;
10953             inonz++;
10954         }
10955
10956
10957         // DIAGONAL
10958         irow = 11;
10959         irow = 1;
10960
10961
10962         if (*flag == 0) {
10963             VAT(values, inonz) = VAT3(oC, i, j, k);
10964         } else if (*flag == 1) {
10965             VAT(values, inonz) = VAT3(oC, i, j, k)
10966                 + VAT3(cc, i, j, k);
10967         } else {
10968             VABORT_MSG0("PMGF1");
10969         }
10970
10971         VAT(rowind, inonz) = irow;
10972         inonz++;
10973
10974         // SUPER-DIAGONAL 1
10975         irow = 11 + 1;
10976         irow = 1 + 1;
10977         doit = (irow >= 1) && (irow <= nn);
10978         doit = doit && (irow >= 1) && (irow <= n);
10979         if (doit) {
10980             VAT(values, inonz) = -VAT3(oE, i, j, k);
10981             VAT(rowind, inonz) = irow;
10982             inonz++;
10983         }
10984
10985
10986         // SUPER-DIAGONAL 2
10987         irow = 11 + nxm2;
10988         irow = 1 + *nx;
10989         doit = (irow >= 1) && (irow <= nn);
10990         doit = doit && (irow >= 1) && (irow <= n);
10991         if (doit) {
10992             VAT(values, inonz) = -VAT3(oN, i, j, k);
10993             VAT(rowind, inonz) = irow;
10994             inonz++;
10995         }
10996
10997
10998         // SUPER-DIAGONAL 3
10999         irow = 11 + nxm2 * nym2;
11000         irow = 1 + *nx * *ny;
11001         doit = (irow >= 1) && (irow <= nn);
11002         doit = doit && (irow >= 1) && (irow <= n);
11003         if (doit) {
11004             VAT(values, inonz) = -VAT3(uC, i, j, k);
11005             VAT(rowind, inonz) = irow;
11006             inonz++;
11007         }
11008     }
11009 }
11010 }
11011

```

```

11012     }
11013
11014     VAT(colptr, ncol + 1) = inonz;
11015
11016     if (inonz != (nonz + 1)) {
11017         VABORT_MSG2("BCOLCOMP4:  ERROR -- INONZ = %d, NONZ = %d", inonz, nonz);
11018     }
11019 }
11020
11021
11022
11023 VPRIVATE void pcolcomp(int *nrow, int *ncol, int *nnzero,
11024     double *values, int *rowind, int *colptr,
11025     char *path, char *title, char *mxttype) {
11026
11027     char key[] = "key";
11028     char ptrfmt[] = "(10I8)";
11029     char indfmt[] = "(10I8)";
11030     char valfmt[] = "(5E15.8)";
11031     char rhsfmt[] = "(5E15.8)";
11032
11033     int i, totcrd, ptrcrd, indcrd, valcrd, neltvl, rhscrd;
11034
11035     FILE *outFile;
11036
11037     WARN_UNTESTED;
11038
11039     // Open the file for reading
11040     outFile = fopen(path, "w");
11041
11042     // Set some default values
11043     ptrcrd = (int)(*ncol / 10 + 1) - 1;
11044     indcrd = (int)(*nnzero / 10 + 1) - 1;
11045     valcrd = (int)(*nnzero / 10 + 1) - 1;
11046     totcrd = ptrcrd + indcrd + valcrd;
11047     rhscrd = 0;
11048     neltvl = 0;
11049
11050     // Print the header
11051     fprintf(outFile, "%72s%8s\n",
11052         title, key);
11053     fprintf(outFile, "%14d%14d%14d%14d%14d\n",
11054         totcrd, ptrcrd, indcrd, valcrd, rhscrd);
11055     fprintf(outFile, "%3s\n", mxttype);
11056     fprintf(outFile, "          %14d%14d%14d%14d\n",
11057         *nrow, *ncol, *nnzero, neltvl);
11058     fprintf(outFile, "%16s%16s%20s%20s\n",
11059         ptrfmt, indfmt, valfmt, rhsfmt);
11060
11061     // Write the matrix structure
11062     for (i=1; i<=*ncol+1; i++)
11063         fprintf(outFile, "%8d", VAT(colptr, i));
11064     fprintf(outFile, "\n");
11065
11066     for (i=1; i<=*nnzero; i++)
11067         fprintf(outFile, "%8d", VAT(rowind, i));
11068     fprintf(outFile, "\n");
11069
11070     // Write out the values
11071     if (valcrd > 0) {
11072         for (i=1; i<=*nnzero; i++)
11073             fprintf(outFile, "%15.8e", VAT(values, i));
11074         fprintf(outFile, "\n");
11075     }
11076
11077     // Close the file
11078     fclose (outFile);
11079 }

```

9.108 src/mg/vpmg.h File Reference

Contains declarations for class Vpmg.

```

#include "apbscfg.h"
#include "malloc/malloc.h"
#include "generic/vhal.h"
#include "generic/vacc.h"

```



```

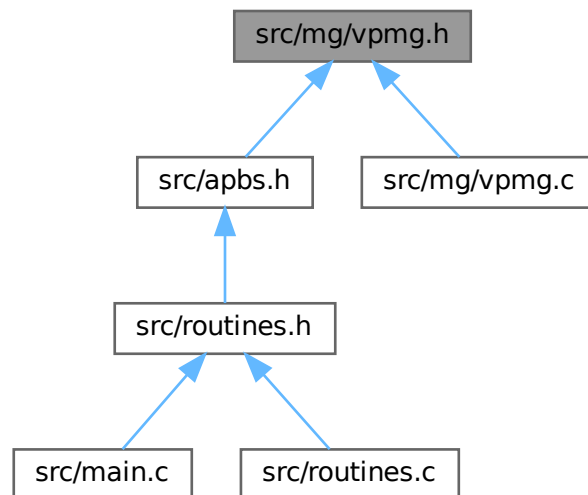
#include "generic/vcap.h"
#include "generic/vpbe.h"
#include "generic/mgparm.h"
#include "generic/pbeparm.h"
#include "generic/vmatrix.h"
#include "pmgc/mgdrvd.h"
#include "pmgc/newdrvd.h"
#include "pmgc/mgsubd.h"
#include "pmgc/mikpckd.h"
#include "pmgc/matvecd.h"
#include "mg/vpmgp.h"
#include "mg/vgrid.h"

```

Include dependency graph for vpmg.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVpmg](#)
Contains public data members for Vpmg class/module.

Macros

- #define [VPMGMAXPART](#) 2000

- `#define VCUB(x) ((x)*(x)*(x))`
- `#define VLOG(x) (log(x))`
- `#define IJK(i, j, k) (((k)*(nx)*(ny))+((j)*(nx))+i)`
- `#define IJKx(j, k, i) (((i)*(ny)*(nz))+((k)*(ny))+j)`
- `#define IJKy(i, k, j) (((j)*(nx)*(nz))+((k)*(nx))+i)`
- `#define IJKz(i, j, k) (((k)*(nx)*(ny))+((j)*(nx))+i)`
- `#define VFCHI(iint, iflt) (1.5+((double)(iint)-(iflt)))`

Typedefs

- typedef struct `sVpmg` `Vpmg`
Declaration of the Vpmg class as the Vpmg structure.

Functions

- VEXTERNC unsigned long int `Vpmg_memChk` (`Vpmg *thee`)
Return the memory used by this structure (and its contents) in bytes.
- VEXTERNC `Vpmg * Vpmg_ctor` (`Vpmgp *parms`, `Vpbe *pbe`, int focusFlag, `Vpmg *pmgOLD`, `MGparm *mgparm`, `PBEparm_calcEnergy` energyFlag)
Constructor for the Vpmg class (allocates new memory)
- VEXTERNC int `Vpmg_ctor2` (`Vpmg *thee`, `Vpmgp *parms`, `Vpbe *pbe`, int focusFlag, `Vpmg *pmgOLD`, `MGparm *mgparm`, `PBEparm_calcEnergy` energyFlag)
FORTTRAN stub constructor for the Vpmg class (uses previously-allocated memory)
- VEXTERNC void `Vpmg_dtor` (`Vpmg **thee`)
Object destructor.
- VEXTERNC void `Vpmg_dtor2` (`Vpmg *thee`)
FORTTRAN stub object destructor.
- VEXTERNC int `Vpmg_fillco` (`Vpmg *thee`, `Vsurf_Meth` surfMeth, double splineWin, `Vchrg_Meth` chargeMeth, int useDielXMap, `Vgrid *dielXMap`, int useDielYMap, `Vgrid *dielYMap`, int useDielZMap, `Vgrid *dielZMap`, int useKappaMap, `Vgrid *kappaMap`, int usePotMap, `Vgrid *potMap`, int useChargeMap, `Vgrid *chargeMap`)
Fill the coefficient arrays prior to solving the equation.
- VEXTERNC int `Vpmg_solve` (`Vpmg *thee`)
Solve the PBE using PMG.
- VEXTERNC int `Vpmg_solveLaplace` (`Vpmg *thee`)
Solve Poisson's equation with a homogeneous Laplacian operator using the solvent dielectric constant. This solution is performed by a sine wave decomposition.
- VEXTERNC double `Vpmg_energy` (`Vpmg *thee`, int extFlag)
Get the total electrostatic energy.
- VEXTERNC double `Vpmg_qfEnergy` (`Vpmg *thee`, int extFlag)
Get the "fixed charge" contribution to the electrostatic energy.
- VEXTERNC double `Vpmg_qfAtomEnergy` (`Vpmg *thee`, `Vatom *atom`)
Get the per-atom "fixed charge" contribution to the electrostatic energy.
- VEXTERNC double `Vpmg_qmEnergy` (`Vpmg *thee`, int extFlag)
Get the "mobile charge" contribution to the electrostatic energy.
- VEXTERNC double `Vpmg_dielEnergy` (`Vpmg *thee`, int extFlag)
Get the "polarization" contribution to the electrostatic energy.
- VEXTERNC double `Vpmg_dielGradNorm` (`Vpmg *thee`)
Get the integral of the gradient of the dielectric function.
- VEXTERNC int `Vpmg_force` (`Vpmg *thee`, double *force, int atomID, `Vsurf_Meth` srfrm, `Vchrg_Meth` chgm)

- Calculate the total force on the specified atom in units of $k_B T/AA$.*

 - VEXTERNC int [Vpmg_qfForce](#) ([Vpmg](#) *thee, double *force, int atomID, [Vchrg_Meth](#) chgm)
- Calculate the "charge-field" force on the specified atom in units of $k_B T/AA$.*

 - VEXTERNC int [Vpmg_dbForce](#) ([Vpmg](#) *thee, double *dbForce, int atomID, [Vsurf_Meth](#) srfm)
- Calculate the dielectric boundary forces on the specified atom in units of $k_B T/AA$.*

 - VEXTERNC int [Vpmg_ibForce](#) ([Vpmg](#) *thee, double *force, int atomID, [Vsurf_Meth](#) srfm)
- Calculate the osmotic pressure on the specified atom in units of $k_B T/AA$.*

 - VEXTERNC void [Vpmg_setPart](#) ([Vpmg](#) *thee, double lowerCorner[3], double upperCorner[3], int bflags[6])

Set partition information which restricts the calculation of observables to a (rectangular) subset of the problem domain.

 - VEXTERNC void [Vpmg_unsetPart](#) ([Vpmg](#) *thee)

Remove partition restrictions.
- VEXTERNC int [Vpmg_fillArray](#) ([Vpmg](#) *thee, double *vec, [Vdata_Type](#) type, double parm, [Vhal_PBEType](#) pbe-type, [PBEparm](#) *pbeparm)

Fill the specified array with accessibility values.
- VPUBLIC void [Vpmg_fieldSpline4](#) ([Vpmg](#) *thee, int atomID, double field[3])

Computes the field at an atomic center using a stencil based on the first derivative of a 5th order B-spline.
- VEXTERNC double [Vpmg_qfPermanentMultipoleEnergy](#) ([Vpmg](#) *thee, int atomID)

Computes the permanent multipole electrostatic hydration energy (the polarization component of the hydration energy currently computed in TINKER).
- VEXTERNC void [Vpmg_qfPermanentMultipoleForce](#) ([Vpmg](#) *thee, int atomID, double force[3], double torque[3])

Computes the q-Phi Force for permanent multipoles based on 5th order B-splines.
- VEXTERNC void [Vpmg_ibPermanentMultipoleForce](#) ([Vpmg](#) *thee, int atomID, double force[3])

Compute the ionic boundary force for permanent multipoles.
- VEXTERNC void [Vpmg_dbPermanentMultipoleForce](#) ([Vpmg](#) *thee, int atomID, double force[3])

Compute the dielectric boundary force for permanent multipoles.
- VEXTERNC void [Vpmg_qfDirectPolForce](#) ([Vpmg](#) *thee, [Vgrid](#) *perm, [Vgrid](#) *induced, int atomID, double force[3], double torque[3])

q-Phi direct polarization force between permanent multipoles and induced dipoles, which are induced by the sum of the permanent intramolecular field and the permanent reaction field.
- VEXTERNC void [Vpmg_qfNLDirectPolForce](#) ([Vpmg](#) *thee, [Vgrid](#) *perm, [Vgrid](#) *nlInduced, int atomID, double force[3], double torque[3])

q-Phi direct polarization force between permanent multipoles and non-local induced dipoles based on 5th Order B-Splines. Keep in mind that the "non-local" induced dipoles are just a mathematical quantity that result from differentiation of the AMOEBA polarization energy.
- VEXTERNC void [Vpmg_ibDirectPolForce](#) ([Vpmg](#) *thee, [Vgrid](#) *perm, [Vgrid](#) *induced, int atomID, double force[3])

Ionic boundary direct polarization force between permanent multipoles and induced dipoles, which are induced by the sum of the permanent intramolecular field and the permanent reaction field.
- VEXTERNC void [Vpmg_ibNLDirectPolForce](#) ([Vpmg](#) *thee, [Vgrid](#) *perm, [Vgrid](#) *nlInduced, int atomID, double force[3])

Ionic boundary direct polarization force between permanent multipoles and non-local induced dipoles based on 5th order. Keep in mind that the "non-local" induced dipoles are just a mathematical quantity that result from differentiation of the AMOEBA polarization energy.
- VEXTERNC void [Vpmg_dbDirectPolForce](#) ([Vpmg](#) *thee, [Vgrid](#) *perm, [Vgrid](#) *induced, int atomID, double force[3])

Dielectric boundary direct polarization force between permanent multipoles and induced dipoles, which are induced by the sum of the permanent intramolecular field and the permanent reaction field.
- VEXTERNC void [Vpmg_dbNLDirectPolForce](#) ([Vpmg](#) *thee, [Vgrid](#) *perm, [Vgrid](#) *nlInduced, int atomID, double force[3])

Dielectric boundary direct polarization force between permanent multipoles and non-local induced dipoles. Keep in mind that the "non-local" induced dipoles are just a mathematical quantity that result from differentiation of the AMOEBA polarization energy.

- VEXTERNC void [Vpmg_qfMutualPolForce](#) ([Vpmg](#) *thee, [Vgrid](#) *induced, [Vgrid](#) *nllInduced, int atomID, double force[3])
Mutual polarization force for induced dipoles based on 5th order B-Splines. This force arises due to self-consistent convergence of the solute induced dipoles and reaction field.
- VEXTERNC void [Vpmg_ibMutualPolForce](#) ([Vpmg](#) *thee, [Vgrid](#) *induced, [Vgrid](#) *nllInduced, int atomID, double force[3])
Ionic boundary mutual polarization force for induced dipoles based on 5th order B-Splines. This force arises due to self-consistent convergence of the solute induced dipoles and reaction field.
- VEXTERNC void [Vpmg_dbMutualPolForce](#) ([Vpmg](#) *thee, [Vgrid](#) *induced, [Vgrid](#) *nllInduced, int atomID, double force[3])
Dielectric boundary mutual polarization force for induced dipoles based on 5th order B-Splines. This force arises due to self-consistent convergence of the solute induced dipoles and reaction field.
- VEXTERNC void [Vpmg_printColComp](#) ([Vpmg](#) *thee, char path[72], char title[72], char mxtype[3], int flag)
Print out a column-compressed sparse matrix in Harwell-Boeing format.
- VPRIVATE void [bcolcomp](#) (int *iparm, double *rparm, int *iwork, double *rwork, double *values, int *rowind, int *colptr, int *flag)
Build a column-compressed matrix in Harwell-Boeing format.
- VPRIVATE void [bcolcomp2](#) (int *iparm, double *rparm, int *nx, int *ny, int *nz, int *iz, int *ipc, double *rpc, double *ac, double *cc, double *values, int *rowind, int *colptr, int *flag)
Build a column-compressed matrix in Harwell-Boeing format.
- VPRIVATE void [bcolcomp3](#) (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac, double *cc, double *values, int *rowind, int *colptr, int *flag)
Build a column-compressed matrix in Harwell-Boeing format.
- VPRIVATE void [bcolcomp4](#) (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *oC, double *cc, double *oE, double *oN, double *uC, double *values, int *rowind, int *colptr, int *flag)
Build a column-compressed matrix in Harwell-Boeing format.
- VPRIVATE void [pcolcomp](#) (int *nrow, int *ncol, int *nnzero, double *values, int *rowind, int *colptr, char *path, char *title, char *mxtype)
Print a column-compressed matrix in Harwell-Boeing format.
- VPRIVATE double [bspline2](#) (double x)
Evaluate a cubic B-spline.
- VPRIVATE double [dbspline2](#) (double x)
Evaluate a cubic B-spline derivative.
- VPRIVATE double [VFCHI4](#) (int i, double f)
Return 2.5 plus difference of i - f.
- VPRIVATE double [bspline4](#) (double x)
Evaluate a 5th Order B-Spline (4th order polynomial)
- VPRIVATE double [dbspline4](#) (double x)
Evaluate a 5th Order B-Spline derivative (4th order polynomial)
- VPRIVATE double [d2bspline4](#) (double x)
Evaluate the 2nd derivative of a 5th Order B-Spline.
- VPRIVATE double [d3bspline4](#) (double x)
Evaluate the 3rd derivative of a 5th Order B-Spline.
- VPRIVATE double [Vpmg_polarizEnergy](#) ([Vpmg](#) *thee, int extFlag)
Determines energy from polarizeable charge and interaction with fixed charges according to Rocchia et al.
- VPRIVATE double [Vpmg_qfEnergyPoint](#) ([Vpmg](#) *thee, int extFlag)
Calculates charge-potential energy using summation over delta function positions (i.e. something like an Linf norm)
- VPRIVATE double [Vpmg_qfEnergyVolume](#) ([Vpmg](#) *thee, int extFlag)
Calculates charge-potential energy as integral over a volume.

- VPRIVATE void [Vpmg_splineSelect](#) (int srfm, [Vacc](#) *acc, double *gpos, double win, double infrad, [Vatom](#) *atom, double *force)
Selects a spline based surface method from either VSM_SPLINE, VSM_SPLINE5 or VSM_SPLINE7.
- VPRIVATE void [bcfl1](#) (double size, double *apos, double charge, double xkappa, double pre1, double *gxcf, double *gycf, double *gzcf, double *xf, double *yf, double *zf, int nx, int ny, int nz)
*Increment all boundary points by $pre1 * (charge/d) * (exp(-xkappa * (d-size)) / (1 + xkappa * size))$ to add the effect of the Debye-Huckel potential due to a single charge.*
- VPRIVATE void [multipolebc](#) (double r, double kappa, double eps_p, double eps_w, double rad, double tsr[3])
This routine serves bcfl2. It returns (in tsr) the contraction independent portion of the Debye-Huckel potential tensor for a spherical ion with a central charge, dipole and quadrupole. See the code for an in depth description.
- VPRIVATE void [bcCalc](#) ([Vpmg](#) *thee)
Fill boundary condition arrays.
- VPRIVATE void [fillcoCoef](#) ([Vpmg](#) *thee)
Top-level driver to fill all operator coefficient arrays.
- VPRIVATE void [fillcoCoefMap](#) ([Vpmg](#) *thee)
Fill operator coefficient arrays from pre-calculated maps.
- VPRIVATE void [fillcoCoefMol](#) ([Vpmg](#) *thee)
Fill operator coefficient arrays from a molecular surface calculation.
- VPRIVATE void [fillcoCoefMollon](#) ([Vpmg](#) *thee)
Fill ion (nonlinear) operator coefficient array from a molecular surface calculation.
- VPRIVATE void [fillcoCoefMolDiel](#) ([Vpmg](#) *thee)
Fill differential operator coefficient arrays from a molecular surface calculation.
- VPRIVATE void [fillcoCoefMolDielNoSmooth](#) ([Vpmg](#) *thee)
Fill differential operator coefficient arrays from a molecular surface calculation without smoothing.
- VPRIVATE void [fillcoCoefMolDielSmooth](#) ([Vpmg](#) *thee)
Fill differential operator coefficient arrays from a molecular surface calculation with smoothing.
- VPRIVATE void [fillcoCoefSpline](#) ([Vpmg](#) *thee)
Fill operator coefficient arrays from a spline-based surface calculation.
- VPRIVATE void [fillcoCoefSpline3](#) ([Vpmg](#) *thee)
Fill operator coefficient arrays from a 5th order polynomial based surface calculation.
- VPRIVATE void [fillcoCoefSpline4](#) ([Vpmg](#) *thee)
Fill operator coefficient arrays from a 7th order polynomial based surface calculation.
- VPRIVATE Vrc_Codes [fillcoCharge](#) ([Vpmg](#) *thee)
Top-level driver to fill source term charge array.
- VPRIVATE Vrc_Codes [fillcoChargeMap](#) ([Vpmg](#) *thee)
Fill source term charge array from a pre-calculated map.
- VPRIVATE void [fillcoChargeSpline1](#) ([Vpmg](#) *thee)
Fill source term charge array from linear interpolation.
- VPRIVATE void [fillcoChargeSpline2](#) ([Vpmg](#) *thee)
Fill source term charge array from cubic spline interpolation.
- VPRIVATE void [fillcoPermanentMultipole](#) ([Vpmg](#) *thee)
Fill source term charge array for the use of permanent multipoles.
- VPRIVATE void [fillcoInducedDipole](#) ([Vpmg](#) *thee)
Fill source term charge array for use of induced dipoles.
- VPRIVATE void [fillcoNLInducedDipole](#) ([Vpmg](#) *thee)
Fill source term charge array for non-local induced dipoles.
- VPRIVATE void [qfForceSpline1](#) ([Vpmg](#) *thee, double *force, int atomID)
Charge-field force due to a linear spline charge function.

- VPRIVATE void [qfForceSpline2](#) ([Vpmg](#) *thee, double *force, int atomID)
Charge-field force due to a cubic spline charge function.
- VPRIVATE void [qfForceSpline4](#) ([Vpmg](#) *thee, double *force, int atomID)
Charge-field force due to a quintic spline charge function.
- VPRIVATE void [zlapSolve](#) ([Vpmg](#) *thee, double **solution, double **source, double **work1)
Calculate the solution to Poisson's equation with a simple Laplacian operator and zero-valued Dirichlet boundary conditions. Store the solution in thee->u.
- VPRIVATE void [markSphere](#) (double rtot, double *tpos, int nx, int ny, int nz, double hx, double hy, double hzed, double xmin, double ymin, double zmin, double *array, double markVal)
Mark the grid points inside a sphere with a particular value. This marks by resetting the the grid points inside the sphere to the specified value.
- VPRIVATE double [Vpmg_qmEnergySMPBE](#) ([Vpmg](#) *thee, int extFlag)
Vpmg_qmEnergy for SMPBE.
- VPRIVATE double [Vpmg_qmEnergyNONLIN](#) ([Vpmg](#) *thee, int extFlag)

9.108.1 Detailed Description

Contains declarations for class [Vpmg](#).

Version

\$Id\$

Author

Nathan A. Baker

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
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* Pacific Northwest National Laboratory
*
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*
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```

```

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*

```

Definition in file [vpmg.h](#).

9.108.2 Macro Definition Documentation

9.108.2.1 IJK

```

#define IJK(
    i,
    j,
    k ) ((k)*(nx)*(ny)) + ((j)*(nx)) + (i))

```

Definition at line 1395 of file [vpmg.h](#).

9.108.2.2 IJKx

```

#define IJKx(
    j,
    k,
    i ) ((i)*(ny)*(nz)) + ((k)*(ny)) + (j))

```

Definition at line 1396 of file [vpmg.h](#).

9.108.2.3 IJKy

```

#define IJKy(
    i,
    k,
    j ) ((j)*(nx)*(nz)) + ((k)*(nx)) + (i))

```

Definition at line 1397 of file [vpmg.h](#).

9.108.2.4 IJKz

```
#define IJKz(
    i,
    j,
    k ) ((k)*(nx)*(ny)) + ((j)*(nx)) + (i))
```

Definition at line 1398 of file [vpmg.h](#).

9.108.2.5 VCUB

```
#define VCUB(
    x ) ((x)*(x)*(x))
```

Definition at line 1392 of file [vpmg.h](#).

9.108.2.6 VFCHI

```
#define VFCHI(
    iint,
    iflt ) (1.5+((double)(iint)-(iflt)))
```

Definition at line 1399 of file [vpmg.h](#).

9.108.2.7 VLOG

```
#define VLOG(
    x ) (log(x))
```

Definition at line 1393 of file [vpmg.h](#).

9.108.2.8 VPMGMAXPART

```
#define VPMGMAXPART 2000
```

Definition at line 105 of file [vpmg.h](#).

9.108.3 Function Documentation

9.108.3.1 bcCalc()

```
VPRIVATE void bcCalc (
    Vpmg * thee )
```

Fill boundary condition arrays.

Author

Nathan Baker

Definition at line 4382 of file [vpmg.c](#).

9.108.3.2 bcf11()

```
VPRIVATE void bcf11 (
    double size,
    double * apos,
    double charge,
    double xkappa,
    double pre1,
    double * gxcf,
    double * gycf,
    double * gzcf,
    double * xf,
    double * yf,
    double * zf,
    int nx,
    int ny,
    int nz )
```

Increment all boundary points by $pre1 * (charge/d) * (exp(-xkappa * (d-size)) / (1+xkappa * size))$ to add the effect of the Debye-Huckel potential due to a single charge.

Author

Nathan Baker

Parameters

<i>apos</i>	Size of the ion
<i>charge</i>	Position of the ion
<i>xkappa</i>	Charge of the ion
<i>pre1</i>	Exponential screening factor
<i>gxcf</i>	Unit- and dielectric-dependent prefactor
<i>gycf</i>	Set to x-boundary values
<i>gzcf</i>	Set to y-boundary values
<i>xf</i>	Set to z-boundary values
<i>yf</i>	Boundary point x-coordinates
<i>zf</i>	Boundary point y-coordinates
<i>nx</i>	Boundary point z-coordinates
<i>ny</i>	Number of grid points in x-direction
<i>nz</i>	Number of grid points in y-direction Number of grid points in y-direction

Definition at line [2564](#) of file [vpmg.c](#).

9.108.3.3 bspline2()

```
VPRIVATE double bspline2 (
    double x )
```

Evaluate a cubic B-spline.

Author

Nathan Baker

Returns

Cubic B-spline value

Parameters

x	Position
-----	----------

Definition at line [5496](#) of file [vpmg.c](#).

9.108.3.4 bspline4()

```
VPRIVATE double bspline4 (  
    double x )
```

Evaluate a 5th Order B-Spline (4th order polynomial)

Author

: Michael Schnieders

Returns

5th Order B-Spline

Parameters

x	Position
-----	----------

Definition at line [7136](#) of file [vpmg.c](#).

9.108.3.5 d2bspline4()

```
VPRIVATE double d2bspline4 (  
    double x )
```

Evaluate the 2nd derivative of a 5th Order B-Spline.

Author

: Michael Schnieders

Returns

2nd derivative of a 5th Order B-Spline

Parameters

x	Position
-----	----------

Definition at line [7202](#) of file [vpmg.c](#).

9.108.3.6 d3bspline4()

```
VPRIVATE double d3bspline4 (  
    double x )
```

Evaluate the 3rd derivative of a 5th Order B-Spline.

Author

: Michael Schnieders

Returns

3rd derivative of a 5th Order B-Spline

Parameters

x	Position
---	----------

Definition at line [7229](#) of file [vpmg.c](#).

9.108.3.7 dbspline2()

```
VPRIVATE double dbspline2 (  
    double x )
```

Evaluate a cubic B-spline derivative.

Author

Nathan Baker

Returns

Cubic B-spline derivative

Parameters

x	Position
---	----------

Definition at line [5512](#) of file [vpmg.c](#).

9.108.3.8 dbspline4()

```
VPRIVATE double dbspline4 (  
    double x )
```

Evaluate a 5th Order B-Spline derivative (4th order polynomial)

Author

: Michael Schnieders

Returns

5th Order B-Spline derivative

Parameters

<i>x</i>	Position
----------	----------

Definition at line 7170 of file [vpmg.c](#).

9.108.3.9 fillcoCharge()

```
VPRIVATE Vrc_Codes fillcoCharge (  
    Vpmg * thee )
```

Top-level driver to fill source term charge array.

Returns

Success/failure status

Author

Nathan Baker

Definition at line 5287 of file [vpmg.c](#).

9.108.3.10 fillcoChargeMap()

```
VPRIVATE Vrc_Codes fillcoChargeMap (  
    Vpmg * thee )
```

Fill source term charge array from a pre-calculated map.

Returns

Success/failure status

Author

Nathan Baker

Definition at line 5343 of file [vpmg.c](#).

9.108.3.11 fillcoChargeSpline1()

```
VPRIVATE void fillcoChargeSpline1 (  
    Vpmg * thee )
```

Fill source term charge array from linear interpolation.

Author

Nathan Baker

Definition at line 5391 of file [vpmg.c](#).

9.108.3.12 fillcoChargeSpline2()

```
VPRIVATE void fillcoChargeSpline2 (  
    Vpmg * thee )
```

Fill source term charge array from cubic spline interpolation.

Author

Nathan Baker

Definition at line 5528 of file [vpmg.c](#).

9.108.3.13 fillcoCoef()

```
VPRIVATE void fillcoCoef (  
    Vpmg * thee )
```

Top-level driver to fill all operator coefficient arrays.

Author

Nathan Baker

Definition at line 5247 of file [vpmg.c](#).

9.108.3.14 fillcoCoefMap()

```
VPRIVATE void fillcoCoefMap (  
    Vpmg * thee )
```

Fill operator coefficient arrays from pre-calculated maps.

Author

Nathan Baker

Definition at line 4489 of file [vpmg.c](#).

9.108.3.15 fillcoCoefMol()

```
VPRIVATE void fillcoCoefMol (  
    Vpmg * thee )
```

Fill operator coefficient arrays from a molecular surface calculation.

Author

Nathan Baker

Definition at line 4612 of file [vpmg.c](#).

9.108.3.16 fillcoCoefMolDiel()

```
VPRIVATE void fillcoCoefMolDiel (  
    Vpmg * thee )
```

Fill differential operator coefficient arrays from a molecular surface calculation.

Author

Nathan Baker

Definition at line 4726 of file [vpmg.c](#).

9.108.3.17 fillcoCoefMolDielNoSmooth()

```
VPRIVATE void fillcoCoefMolDielNoSmooth (
    Vpmg * thee )
```

Fill differential operator coefficient arrays from a molecular surface calculation without smoothing.

Author

Nathan Baker

Definition at line 4737 of file [vpmg.c](#).

9.108.3.18 fillcoCoefMolDielSmooth()

```
VPRIVATE void fillcoCoefMolDielSmooth (
    Vpmg * thee )
```

Fill differential operator coefficient arrays from a molecular surface calculation with smoothing.

Molecular surface, dielectric smoothing following an implementation of Bruccoleri, et al. J Comput Chem 18 268-276 (1997).

This algorithm uses a 9 point harmonic smoothing technique - the point in question and all grid points 1/sqrt(2) grid spacings away.

Note

This uses thee->a1cf, thee->a2cf, thee->a3cf as temporary storage.

Author

Todd Dolinsky

Definition at line 4891 of file [vpmg.c](#).

9.108.3.19 fillcoCoefMolIon()

```
VPRIVATE void fillcoCoefMolIon (
    Vpmg * thee )
```

Fill ion (nonlinear) operator coefficient array from a molecular surface calculation.

Author

Nathan Baker

Definition at line 4628 of file [vpmg.c](#).

9.108.3.20 fillcoCoefSpline()

```
VPRIVATE void fillcoCoefSpline (
    Vpmg * thee )
```

Fill operator coefficient arrays from a spline-based surface calculation.

Author

Nathan Baker

Definition at line 5022 of file [vpmg.c](#).

9.108.3.21 fillcoCoefSpline3()

```
VPRIVATE void fillcoCoefSpline3 (  
    Vpmg * thee )
```

Fill operator coefficient arrays from a 5th order polynomial based surface calculation.

Author

Michael Schnieders

Definition at line 10430 of file [vpmg.c](#).

9.108.3.22 fillcoCoefSpline4()

```
VPRIVATE void fillcoCoefSpline4 (  
    Vpmg * thee )
```

Fill operator coefficient arrays from a 7th order polynomial based surface calculation.

Author

Michael Schnieders

Definition at line 9939 of file [vpmg.c](#).

9.108.3.23 fillcoInducedDipole()

```
VPRIVATE void fillcoInducedDipole (  
    Vpmg * thee )
```

Fill source term charge array for use of induced dipoles.

Author

Michael Schnieders

9.108.3.24 fillcoNLInducedDipole()

```
VPRIVATE void fillcoNLInducedDipole (  
    Vpmg * thee )
```

Fill source term charge array for non-local induced dipoles.

Author

Michael Schnieders

9.108.3.25 fillcoPermanentMultipole()

```
VPRIVATE void fillcoPermanentMultipole (  
    Vpmg * thee )
```

Fill source term charge array for the use of permanent multipoles.

Author

Michael Schnieders

Definition at line 7240 of file [vpmg.c](#).

9.108.3.26 markSphere()

```

VPRIVATE void markSphere (
    double rtot,
    double * tpos,
    int nx,
    int ny,
    int nz,
    double hx,
    double hy,
    double hzed,
    double xmin,
    double ymin,
    double zmin,
    double * array,
    double markVal )

```

Mark the grid points inside a sphere with a particular value. This marks by resetting the the grid points inside the sphere to the specified value.

Author

Nathan Baker

Parameters

<i>tpos</i>	Sphere radius
<i>nx</i>	Sphere position
<i>ny</i>	Number of grid points
<i>nz</i>	Number of grid points
<i>hx</i>	Number of grid points
<i>hy</i>	Grid spacing
<i>hzed</i>	Grid spacing
<i>xmin</i>	Grid spacing
<i>ymin</i>	Grid lower corner
<i>zmin</i>	Grid lower corner
<i>array</i>	Grid lower corner
<i>markVal</i>	Grid values Value to mark with

Definition at line [6849](#) of file [vpmg.c](#).

9.108.3.27 multipolebc()

```

VPRIVATE void multipolebc (
    double r,
    double kappa,
    double eps_p,
    double eps_w,
    double rad,
    double tsr[3] )

```

This routine serves bcf2. It returns (in tsr) the contraction independent portion of the Debye-Huckel potential tensor for a spherical ion with a central charge, dipole and quadrupole. See the code for an in depth description.

Author

Michael Schnieders

Parameters

<i>kappa</i>	Distance to the boundary
<i>eps</i> _{← _p}	Exponential screening factor
<i>eps</i> _{← _w}	Solute dielectric
<i>rad</i>	Solvent dielectric
<i>tsr</i>	Radius of the sphere Contraction-independent portion of each tensor

Definition at line 3487 of file [vpmg.c](#).**9.108.3.28 qfForceSpline1()**

```
VPRIVATE void qfForceSpline1 (  
    Vpmg * thee,  
    double * force,  
    int atomID )
```

Charge-field force due to a linear spline charge function.

Author

Nathan Baker

Parameters

<i>atomID</i>	Set to force Valist atom ID
---------------	-----------------------------

Definition at line 6311 of file [vpmg.c](#).**9.108.3.29 qfForceSpline2()**

```
VPRIVATE void qfForceSpline2 (  
    Vpmg * thee,  
    double * force,  
    int atomID )
```

Charge-field force due to a cubic spline charge function.

Author

Nathan Baker

Parameters

<i>atomID</i>	Set to force Valist atom ID
---------------	-----------------------------

Definition at line 6448 of file [vpmg.c](#).

9.108.3.30 qfForceSpline4()

```
VPRIVATE void qfForceSpline4 (
    Vpmg * thee,
    double * force,
    int atomID )
```

Charge-field force due to a quintic spline charge function.

Author

Michael Schnieders

Parameters

<i>atomID</i>	Set to force Valist atom ID
---------------	-----------------------------

Definition at line 6561 of file [vpmg.c](#).

9.108.3.31 VFCHI4()

```
VPRIVATE double VFCHI4 (
    int i,
    double f )
```

Return 2.5 plus difference of i - f.

Author

Michael Schnieders

Returns

$(2.5 + ((\text{double})(i) - f))$

Definition at line 7132 of file [vpmg.c](#).

9.108.3.32 Vpmg_polarizEnergy()

```
VPRIVATE double Vpmg_polarizEnergy (
    Vpmg * thee,
    int extFlag )
```

Determines energy from polarizeable charge and interaction with fixed charges according to Rocchia et al.

Author

Nathan Baker

Returns

Energy in kT

Parameters

<i>extFlag</i>	If 1, add external energy contributions to result
----------------	---

Definition at line 1148 of file [vpmg.c](#).

9.108.3.33 Vpmg_qfEnergyPoint()

```
VPRIVATE double Vpmg_qfEnergyPoint (
    Vpmg * thee,
    int extFlag )
```

Calculates charge-potential energy using summation over delta function positions (i.e. something like an Linf norm)

Author

Nathan Baker

Returns

Energy in kT

Parameters

<i>extFlag</i>	If 1, add external energy contributions to result
----------------	---

Definition at line 1704 of file [vpmg.c](#).

9.108.3.34 Vpmg_qfEnergyVolume()

```
VPRIVATE double Vpmg_qfEnergyVolume (
    Vpmg * thee,
    int extFlag )
```

Calculates charge-potential energy as integral over a volume.

Author

Nathan Baker

Returns

Energy in kT

Parameters

<i>extFlag</i>	If 1, add external energy contributions to result
----------------	---

Definition at line 1861 of file [vpmg.c](#).

9.108.3.35 Vpmg_qmEnergyNONLIN()

```
VPRIVATE double Vpmg_qmEnergyNONLIN (
    Vpmg * thee,
    int extFlag )
```

Definition at line 1401 of file [vpmg.c](#).

9.108.3.36 Vpmg_qmEnergySMPBE()

```
VPRIVATE double Vpmg_qmEnergySMPBE (
    Vpmg * thee,
    int extFlag )
```

Vpmg_qmEnergy for SMPBE.

Author

Vincent Chu

Definition at line 1490 of file [vpmg.c](#).

9.108.3.37 Vpmg_splineSelect()

```
VPRIVATE void Vpmg_splineSelect (
    int srfm,
    Vacc * acc,
    double * gpos,
    double win,
    double infrad,
    Vatom * atom,
    double * force )
```

Selects a spline based surface method from either VSM_SPLINE, VSM_SPLINE5 or VSM_SPLINE7.

Author

David Gohara

Parameters

<i>acc</i>	Surface method, currently VSM_SPLINE, VSM_SPLINE5, or VSM_SPLINE7
<i>gpos</i>	Accessibility object
<i>win</i>	Position array -> array[3]
<i>infrad</i>	Spline window
<i>atom</i>	Inflation radius
<i>force</i>	Atom object Force array -> array[3]

Definition at line 1893 of file [vpmg.c](#).

9.108.3.38 zlapSolve()

```
VPRIVATE void zlapSolve (
    Vpmg * thee,
    double ** solution,
    double ** source,
    double ** work1 )
```

Calculate the solution to Poisson's equation with a simple Laplacian operator and zero-valued Dirichlet boundary conditions. Store the solution in thee->u.

Author

Nathan Baker

Note

Vpmg_fillco must be called first

Parameters

<i>source</i>	Solution term vector
<i>work1</i>	Source term vector Work vector

Definition at line 6898 of file vpmg.c.

9.109 vpmg.h

[Go to the documentation of this file.](#)

```

00001
00080 #ifndef _VPMG_H_
00081 #define _VPMG_H_
00082
00083 #include "apbscfg.h"
00084
00085 #include "malloc/malloc.h"
00086
00087 #include "generic/vhal.h"
00088 #include "generic/vacc.h"
00089 #include "generic/vcap.h"
00090 #include "generic/vpbe.h"
00091 #include "generic/mgparm.h"
00092 #include "generic/pbeparm.h"
00093 #include "generic/vmatrix.h"
00094 #include "pmgc/mgdrvd.h"
00095 #include "pmgc/newdrvd.h"
00096 #include "pmgc/mgsubd.h"
00097 #include "pmgc/mikpckd.h"
00098 #include "pmgc/matvecd.h"
00099 #include "mg/vpmgp.h"
00100 #include "mg/vgrid.h"
00101
00105 #define VPMGMAXPART 2000
00106
00116 struct sVpmg {
00117
00118     Vmem *vmem;
00119     Vpmgp *pmgp;
00120     Vpbe *pbe;
00122 #ifdef BURY_FORTRAN
00123     Vpde *pde;
00124     Vmgdriver *mgdriver;
00125 #endif
00126
00127     double *epsx;
00128     double *epsy;
00129     double *epsz;
00130     double *kappa;
00131     double *pot;
00132     double *charge;
00133     int *iparm;
00134     double *rparm;
00135     int *iwork;
00136     double *rwork;
00137     double *alcf;
00138     double *a2cf;
00142     double *a3cf;
00144     double *ccf;
00145     double *fcf;
00146     double *tcf;
00147     double *u;
00148     double *xf;
00149     double *yf;
00150     double *zf;
00151     double *gxcf;
00152     double *gycf;
00153     double *gzcf;
00154     double *pvec;

```

```

00155     double extDiEnergy;
00157     double extQmEnergy;
00159     double extQfEnergy;
00161     double extNpEnergy;
00163     Vsurf_Meth surfMeth;
00164     double splineWin;
00165     Vchrg_Meth chargeMeth;
00166     Vchrg_Src chargeSrc;
00168     int filled;
00170     int useDielXMap;
00172     Vgrid *dielXMap;
00173     int useDielYMap;
00175     Vgrid *dielYMap;
00176     int useDielZMap;
00178     Vgrid *dielZMap;
00179     int useKappaMap;
00181     Vgrid *kappaMap;
00182     int usePotMap;
00184     Vgrid *potMap;
00186     int useChargeMap;
00188     Vgrid *chargeMap;
00189 };
00190
00195 typedef struct sVpmg Vpmg;
00196
00197 /* ////////////////////////////////////////////////////////////////////
00200 #if !defined(VINLINE_VPMG)
00201
00208     VEXTERNC unsigned long int Vpmg_memChk(
00209         Vpmg *thee /**< Object for memory check */
00210     );
00211
00212 #else /* if defined(VINLINE_VPMG) */
00213 #    define Vpmg_memChk(thee) (Vmem_bytes((thee)->vmem))
00215 #endif /* if !defined(VINLINE_VPMG) */
00217 /* ////////////////////////////////////////////////////////////////////
00221
00226 VEXTERNC Vpmg* Vpmg_ctor(
00227     Vpmgp *parms, /**< PMG parameter object */
00228     Vpbe *pbe,
00229     int focusFlag,
00230     Vpmg *pmgOLD,
00231     MGparm *mgparm,
00232     PBEparm_calcEnergy energyFlag
00233 );
00234
00242 VEXTERNC int Vpmg_ctor2(
00243     Vpmg *thee,
00244     Vpmgp *parms,
00245     Vpbe *pbe,
00246     int focusFlag,
00247     Vpmg *pmgOLD,
00249     MGparm *mgparm,
00251     PBEparm_calcEnergy energyFlag
00254 );
00255
00260 VEXTERNC void Vpmg_dtor(
00261     Vpmg **thee
00263 );
00264
00269 VEXTERNC void Vpmg_dtor2(
00270     Vpmg *thee
00271 );
00272
00281 VEXTERNC int Vpmg_fillco(
00282     Vpmg *thee,
00283     Vsurf_Meth surfMeth,
00284     double splineWin,
00286     Vchrg_Meth chargeMeth,
00287     int useDielXMap,
00288     Vgrid *dielXMap,
00289     int useDielYMap,
00290     Vgrid *dielYMap,
00291     int useDielZMap,
00292     Vgrid *dielZMap,
00293     int useKappaMap,
00294     Vgrid *kappaMap,
00295     int usePotMap,

```

```
00296         Vgrid *potMap,
00297         int useChargeMap,
00298         Vgrid *chargeMap
00299     );
00300
00306 VEXTERNC int Vpmg_solve(
00307     Vpmg *thee
00308 );
00309
00321 VEXTERNC int Vpmg_solveLaplace(
00322     Vpmg *thee
00323 );
00324
00334 VEXTERNC double Vpmg_energy(
00335     Vpmg *thee,
00336     int extFlag
00340 );
00341
00359 VEXTERNC double Vpmg_qfEnergy(
00360     Vpmg *thee,
00361     int extFlag
00365 );
00366
00386 VEXTERNC double Vpmg_qfAtomEnergy(
00387     Vpmg *thee,
00388     Vatom *atom
00389 );
00390
00415 VEXTERNC double Vpmg_qmEnergy(
00416     Vpmg *thee,
00417     int extFlag
00421 );
00422
00423
00442 VEXTERNC double Vpmg_dielEnergy(
00443     Vpmg *thee,
00444     int extFlag
00448 );
00449
00450
00467 VEXTERNC double Vpmg_dielGradNorm(
00468     Vpmg *thee
00469 );
00470
00482 VEXTERNC int Vpmg_force(
00483     Vpmg *thee,
00484     double *force,
00486     int atomID,
00487     Vsurf_Meth srfm,
00488     Vchrg_Meth chgm
00489 );
00490
00502 VEXTERNC int Vpmg_qfForce(
00503     Vpmg *thee,
00504     double *force,
00506     int atomID,
00507     Vchrg_Meth chgm
00508 );
00509
00521 VEXTERNC int Vpmg_dbForce(
00522     Vpmg *thee,
00523     double *dbForce,
00525     int atomID,
00526     Vsurf_Meth srfm
00527 );
00528
00540 VEXTERNC int Vpmg_ibForce(
00541     Vpmg *thee,
00542     double *force,
00544     int atomID,
00545     Vsurf_Meth srfm
00546 );
00547
00553 VEXTERNC void Vpmg_setPart(
00554     Vpmg *thee,
00555     double lowerCorner[3],
00556     double upperCorner[3],
00557     int bflags[6]
00561 );
00562
00567 VEXTERNC void Vpmg_unsetPart(
```

```
00568         Vpmg *thee
00569     );
00570
00576 VEXTERNC int Vpmg_fillArray(
00577     Vpmg *thee,
00578     double *vec,
00580     Vdata_Type type,
00581     double parm,
00582     Vhal_PBEType pbetype,
00583     PBEparm * pbeparm
00584 );
00585
00591 VPUBLIC void Vpmg_fieldSpline4(
00592     Vpmg *thee,
00593     int atomID,
00594     double field[3]
00595 );
00596
00604 VEXTERNC double Vpmg_qfPermanentMultipoleEnergy(
00605     Vpmg *thee,
00606     int atomID
00607 );
00608
00614 VEXTERNC void Vpmg_qfPermanentMultipoleForce(
00615     Vpmg *thee,
00616     int atomID,
00617     double force[3],
00618     double torque[3]
00619 );
00620
00625 VEXTERNC void Vpmg_ibPermanentMultipoleForce(
00626     Vpmg *thee,
00627     int atomID,
00628     double force[3]
00629 );
00630
00635 VEXTERNC void Vpmg_dbPermanentMultipoleForce(
00636     Vpmg *thee,
00637     int atomID,
00638     double force[3]
00639 );
00640
00647 VEXTERNC void Vpmg_qfDirectPolForce(
00648     Vpmg *thee,
00649     Vgrid *perm,
00650     Vgrid *induced,
00651     int atomID,
00652     double force[3],
00653     double torque[3]
00654 );
00655
00664 VEXTERNC void Vpmg_qfNLDirectPolForce(
00665     Vpmg *thee,
00666     Vgrid *perm,
00667     Vgrid *nlInduced,
00668     int atomID,
00669     double force[3],
00670     double torque[3]
00671 );
00672
00680 VEXTERNC void Vpmg_ibDirectPolForce(
00681     Vpmg *thee,
00682     Vgrid *perm,
00683     Vgrid *induced,
00684     int atomID,
00685     double force[3]
00686 );
00687
00696 VEXTERNC void Vpmg_ibNLDirectPolForce(
00697     Vpmg *thee,
00698     Vgrid *perm,
00699     Vgrid *nlInduced,
00700     int atomID,
00701     double force[3]
00702 );
00703
00711 VEXTERNC void Vpmg_dbDirectPolForce(
00712     Vpmg *thee,
00713     Vgrid *perm,
00714     Vgrid *induced,
00715     int atomID,
```



```
00716         double force[3]
00717     );
00718
00727 VEXTERNC void Vpmg_dbNLDirectPolForce(
00728     Vpmg *thee,
00729     Vgrid *perm,
00730     Vgrid *nlInduced,
00731     int atomID,
00732     double force[3]
00733 );
00734
00741 VEXTERNC void Vpmg_qfMutualPolForce(
00742     Vpmg *thee,
00743     Vgrid *induced,
00744     Vgrid *nlInduced,
00745     int atomID,
00746     double force[3]
00747 );
00748
00756 VEXTERNC void Vpmg_ibMutualPolForce(
00757     Vpmg *thee,
00758     Vgrid *induced,
00759     Vgrid *nlInduced,
00760     int atomID,
00761     double force[3]
00762 );
00763
00771 VEXTERNC void Vpmg_dbMutualPolForce(
00772     Vpmg *thee,
00773     Vgrid *induced,
00774     Vgrid *nlInduced,
00775     int atomID,
00776     double force[3]
00777 );
00778
00785 VEXTERNC void Vpmg_printColComp(
00786     Vpmg *thee,
00787     char path[72],
00788     char title[72],
00789     char mxtype[3],
00797     int flag
00801 );
00802
00803
00804
00811 VPRIVATE void bcolcomp(
00812     int *iparm,
00813     double *rparm,
00814     int *iwork,
00815     double *rwork,
00816     double *values,
00817     int *rowind,
00818     int *colptr,
00819     int *flag
00824 );
00825
00826
00827
00834 VPRIVATE void bcolcomp2(
00835     int *iparm,
00836     double *rparm,
00837     int *nx,
00838     int *ny,
00839     int *nz,
00840     int *iz,
00841     int *ipc,
00842     double *rpc,
00843     double *ac,
00844     double *cc,
00845     double *values,
00846     int *rowind,
00847     int *colptr,
00848     int *flag
00853 );
00854
00855
00856
00863 VPRIVATE void bcolcomp3(
00864     int *nx,
00865     int *ny,
00866     int *nz,
```

```
00867         int      *ipc,
00868         double *rpc,
00869         double *ac,
00870         double *cc,
00871         double *values,
00872         int      *rowind,
00873         int      *colptr,
00874         int      *flag
00875     );
00876
00877
00878
00885 VPRIVATE void bcolcomp4(
00886     int      *nx,
00887     int      *ny,
00888     int      *nz,
00889     int      *ipc,
00890     double *rpc,
00891     double *oC,
00892     double *cc,
00893     double *oE,
00894     double *oN,
00895     double *uC,
00896     double *values,
00897     int      *rowind,
00898     int      *colptr,
00899     int      *flag
00900 );
00901
00902
00903
00910 VPRIVATE void pcolcomp(
00911     int      *nrow,
00912     int      *ncol,
00913     int      *nnzero,
00914     double *values,
00915     int      *rowind,
00916     int      *colptr,
00917     char      *path,
00918     char      *title,
00919     char      *mxtype
00920 );
00921
00922
00923
00924 /* ////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////
00925 // Internal routines
00926
00927
00933 VPRIVATE double bspline2(
00934     double x /** Position */
00935 );
00936
00942 VPRIVATE double dbspline2(
00943     double x
00944 );
00945
00951 VPRIVATE double VFCHI4(
00952     int i,
00953     double f
00954 );
00955
00961 VPRIVATE double bspline4(
00962     double x
00963 );
00964
00970 VPRIVATE double dbspline4(
00971     double x
00972 );
00973
00979 VPRIVATE double d2bspline4(
00980     double x
00981 );
00982
00988 VPRIVATE double d3bspline4(
00989     double x
00990 );
00991
00998 VPRIVATE double Vpmg_polarizEnergy(
00999     Vpmg *thee,
01000     int extFlag
01001 );
01002
```

```
01009 VPRIVATE double Vpmg_qfEnergyPoint (
01010     Vpmg *thee,
01011     int extFlag
01013 );
01014
01020 VPRIVATE double Vpmg_qfEnergyVolume (
01021     Vpmg *thee,
01022     int extFlag
01024 );
01025
01031 VPRIVATE void Vpmg_splineSelect (
01032     int srfm,
01034     Vacc *acc,
01035     double *gpos,
01036     double win,
01037     double infrad,
01038     Vatom *atom,
01039     double *force
01040 );
01041
01047 VPRIVATE void focusFillBound(
01048     Vpmg *thee,
01049     Vpmg *pmg
01050 );
01051
01058 VPRIVATE void bcfl1(
01059     double size,
01060     double *apos,
01061     double charge,
01062     double xkappa,
01063     double prel,
01064     double *gxcf,
01065     double *gycf,
01066     double *gzcf,
01067     double *xf,
01068     double *yf,
01069     double *zf,
01070     int nx,
01071     int ny,
01072     int nz
01073 );
01074
01080 VPRIVATE void bcfl2(
01081     double size,
01082     double *apos,
01083     double charge,
01084     double *dipole,
01085     double *quad,
01086     double xkappa,
01087     double eps_p,
01088     double eps_w,
01089     double T,
01090     double *gxcf,
01091     double *gycf,
01092     double *gzcf,
01093     double *xf,
01094     double *yf,
01095     double *zf,
01096     int nx,
01097     int ny,
01098     int nz
01099 );
01100
01109 VPRIVATE void multipolebc(
01110     double r,
01111     double kappa,
01112     double eps_p,
01113     double eps_w,
01114     double rad,
01115     double tsr[3]
01116 );
01117
01126 VPRIVATE double bcfl1sp(
01127     double size,
01128     double *apos,
01129     double charge,
01130     double xkappa,
01131     double prel,
01132     double *pos
01133 );
01134
```

```
01139 VPRIVATE void bcCalc(  
01140     Vpmg *thee  
01141 );  
01142  
01147 VPRIVATE void fillcoCoef(  
01148     Vpmg *thee  
01149 );  
01150  
01155 VPRIVATE void fillcoCoefMap(  
01156     Vpmg *thee  
01157 );  
01158  
01164 VPRIVATE void fillcoCoefMol(  
01165     Vpmg *thee  
01166 );  
01167  
01173 VPRIVATE void fillcoCoefMolIon(  
01174     Vpmg *thee  
01175 );  
01176  
01182 VPRIVATE void fillcoCoefMolDiel(  
01183     Vpmg *thee  
01184 );  
01185  
01191 VPRIVATE void fillcoCoefMolDielNoSmooth(  
01192     Vpmg *thee  
01193 );  
01194  
01208 VPRIVATE void fillcoCoefMolDielSmooth(  
01209     Vpmg *thee  
01210 );  
01211  
01217 VPRIVATE void fillcoCoefSpline(  
01218     Vpmg *thee  
01219 );  
01220  
01226 VPRIVATE void fillcoCoefSpline3(  
01227     Vpmg *thee  
01228 );  
01229  
01235 VPRIVATE void fillcoCoefSpline4(  
01236     Vpmg *thee  
01237 );  
01238  
01244 VPRIVATE Vrc_Codes fillcoCharge(  
01245     Vpmg *thee  
01246 );  
01247  
01253 VPRIVATE Vrc_Codes fillcoChargeMap(  
01254     Vpmg *thee  
01255 );  
01256  
01261 VPRIVATE void fillcoChargeSpline1(  
01262     Vpmg *thee  
01263 );  
01264  
01269 VPRIVATE void fillcoChargeSpline2(  
01270     Vpmg *thee  
01271 );  
01272  
01277 VPRIVATE void fillcoPermanentMultipole(  
01278     Vpmg *thee  
01279 );  
01280  
01285 VPRIVATE void fillcoInducedDipole(  
01286     Vpmg *thee  
01287 );  
01288  
01294 VPRIVATE void fillcoNLInducedDipole(  
01295     Vpmg *thee  
01296 );  
01297  
01304 VPRIVATE void extEnergy(  
01305     Vpmg *thee,  
01306     Vpmg *pmgOLD,  
01307     PBEparm_calcEnergy extFlag,  
01308     double partMin[3],  
01309     double partMax[3],  
01310     int bflags[6]  
01311 );  
01312
```

```

01317 VPRIVATE void qfForceSpline1(
01318     Vpmg *thee,
01319     double *force,
01320     int atomID
01321 );
01322
01327 VPRIVATE void qfForceSpline2(
01328     Vpmg *thee,
01329     double *force,
01330     int atomID
01331 );
01332
01337 VPRIVATE void qfForceSpline4(
01338     Vpmg *thee,
01339     double *force,
01340     int atomID
01341 );
01342
01343
01351 VPRIVATE void zlapSolve(
01352     Vpmg *thee,
01353     double **solution,
01354     double **source,
01355     double **work1
01356 );
01357
01364 VPRIVATE void markSphere(
01365     double rtot,
01366     double *tpos,
01367     int nx,
01368     int ny,
01369     int nz,
01370     double hx,
01371     double hy,
01372     double hzed,
01373     double xmin,
01374     double ymin,
01375     double zmin,
01376     double *array,
01377     double markVal
01378 );
01379
01384 VPRIVATE double Vpmg_qmEnergySMPBE(Vpmg *thee, int extFlag);
01385 VPRIVATE double Vpmg_qmEnergyNONLIN(Vpmg *thee, int extFlag);
01386
01387
01388
01389 // Additional macros and definitions. May not be needed
01390
01391 // Added by Vincent Chu 9/13/06 for SMPB
01392 #define VCUB(x) ((x)*(x)*(x))
01393 #define VLOG(x) (log(x))
01394
01395 #define IJK(i,j,k) (((k)*(nx)*(ny))+((j)*(nx))+i))
01396 #define IJKx(j,k,i) (((i)*(ny)*(nz))+((k)*(ny))+j))
01397 #define IJKy(i,k,j) (((j)*(nx)*(nz))+((k)*(nx))+i))
01398 #define IJKz(i,j,k) (((k)*(nx)*(ny))+((j)*(nx))+i))
01399 #define VFCHI(iint,iflt) (1.5+((double)(iint)-(iflt)))
01400
01401
01402 #endif /* ifndef _VPMG_H_ */
01403

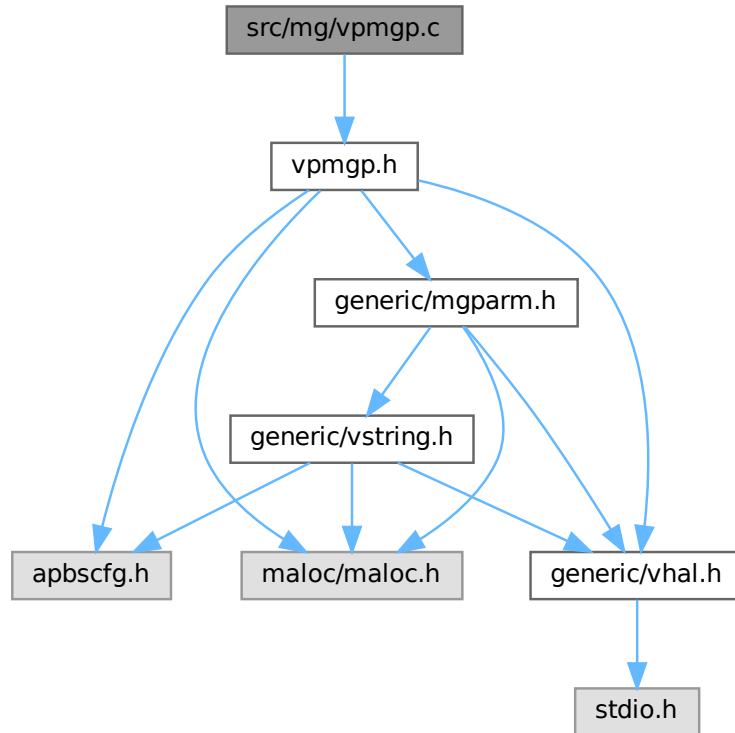
```

9.110 src/mg/vpmgp.c File Reference

Class Vpmgp methods.

```
#include "vpmgp.h"
```

Include dependency graph for vpmgp.c:



Functions

- `VPUBLIC Vpmgp * Vpmgp_ctor (MGparm *mgparm)`
Construct PMG parameter object and initialize to default values.
- `VPUBLIC int Vpmgp_ctor2 (Vpmgp *thee, MGparm *mgparm)`
FORTTRAN stub to construct PMG parameter object and initialize to default values.
- `VPUBLIC void Vpmgp_dtor (Vpmgp **thee)`
Object destructor.
- `VPUBLIC void Vpmgp_dtor2 (Vpmgp *thee)`
FORTTRAN stub for object destructor.
- `VPUBLIC void Vpmgp_size (Vpmgp *thee)`
Determine array sizes and parameters for multigrid solver.
- `VPPRIVATE int coarsenThis (int nOld)`
- `VPUBLIC void Vpmgp_makeCoarse (int numLevel, int nxOld, int nyOld, int nzOld, int *nxNew, int *nyNew, int *nzNew)`
Coarsen the grid by the desired number of levels and determine the resulting numbers of grid points.

9.110.1 Detailed Description

Class Vpmgp methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
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*
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*
*
```

Definition in file [vpmgp.c](#).

9.110.2 Function Documentation

9.110.2.1 coarsenThis()

```
VPRIVATE int coarsenThis (
    int nOld )
```

Definition at line 294 of file [vpmgp.c](#).

9.111 vpmgp.c

[Go to the documentation of this file.](#)

```
00001
00057 #include "vpmgp.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 /* ////////////////////////////////////////
00062 // Class Vpmgp: Inlineable methods
00064 #if !defined(VINLINE_VACC)
00065 #endif /* if !defined(VINLINE_VACC) */
00066
00067 /* ////////////////////////////////////////
00068 // Class Vpmgp: Non-inlineable methods
00070
00071 /* ////////////////////////////////////////
00072 // Routine: Vpmgp_ctor
00073 //
00074 // Author: Nathan Baker
00076 VPUBLIC Vpmgp* Vpmgp_ctor(MGparm *mgparm) {
00077
00078     Vpmgp *thee = VNULL;
00079
00080     /* Set up the structure */
00081     thee = (Vpmgp*)Vmem_malloc(VNULL, 1, sizeof(Vpmgp) );
00082     VASSERT( thee != VNULL);
00083     VASSERT(Vpmgp_ctor2(thee,mgparm));
00084
00085     return thee;
00086 }
00087
00088 /* ////////////////////////////////////////
00089 // Routine: Vpmgp_ctor2
00090 //
00091 // Author: Nathan Baker
00093 VPUBLIC int Vpmgp_ctor2(Vpmgp *thee,MGparm *mgparm) {
00094
00095     /* Specified parameters */
00096     thee->nx = mgparm->dime[0];
00097     thee->ny = mgparm->dime[1];
00098     thee->nz = mgparm->dime[2];
00099     thee->hx = mgparm->grid[0];
00100     thee->hy = mgparm->grid[1];
00101     thee->hzcd = mgparm->grid[2];
00102     thee->xlen = ((double) (mgparm->dime[0]-1))*mgparm->grid[0];
00103     thee->ylen = ((double) (mgparm->dime[1]-1))*mgparm->grid[1];
00104     thee->zlen = ((double) (mgparm->dime[2]-1))*mgparm->grid[2];
00105     thee->nlev = mgparm->nlev;
00106
00107     thee->nonlin = mgparm->nonlintype;
00108     thee->meth = mgparm->method;
00109
00110 #ifdef DEBUG_MAC_OSX_OCL
00111 #include "mach_chud.h"
00112     if(kOpenCLAvailable)
00113         thee->meth = 4;
00114 #endif
00115
00116     if (thee->nonlin == NONLIN_LPBE) thee->ipkey = IPKEY_LPBE; /* LPBE case */
00117     else if(thee->nonlin == NONLIN_SMPBE) thee->ipkey = IPKEY_SMPBE; /* SMPBE case */
00118     else thee->ipkey = IPKEY_NPBE; /* NPBE standard case */
00119
00120     /* Default parameters */
00121     if (mgparm->setetol) { /* If etol is set by the user in APBS input file, then use this custom-defined
    etol */
00122         thee->errtol = mgparm->etol;
00123         Vnm_print(1, " Error tolerance (etol) is now set to user-defined \
00124 value: %g \n", thee->errtol);
00125         Vnm_print(0, "Error tolerance (etol) is now set to user-defined \
```



```

00126 value: %g \n", thee->errtol);
00127     } else thee->errtol = 1.0e-6; /* Here are a few comments. Mike had this set to
00128         * 1e-9; conventional wisdom sets this at 1e-6 for
00129         * the PBE; Ray Luo sets this at 1e-3 for his
00130         * accelerated PBE (for dynamics, etc.) */
00131     thee->itmax = 200;
00132     thee->istop = 1;
00133     thee->iinfo = 1; /* I'd recommend either 1 (for debugging LPBE) or 2 (for debugging NPBE),
higher values give too much output */
00134
00135     thee->bcfl = BCFL_SDH;
00136     thee->key = 0;
00137     thee->iperf = 0;
00138     thee->mgcoar = 2;
00139     thee->mgkey = 0;
00140     thee->nul = 2;
00141     thee->nu2 = 2;
00142     thee->mgprol = 0;
00143     thee->mgdisc = 0;
00144     thee->omegal = 19.4e-1;
00145     thee->omegan = 9.0e-1;
00146     thee->ipcon = 3;
00147     thee->irite = 8;
00148     thee->xcen = 0.0;
00149     thee->ycen = 0.0;
00150     thee->zcen = 0.0;
00151
00152     /* Default value for all APBS runs */
00153     thee->mgsmoo = 1;
00154     if (thee->nonlin == NONLIN_NPBE || thee->nonlin == NONLIN_SMPBE) {
00155         /* SMPBE Added - SMPBE needs to mimic NPBE */
00156         Vnm_print(0, "Vpmp_ctor2: Using meth = 1, mgsolv = 0\n");
00157         thee->mgsolv = 0;
00158     } else {
00159         /* Most rigorous (good for testing) */
00160         Vnm_print(0, "Vpmp_ctor2: Using meth = 2, mgsolv = 1\n");
00161         thee->mgsolv = 1;
00162     }
00163
00164     /* TEMPORARY USEAQUA */
00165     /* If we are using aqua, our solution method is either VSOL_CGMAqua or VSOL_NewtonAqua
00166        * so we need to temporarily override the mgsolve value and set it to 0
00167        */
00168     if(mgparm->useAqua == 1) thee->mgsolv = 0;
00169
00170     return 1;
00171 }
00172
00173 /* ////////////////////////////////////////
00174 // Routine: Vpmpg_dtor
00175 //
00176 // Author: Nathan Baker
00177 VPUBLIC void Vpmpg_dtor(Vpmpg **thee) {
00178
00179     if ((*thee) != VNULL) {
00180         Vpmpg_dtor2(*thee);
00181         Vmem_free(VNULL, 1, sizeof(Vpmpg), (void **)thee);
00182         (*thee) = VNULL;
00183     }
00184 }
00185
00186 }
00187
00188 /* ////////////////////////////////////////
00189 // Routine: Vpmpg_dtor2
00190 //
00191 // Author: Nathan Baker
00192 VPUBLIC void Vpmpg_dtor2(Vpmpg *thee) { ; }
00193
00194
00195
00196 VPUBLIC void Vpmpg_size(
00197     Vpmpg *thee
00198 )
00199 {
00200
00201     int num_nf = 0;
00202     int num_narr = 2;
00203     int num_narrc = 27;
00204     int nxf, nyf, nzf, level, num_nf_oper, num_narrc_oper, n_band, nc_band, num_band, iretot;
00205
00206     thee->nf = thee->nxf * thee->ny * thee->nz;
00207     thee->narr = thee->nf;

```

```

00208     nxf = thee->nxf;
00209     nyf = thee->nyf;
00210     nzf = thee->nzf;
00211     thee->nxc = thee->nxf;
00212     thee->nyc = thee->nyf;
00213     thee->nzc = thee->nzf;
00214
00215     for (level=2; level<=thee->nlev; level++) {
00216         Vpmgp_makeCoarse(1, nxf, nyf, nzf, &(thee->nxc), &(thee->nyc), &(thee->nzc)); /* NAB TO-DO --
implement this function and check which variables need to be passed by reference... */
00217         nxf = thee->nxc;
00218         nyf = thee->nyc;
00219         nzf = thee->nzc;
00220         thee->narr = thee->narr + (nxf * nyf * nzf);
00221     }
00222
00223     thee->nc = thee->nxc * thee->nyc * thee->nzc;
00224     thee->narrc = thee->narr - thee->nf;
00225
00226     /* Box or FEM discretization on fine grid? */
00227     switch (thee->mgdisc) { /* NAB TO-DO: This needs to be changed into an enumeration */
00228     case 0:
00229         num_nf_oper = 4;
00230         break;
00231     case 1:
00232         num_nf_oper = 14;
00233         break;
00234     default:
00235         Vnm_print(2, "Vpmgp_size: Invalid mgdisc value (%d)!\n", thee->mgdisc);
00236         VASSERT(0);
00237     }
00238
00239     /* Galerkin or standard coarsening? */
00240     switch (thee->mgcoar) { /* NAB TO-DO: This needs to be changed into an enumeration */
00241     case 0:
00242         if (thee->mgdisc != 0) {
00243             Vnm_print(2, "Vpmgp_size: Invalid mgcoar value (%d); must be used with mgdisc 0!\n",
thee->mgcoar);
00244             VASSERT(0);
00245         }
00246         num_narrc_oper = 4;
00247         break;
00248     case 1:
00249         if (thee->mgdisc != 0) {
00250             Vnm_print(2, "Vpmgp_size: Invalid mgcoar value (%d); must be used with mgdisc 0!\n",
thee->mgcoar);
00251             VASSERT(0);
00252         }
00253         num_narrc_oper = 14;
00254         break;
00255     case 2:
00256         num_narrc_oper = 14;
00257         break;
00258     default:
00259         Vnm_print(2, "Vpmgp_size: Invalid mgcoar value (%d)!\n", thee->mgcoar);
00260         VASSERT(0);
00261     }
00262
00263     /* LINPACK storage on coarse grid */
00264     switch (thee->mgsolv) { /* NAB TO-DO: This needs to be changed into an enumeration */
00265     case 0:
00266         n_band = 0;
00267         break;
00268     case 1:
00269         if ( ( (thee->mgcoar == 0) || (thee->mgcoar == 1)) && (thee->mgdisc == 0) ) {
00270             num_band = 1 + (thee->nxc-2)*(thee->nyc-2);
00271         } else {
00272             num_band = 1 + (thee->nxc-2)*(thee->nyc-2) + (thee->nxc-2) + 1;
00273         }
00274         nc_band = (thee->nxc-2)*(thee->nyc-2)*(thee->nzc-2);
00275         n_band = nc_band * num_band;
00276         break;
00277     default:
00278         Vnm_print(2, "Vpmgp_size: Invalid mgsolv value (%d)!\n", thee->mgsolv);
00279         VASSERT(0);
00280     }
00281
00282     /* Real storage parameters */
00283     thee->n_rpc = 100*(thee->nlev+1);
00284
00285     /* Resulting total required for real storage */

```

```

00286     thee->nwrk = num_narr*thee->narr + (size_t)(num_nf + num_nf_oper)*thee->nf + (size_t)(num_narrc +
num_narrc_oper)*thee->narrc + n_band + thee->n_rpc;
00287
00288     /* Integer storage parameters */
00289     thee->n_iz = 50*(thee->nlev+1);
00290     thee->n_ipc = 100*(thee->nlev+1);
00291     thee->n_iwk = thee->n_iz + thee->n_ipc;
00292 }
00293
00294 VPRIVATE int coarsenThis(int nOld) {
00295     int nOut;
00296
00297     nOut = (nOld - 1) / 2 + 1;
00298
00299     if (((nOut-1)*2) != (nOld-1)) {
00300         Vnm_print(2, "Vpmgp_makeCoarse: Warning! The grid dimensions you have chosen are not consistent
00301 with the nlev you have specified!\n");
00302         Vnm_print(2, "Vpmgp_makeCoarse: This calculation will only work if you are running with mg-dummy
type.\n");
00303     }
00304     if (nOut < 1) {
00305         Vnm_print(2, "D'oh! You coarsened the grid below zero! How did you do that?\n");
00306         VASSERT(0);
00307     }
00308
00309     return nOut;
00310 }
00311
00312 VPUBLIC void Vpmgp_makeCoarse(
00313     int numLevel,
00314     int nxOld,
00315     int nyOld,
00316     int nzOld,
00317     int *nxNew,
00318     int *nyNew,
00319     int *nzNew
00320 )
00321 {
00322     int ntmp, nytmp, nztmp, iLevel;
00323
00324     for (iLevel=0; iLevel<numLevel; iLevel++) {
00325         ntmp = *nxNew;
00326         nytmp = *nyNew;
00327         nztmp = *nzNew;
00328         *nxNew = coarsenThis(ntmp);
00329         *nyNew = coarsenThis(nytmp);
00330         *nzNew = coarsenThis(nztmp);
00331     }
00332
00333
00334 }

```

9.112 src/mg/vpmgp.h File Reference

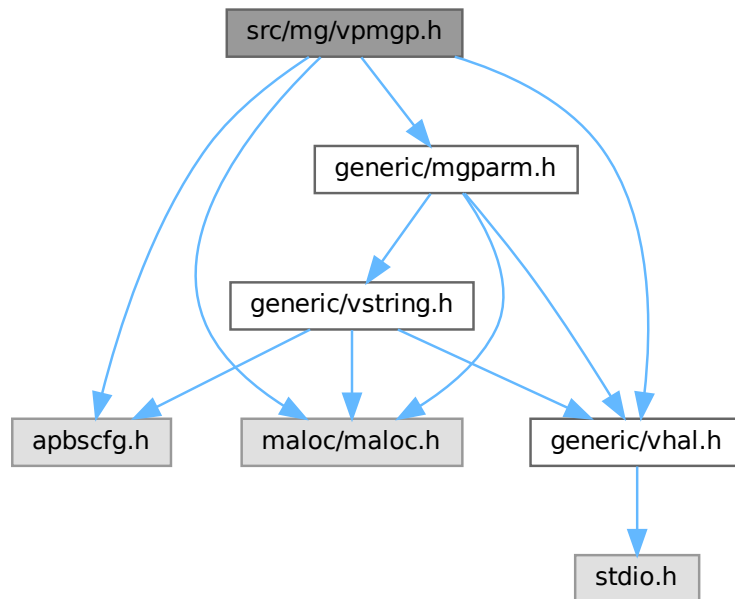
Contains declarations for class Vpmgp.

```

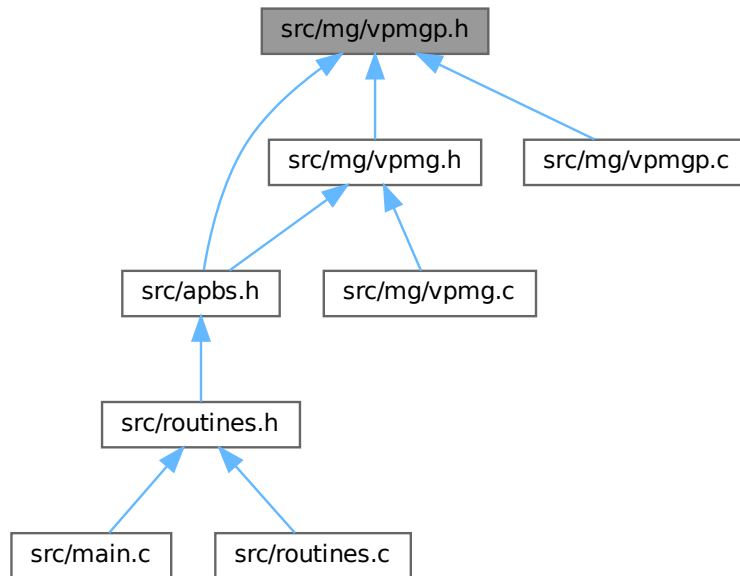
#include "apbscfg.h"
#include "maloc/maloc.h"
#include "generic/vhal.h"
#include "generic/mgparm.h"

```

Include dependency graph for `vpmgp.h`:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVpmgp](#)
Contains public data members for Vpmgp class/module.

Typedefs

- typedef struct [sVpmgp](#) [Vpmgp](#)
Declaration of the Vpmgp class as the [sVpmgp](#) structure.

Functions

- VEXTERNC [Vpmgp](#) * [Vpmgp_ctor](#) ([MGparm](#) *mgparm)
Construct PMG parameter object and initialize to default values.
- VEXTERNC int [Vpmgp_ctor2](#) ([Vpmgp](#) *thee, [MGparm](#) *mgparm)
FORTTRAN stub to construct PMG parameter object and initialize to default values.
- VEXTERNC void [Vpmgp_dtor](#) ([Vpmgp](#) **thee)
Object destructor.
- VEXTERNC void [Vpmgp_dtor2](#) ([Vpmgp](#) *thee)
FORTTRAN stub for object destructor.
- VEXTERNC void [Vpmgp_size](#) ([Vpmgp](#) *thee)
Determine array sizes and parameters for multigrid solver.
- VEXTERNC void [Vpmgp_makeCoarse](#) (int numLevel, int nxOld, int nyOld, int nzOld, int *nxNew, int *nyNew, int *nzNew)
Coarsen the grid by the desired number of levels and determine the resulting numbers of grid points.

9.112.1 Detailed Description

Contains declarations for class Vpmgp.

Version

\$Id\$

Author

Nathan A. Baker

Note

Variables and many default values taken directly from PMG

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
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*   Pacific Northwest National Laboratory
*
*   Additional contributing authors listed in the code documentation.
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*   THE POSSIBILITY OF SUCH DAMAGE.
*
*
```

Definition in file [vpmgp.h](#).

9.113 vpmgp.h

[Go to the documentation of this file.](#)

```

00001
00064 #ifndef _VPMGP_H_
00065 #define _VPMGP_H_
00066
00067 #include "apbscfg.h"
00068
00069 #include "malloc/malloc.h"
00070
00071 #include "generic/vhal.h"
00072 #include "generic/mgparm.h"
00073
00080 struct sVpmgp {
00081
00082     /* ***** USER-SPECIFIED PARAMETERS ***** */
00083     int nx;
00084     int ny;
00085     int nz;
00086     int nlev;
00087     double hx;
00088     double hy;
00089     double hzed;
00090     int nonlin;
00095     /* ***** DERIVED PARAMETERS ***** */
00096     int nxc;
00097     int nyc;
00098     int nzc;
00099     int nf;
00100     int nc;
00101     int narrc;
00102     int n_rpc;
00103     int n_iz;
00104     int n_ipc;
00106     size_t nrw;
00107     int niwk;
00108     int narr;
00109     int ipkey;
00117     /* ***** PARAMETERS WITH DEFAULT VALUES ***** */
00118     double xcent;
00119     double ycent;
00120     double zcent;
00121     double errtol;
00122     int itmax;
00123     int istop;
00130     int iinfo;
00135     Vbcfl bcf1;
00136     int key;
00139     int iperf;
00144     int meth;
00155     int mgkey;
00158     int nul;
00159     int nu2;
00160     int mgsmoo;
00166     int mgprol;
00170     int mgcoar;
00174     int mgsolv;
00177     int mgdisc;
00180     double omegal;
00181     double omegan;
00182     int irite;
00183     int ipcon;
00189     double xlen;
00190     double ylen;
00191     double zlen;
00192     double xmin;
00193     double ymin;
00194     double zmin;
00195     double xmax;
00196     double ymax;
00197     double zmax;
00198 };
00199
00204 typedef struct sVpmgp Vpmgp;
00205
00206 /* ////////////////////////////////////////
00207 // Class Vpmgp: Inlineable methods (vpmgp.c)
00209
00210 #if !defined(VINLINE_VPMGP)

```

```

00211 #else /* if defined(VINLINE_VPMGP) */
00212 #endif /* if !defined(VINLINE_VPMGP) */
00213
00214 /* ////////////////////////////////////////
00215 // Class Vpmgp: Non-Inlineable methods (vpmgp.c)
00216 ////////////////////////////////////////
00217
00224 VEXTERNC Vpmgp* Vpmgp_ctor(MGparm *mgparm);
00225
00234 VEXTERNC int Vpmgp_ctor2(Vpmgp *thee, MGparm *mgparm);
00235
00241 VEXTERNC void Vpmgp_dtor(Vpmgp **thee);
00242
00248 VEXTERNC void Vpmgp_dtor2(Vpmgp *thee);
00249
00254 VEXTERNC void Vpmgp_size(
00255     Vpmgp *thee /**< Object to be sized */
00256 );
00257
00262 VEXTERNC void Vpmgp_makeCoarse(
00263     int numLevel,
00264     int nxOld,
00265     int nyOld,
00266     int nzOld,
00267     int *nxNew,
00268     int *nyNew,
00269     int *nzNew
00270 );
00271
00272
00273
00274 #endif /* ifndef _VPMGP_H_ */

```

9.114 buildAd.c

```

00001
00055 #include "buildAd.h"
00056
00057 VPUBLIC void VbuildA(int* nx, int* ny, int* nz,
00058     int* ipkey, int* mgdisc, int* numdia,
00059     int* ipc, double* rpc,
00060     double* ac, double* cc, double* fc,
00061     double* xf, double* yf, double* zf,
00062     double* gxcf, double* gycf, double* gzcf,
00063     double* alcf, double* a2cf, double* a3cf,
00064     double* ccf, double* fcf) {
00065
00066     MAT2(ac, *nx * *ny * *nz, 14);
00067
00068     if (*mgdisc == 0) {
00069
00070         VbuildA_fv(nx, ny, nz,
00071             ipkey, numdia,
00072             ipc, rpc,
00073             RAT2(ac, 1,1), cc, fc,
00074             RAT2(ac, 1,2), RAT2(ac, 1,3), RAT2(ac, 1,4),
00075             xf, yf, zf,
00076             gxcf, gycf, gzcf,
00077             alcf, a2cf, a3cf,
00078             ccf, fcf);
00079
00080     } else if (*mgdisc == 1) {
00081
00082         VbuildA_fe(nx, ny, nz,
00083             ipkey, numdia,
00084             ipc, rpc,
00085             RAT2(ac, 1, 1), cc, fc,
00086             RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4), RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00087             RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1,10),
00088             RAT2(ac, 1,11), RAT2(ac, 1,12), RAT2(ac, 1,13), RAT2(ac, 1,14),
00089             xf, yf, zf,
00090             gxcf, gycf, gzcf,
00091             alcf, a2cf, a3cf,
00092             ccf, fcf);
00093
00094     } else {
00095
00096         Vnm_print(2, "VbuildA: Invalid discretization requested.\n");
00097         exit(EXIT_FAILURE);
00098     }

```



```

00099
00100     }
00101 }
00102
00103
00104
00105 VPUBLIC void VbuildA_fv(int *nx, int *ny, int *nz,
00106     int *ipkey, int *numdia,
00107     int *ipc, double *rpc,
00108     double *oC, double *cc, double *fc, double *oE, double *oN, double *uC,
00109     double *xf, double *yf, double *zf,
00110     double *gxcf, double *gycf, double *gzcf,
00111     double *alcf, double *a2cf, double *a3cf,
00112     double *ccf, double *fcf) {
00113
00114     int i, j, k;           // @todo Document this function
00115
00126     int ike, jke, kke;
00127
00128
00129     int nxml, nym1, nzml;
00130
00131
00132     double hx, hy, hz;
00133
00134
00135     double hxml, hym1, hzml;
00136
00137     double coef_fc;
00138
00139     double bc_cond_e;
00140     double bc_cond_w;
00141     double bc_cond_n;
00142     double bc_cond_s;
00143     double bc_cond_u;
00144     double bc_cond_d;
00145     double coef_oE;
00146     double coef_oN;
00147     double coef_uC;
00148     double coef_oEm1;
00149     double coef_oNm1;
00150     double coef_uCm1;
00151
00152     double diag;
00153
00154     MAT3( fc, *nx, *ny, *nz);
00155     MAT3( fcf, *nx, *ny, *nz);
00156     MAT3( cc, *nx, *ny, *nz);
00157     MAT3( ccf, *nx, *ny, *nz);
00158     MAT3( oC, *nx, *ny, *nz);
00159     MAT3( alcf, *nx, *ny, *nz);
00160     MAT3( a2cf, *nx, *ny, *nz);
00161     MAT3( a3cf, *nx, *ny, *nz);
00162     MAT3( uC, *nx, *ny, *nz);
00163     MAT3( oN, *nx, *ny, *nz);
00164     MAT3( oE, *nx, *ny, *nz);
00165     MAT3( gxcf, *ny, *nz, 2);
00166     MAT3( gyCF, *nx, *nz, 2);
00167     MAT3( gzcf, *nx, *ny, 2);
00168
00169     // Save the problem key with this operator. @todo: What?
00170     VAT(ipc, 10) = *ipkey;
00171
00172     // Note how many nonzeros in this discretization stencil
00173     VAT(ipc, 11) = 7;
00174     VAT(ipc, 12) = 1;
00175     *numdia = 4;
00176
00177     // Define n and determine number of mesh points
00178     nxml = *nx - 1;
00179     nym1 = *ny - 1;
00180     nzml = *nz - 1;
00181
00182     // Determine diag scale factor
00183     // (would like something close to ones on the main diagonal)
00184     // @todo: Make a more meaningful comment
00185     diag = 1.0;
00186
00187
00188
00189     /* *****

```

```

00190      * *** interior points ***
00191      * ***** */
00192
00193      // build the operator
00194      //fprintf(data, "%s\n", PRINT_FUNC);
00195      for(k=2; k<=*nz-1; k++) {
00196
00197          hzm1 = VAT(zf, k) - VAT(zf, k-1);
00198          hz   = VAT(zf, k+1) - VAT(zf, k);
00199
00200          for(j=2; j<=*ny-1; j++) {
00201
00202              hym1 = VAT(yf, j) - VAT(yf, j-1);
00203              hy   = VAT(yf, j+1) - VAT(yf, j);
00204
00205              for(i=2; i<=*nx-1; i++) {
00206
00207                  hxm1 = VAT(xf, i) - VAT(xf, i-1);
00208                  hx    = VAT(xf, i+1) - VAT(xf, i);
00209
00210                  // Calculate some coefficients
00211                  coef_oE = diag * (hym1 + hy) * (hzm1 + hz) / (4.0 * hx);
00212                  coef_oEm1 = diag * (hym1 + hy) * (hzm1 + hz) / (4.0 * hxm1);
00213                  coef_oN = diag * (hxm1 + hx) * (hzm1 + hz) / (4.0 * hy);
00214                  coef_oNm1 = diag * (hxm1 + hx) * (hzm1 + hz) / (4.0 * hym1);
00215                  coef_uC = diag * (hxm1 + hx) * (hym1 + hy) / (4.0 * hz);
00216                  coef_uCm1 = diag * (hxm1 + hx) * (hym1 + hy) / (4.0 * hzm1);
00217                  coef_fc = diag * (hxm1 + hx) * (hym1 + hy) * (hzm1 + hz) / 8.0;
00218
00219                  // Calculate the coefficient and source function
00220                  VAT3(fc, i, j, k) = coef_fc * VAT3(fcf, i, j, k);
00221                  VAT3(cc, i, j, k) = coef_fc * VAT3(ccf, i, j, k);
00222                  //fprintf(data, "%19.12E\n", VAT3(cc, i, j, k));
00223
00224                  // Calculate the diagonal for matvecs and smoothings
00225
00226                  VAT3(oC, i, j, k) = coef_oE * VAT3(alcf, i, j, k) +
00227                      coef_oEm1 * VAT3(alcf, i-1, j, k) +
00228                      coef_oN * VAT3(a2cf, i, j, k) +
00229                      coef_oNm1 * VAT3(a2cf, i, j-1, k) +
00230                      coef_uC * VAT3(a3cf, i, j, k) +
00231                      coef_uCm1 * VAT3(a3cf, i, j, k-1);
00232
00233                  //fprintf(data, "%19.12E\n", VAT3(oC, i, j, k));
00234
00235                  // Calculate the east neighbor
00236                  ike = VMIN2(1, VABS(i - nxm1));
00237                  VAT3(oE, i, j, k) = ike * coef_oE * VAT3(alcf, i, j, k);
00238                  //fprintf(data, "%19.12E\n", VAT3(oE, i, j, k));
00239                  bc_cond_e = (1 - ike) * coef_oE * VAT3(alcf, i, j, k) * VAT3(gxcf, j, k, 2);
00240                  VAT3(fc, i, j, k) += bc_cond_e;
00241
00242                  // Calculate the north neighbor
00243                  jke = VMIN2(1, VABS(j - nym1));
00244                  VAT3(oN, i, j, k) = jke * coef_oN * VAT3(a2cf, i, j, k);
00245                  //fprintf(data, "%19.12E\n", VAT3(oN, i, j, k));
00246                  bc_cond_n = (1 - jke) * coef_oN * VAT3(a2cf, i, j, k) * VAT3(gycf, i, k, 2);
00247                  VAT3(fc, i, j, k) += bc_cond_n;
00248
00249                  // Calculate the up neighbor
00250                  kke = VMIN2(1, VABS(k - nzm1));
00251                  VAT3(uC, i, j, k) = kke * coef_uC * VAT3(a3cf, i, j, k);
00252                  //fprintf(data, "%19.12E\n", VAT3(uC, i, j, k));
00253                  bc_cond_u = (1 - kke) * coef_uC * VAT3(a3cf, i, j, k) * VAT3(gzcf, i, j, 2);
00254                  VAT3(fc, i, j, k) += bc_cond_u;
00255
00256                  // Calculate the west neighbor (just handle b.c.)
00257                  ike = VMIN2(1, VABS(i - 2));
00258                  bc_cond_w = (1 - ike) * coef_oEm1 * VAT3(alcf, i-1, j, k) * VAT3(gxcf, j, k, 1);
00259                  VAT3(fc, i, j, k) += bc_cond_w;
00260
00261                  // Calculate the south neighbor (just handle b.c.)
00262                  jke = VMIN2(1, VABS(j - 2));
00263                  bc_cond_s = (1 - jke) * coef_oNm1 * VAT3(a2cf, i, j-1, k) * VAT3(gycf, i, k, 1);
00264                  VAT3(fc, i, j, k) += bc_cond_s;
00265
00266                  // Calculate the down neighbor (just handle b.c.)
00267                  kke = VMIN2(1, VABS(k - 2));
00268                  bc_cond_d = (1 - kke) * coef_uCm1 * VAT3(a3cf, i, j, k-1) * VAT3(gzcf, i, j, 1);
00269                  VAT3(fc, i, j, k) += bc_cond_d;
00270
00271
00272
00273
00274
00275
00276

```

```

00277             //fprintf(data, "%19.12E\n", VAT3(fc, i, j, k));
00278         }
00279     }
00280 }
00281 }
00282
00283
00284
00285 VPUBLIC void VbuildA_fe(int *nx, int *ny, int *nz,
00286     int *ipkey, int *numdia,
00287     int *ipc, double *rpc,
00288     double *oC, double *cc, double *fc,
00289     double *oE, double *oN, double *uC,
00290     double* oNE, double* oNW,
00291     double* uE, double* uW,
00292     double* uN, double* uS,
00293     double* uNE, double* uNW, double* uSE, double* uSW,
00294     double *xf, double *yf, double *zf,
00295     double *gxcf, double *gycf, double *gzcf,
00296     double *alcf, double *a2cf, double *a3cf,
00297     double *ccf, double *fcf) {
00298     VABORT_MSG0("Untranslated Component: from buildAd.f");
00299 }

```

9.115 buildAd.h

```

00001
00049 #ifndef _VBUILD_A_H_
00050 #define _VBUILD_A_H_
00051
00052 #include "apbscfg.h"
00053
00054 #include "malloc/malloc.h"
00055
00056 #include "generic/vhal.h"
00057 #include "generic/vmatrix.h"
00058
00064 VEXTERNC void VbuildA(
00065     int*    nx,
00066     int*    ny,
00067     int*    nz,
00068     int*    ipkey,
00069     int*    mgdisc,
00070     int*    numdia,
00071     int*    ipc,
00072     double* rpc,
00073     double* ac,
00074     double* cc,
00075     double* fc,
00076     double* xf,
00077     double* yf,
00078     double* zf,
00079     double* gxcf,
00080     double* gycf,
00081     double* gzcf,
00082     double* alcf,
00083     double* a2cf,
00084     double* a3cf,
00085     double* ccf,
00086     double* fcf
00087 );
00088
00089
00090
00161 VEXTERNC void VbuildA_fv(
00162     int*    nx,
00163     int*    ny,
00164     int*    nz,
00165     int*    ipkey,
00166     int*    numdia,
00167     int*    ipc,
00168     double* rpc,
00169     double* oC,
00170     double* cc,
00171     double* fc,
00172     double* oE,
00173     double* oN,
00174     double* uC,

```

```

00175         double* xf,
00176         double* yf,
00177         double* zf,
00178         double* gxcf,
00179         double* gycf,
00180         double* gzcf,
00181         double* alcf,
00182         double* a2cf,
00183         double* a3cf,
00184         double* ccf,
00185         double* fcf
00186     );
00187
00188
00266 VEXTERNC void VbuildA_fe(
00267     int*      nx,
00268     int*      ny,
00269     int*      nz,
00270     int*      ipkey,
00271     int*      numdia,
00272     int*      ipc,
00273     double*   rpc,
00274     double*   oC,
00275     double*   cc,
00276     double*   fc,
00277     double*   oE,
00278     double*   oN,
00279     double*   uC,
00280     double*   oNE,
00281     double*   oNW,
00282     double*   uE,
00283     double*   uW,
00284     double*   uN,
00285     double*   uS,
00286     double*   uNE,
00287     double*   uNW,
00288     double*   uSE,
00289     double*   uSW,
00290     double*   xf,
00291     double*   yf,
00292     double*   zf,
00293     double*   gxcf,
00294     double*   gycf,
00295     double*   gzcf,
00296     double*   alcf,
00297     double*   a2cf,
00298     double*   a3cf,
00299     double*   ccf,
00300     double*   fcf
00301 );
00302
00303
00304
00305
00306
00307
00308
00309
00310
00311
00312
00313 #endif /* _VBUILD_A_H_ */

```

9.116 buildBd.c

```

00001
00055 #include "buildBd.h"
00056
00057 VPUBLIC void Vbuildband(int *key, int *nx, int *ny, int *nz,
00058     int *ipc, double *rpc, double *ac,
00059     int *ipcB, double *rpcB, double *acB) {
00060
00061     int numdia;
00062     int n, m;
00063     int lda, info;
00064
00065     MAT2(ac, *nx * *ny * *nz, 1);
00066

```

```

00067 // Do in one step
00068 numdia = VAT(ipc, 11);
00069 if (numdia == 7) {
00070
00071     n = (*nx - 2) * (*ny - 2) * (*nz - 2);
00072     m = (*nx - 2) * (*ny - 2);
00073     lda = m + 1;
00074
00075     Vbuildband1_7
00076         (nx, ny, nz,
00077          ipc, rpc,
00078          RAT2(ac, 1, 1), RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
00079          ipcB, rpcB, acB,
00080          &n, &m, &lda);
00081
00082 } else if (numdia == 27) {
00083
00084     n = (*nx - 2) * (*ny - 2) * (*nz - 2);
00085     m = (*nx - 2) * (*ny - 2) + (*nx - 2) + 1;
00086     lda = m + 1;
00087
00088     Vbuildband1_27
00089         (nx, ny, nz,
00090          ipc, rpc,
00091          RAT2(ac, 1, 1), RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
00092          RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00093          RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1, 10),
00094          RAT2(ac, 1, 11), RAT2(ac, 1, 12), RAT2(ac, 1, 13), RAT2(ac, 1, 14),
00095          ipcB, rpcB, acB,
00096          &n, &m, &lda);
00097 } else {
00098     Vnm_print(2, "Vbuildband: invalid stencil type given...");
00099 }
00100
00101 // Factor the system
00102 *key = 0;
00103 info = 0;
00104
00105 Vdgbfa(acB, &lda, &n, &m, &info);
00106 VAT(ipcB, 4) = 1;
00107
00108 if (info != 0) {
00109
00110     Vnm_print(2, "Vbuildband: dgbfa problem: %d\n", info);
00111     Vnm_print(2, "Vbuildband: leading principle minor not PD...\n");
00112
00113     *key = 1;
00114 }
00115 }
00116
00117
00118
00119 VPUBLIC void Vbuildband1_7(int *nx, int *ny, int *nz,
00120                             int *ipc, double *rpc,
00121                             double *oC, double *oE, double *oN, double *uC,
00122                             int *ipcB, double *rpcB, double *acB,
00123                             int *n, int *m, int *lda) {
00124
00125     int i, j, k;
00126     int ii, jj, kk;
00127
00128     MAT2(acB, *lda, *ny-1);
00129
00130     MAT3(oC, *nx, *ny, *nz);
00131     MAT3(oE, *nx, *ny, *nz);
00132     MAT3(oN, *nx, *ny, *nz);
00133     MAT3(uC, *nx, *ny, *nz);
00134
00135     WARN_UNTESTED;
00136
00137     // Do it
00138     VAT(ipcB, 1) = *n;
00139     VAT(ipcB, 2) = *m;
00140     VAT(ipcB, 3) = *lda;
00141     VAT(ipcB, 4) = 0;
00142
00143     jj = 0;
00144
00145     //fprintf(data, "%s\n", PRINT_FUNC);
00146
00147     for (k=2; k<=*nz-1; k++) {

```

```

00148
00149     for (j=2; j<=*ny-1; j++) {
00150
00151         for (i=2; i<=*nx-1; i++) {
00152             jj++;
00153
00154             // Diagonal term
00155             ii = jj;
00156             kk = ii - jj + *m + 1;
00157
00158             VAT2(acB, kk, jj) = VAT3(oC, i, j, k);
00159
00160             // East neighbor
00161             ii = jj - 1;
00162             kk = ii - jj + *m + 1;
00163             VAT2(acB, kk, jj) = - VAT3(oE, i-1, j, k);
00164
00165             // North neighbor
00166             ii = jj - (*nx - 2);
00167             kk = ii - jj + *m + 1;
00168             VAT2(acB, kk, jj) = - VAT3(oN, i, j-1, k);
00169
00170             // Up neighbor ***
00171             ii = jj - (*nx - 2) * (*ny - 2);
00172             kk = ii - jj + *m + 1;
00173             VAT2(acB, kk, jj) = - VAT3(uC, i, j, k-1);
00174
00175             //fprintf(data, "%19.12E\n", VAT2(acB, kk, jj));
00176         }
00177     }
00178 }
00179 }
00180
00181
00182
00183 VPUBLIC void Vbuildband1_27(int *nx, int *ny, int *nz,
00184     int *ipc, double *rpc,
00185     double *oC, double *oE, double *oN, double *uC,
00186     double *oNE, double *oNW,
00187     double *uE, double *uW, double *uN, double *uS,
00188     double *uNE, double *uNW, double *uSE, double *uSW,
00189     int *ipcB, double *rpcB, double *acB,
00190     int *n, int *m, int *lda) {
00191
00192     int i, j, k;
00193     int ii, jj, kk;
00194
00195     MAT2(acB, *lda, *ny-1);
00196
00197     MAT3(oC, *nx, *ny, *nz);
00198     MAT3(oE, *nx, *ny, *nz);
00199     MAT3(oN, *nx, *ny, *nz);
00200     MAT3(uC, *nx, *ny, *nz);
00201
00202     MAT3(oNE, *nx, *ny, *nz);
00203     MAT3(oNW, *nx, *ny, *nz);
00204
00205     MAT3(uE, *nx, *ny, *nz);
00206     MAT3(uW, *nx, *ny, *nz);
00207     MAT3(uN, *nx, *ny, *nz);
00208     MAT3(uS, *nx, *ny, *nz);
00209
00210     MAT3(uNE, *nx, *ny, *nz);
00211     MAT3(uNW, *nx, *ny, *nz);
00212     MAT3(uSE, *nx, *ny, *nz);
00213     MAT3(uSW, *nx, *ny, *nz);
00214
00215     // Do it
00216     VAT(ipcB, 1) = *n;
00217     VAT(ipcB, 2) = *m;
00218     VAT(ipcB, 3) = *lda;
00219     VAT(ipcB, 4) = 0;
00220
00221     jj = 0;
00222
00223     //fprintf(data, "%s\n", PRINT_FUNC);
00224
00225     for (k=2; k<=*nz-1; k++) {
00226
00227         for (j=2; j<=*ny-1; j++) {
00228

```

```

00229         for (i=2; i<=*nx-1; i++) {
00230             jj++;
00231
00232             // Diagonal term
00233             ii = jj;
00234             kk = ii - jj + *m + 1;
00235             VAT2(acB, kk, jj) = VAT3(oC, i, j, k);
00236
00237             // East neighbor
00238             ii = jj - 1;
00239             kk = ii - jj + *m + 1;
00240             VAT2(acB, kk, jj) = - VAT3(oE, i-1, j, k);
00241
00242             // North neighbor
00243             ii = jj - (*nx - 2);
00244             kk = ii - jj + *m + 1;
00245             VAT2(acB, kk, jj) = - VAT3(oN, i, j-1, k);
00246
00247             // North-east neighbor
00248             ii = jj - (*nx - 2) + 1;
00249             kk = ii - jj + *m + 1;
00250             VAT2(acB, kk, jj) = - VAT3(oNE, i, j-1, k);
00251
00252             // North-west neighbor
00253             ii = jj - (*nx - 2) - 1;
00254             kk = ii - jj + *m + 1;
00255             VAT2(acB, kk, jj) = - VAT3(oNW, i, j-1, k);
00256
00257             // Up neighbor
00258             ii = jj - (*nx - 2) * (*ny - 2);
00259             kk = ii - jj + *m + 1;
00260             VAT2(acB, kk, jj) = - VAT3(uC, i, j, k-1);
00261
00262             // Up-east neighbor
00263             ii = jj - (*nx - 2) * (*ny - 2) + 1;
00264             kk = ii - jj + *m + 1;
00265             VAT2(acB, kk, jj) = - VAT3(uE, i, j, k-1);
00266
00267             // Up-west neighbor
00268             ii = jj - (*nx - 2) * (*ny - 2) - 1;
00269             kk = ii - jj + *m + 1;
00270             VAT2(acB, kk, jj) = - VAT3(uW, i, j, k-1);
00271
00272             // Up-north neighbor
00273             ii = jj - (*nx - 2) * (*ny - 2) + (*nx - 2);
00274             kk = ii - jj + *m + 1;
00275             VAT2(acB, kk, jj) = - VAT3(uN, i, j, k-1);
00276
00277             // Up-south neighbor
00278             ii = jj - (*nx - 2) * (*ny - 2) - (*nx - 2);
00279             kk = ii - jj + *m + 1;
00280             VAT2(acB, kk, jj) = - VAT3(uS, i, j, k-1);
00281
00282             // Up-north-east neighbor
00283             ii = jj - (*nx - 2) * (*ny - 2) + (*nx - 2) + 1;
00284             kk = ii - jj + *m + 1;
00285             VAT2(acB, kk, jj) = - VAT3(uNE, i, j, k-1);
00286
00287             // Up-north-west neighbor
00288             ii = jj - (*nx - 2) * (*ny - 2) + (*nx - 2) - 1;
00289             kk = ii - jj + *m + 1;
00290             VAT2(acB, kk, jj) = - VAT3(uNW, i, j, k-1);
00291
00292             // Up-south-east neighbor
00293             ii = jj - (*nx - 2) * (*ny - 2) - (*nx - 2) + 1;
00294             kk = ii - jj + *m + 1;
00295             VAT2(acB, kk, jj) = - VAT3(uSE, i, j, k-1);
00296
00297             // Up-south-west neighbor
00298             ii = jj - (*nx - 2) * (*ny - 2) - (*nx - 2) - 1;
00299             kk = ii - jj + *m + 1;
00300             VAT2(acB, kk, jj) = - VAT3(uSW, i, j, k-1);
00301
00302             //fprintf(data, "%19.12E\n", VAT2(acB, kk, jj));
00303         }
00304     }
00305 }
00306 }

```

9.117 buildBd.h

```

00001
00049 #ifndef _BUILDBD_H_
00050 #define _BUILDBD_H_
00051
00052 #include "apbscfg.h"
00053
00054 #include "malloc/malloc.h"
00055
00056 #include "generic/vhal.h"
00057 #include "generic/vmatrix.h"
00058 #include "pmgc/mlinpckd.h"
00059
00065 VEXTERNC void Vbuildband(
00066     int *key,
00067     int *nx,
00068     int *ny,
00069     int *nz,
00070     int *ipc,
00071     double *rpc,
00072     double *ac,
00073     int *ipcB,
00074     double *rpcB,
00075     double *acB
00076 );
00077
00083 VEXTERNC void Vbuildband1_7(
00084     int *nx,
00085     int *ny,
00086     int *nz,
00087     int *ipc,
00088     double *rpc,
00089     double *oC,
00090     double *oE,
00091     double *oN,
00092     double *uC,
00093     int *ipcB,
00094     double *rpcB,
00095     double *acB,
00096     int *n,
00097     int *m,
00098     int *lda
00099 );
00100
00106 VEXTERNC void Vbuildband1_27(
00107     int *nx,
00108     int *ny,
00109     int *nz,
00110     int *ipc,
00111     double *rpc,
00112     double *oC,
00113     double *oE,
00114     double *oN,
00115     double *uC,
00116     double *oNE,
00117     double *oNW,
00118     double *uE,
00119     double *uW,
00120     double *uN,
00121     double *uS,
00122     double *uNE,
00123     double *uNW,
00124     double *uSE,
00125     double *uSW,
00126     int *ipcB,
00127     double *rpcB,
00128     double *acB,
00129     int *n,
00130     int *m,
00131     int *lda
00132 );
00133
00134 #endif /* _BUILDBD_H_ */

```

9.118 buildGd.c

```

00001

```



```

00055 #include "buildGd.h"
00056
00057 VPUBLIC void VbuildG(int *nxf, int *nyf, int *nzf,
00058                     int *nxc, int *nyc, int *nzc,
00059                     int *numdia,
00060                     double *pcFF, double *acFF, double *ac) {
00061
00062     MAT2(pcFF, *nxc * *nyc * *nzc, 27);
00063     MAT2(acFF, *nxf * *nyf * *nzf, 27);
00064     MAT2( ac, *nxc * *nyc * *nzc, 27);
00065
00066     // Call the build routine ***
00067     if (*numdia == 1) {
00068
00069         VbuildG_1(
00070
00071             nxf, nyf, nzf, nxc, nyc, nzc,
00072
00073             RAT2(pcFF, 1, 1), RAT2(pcFF, 1, 2), RAT2(pcFF, 1, 3), RAT2(pcFF, 1, 4), RAT2(pcFF, 1,
00074 5),
00075             RAT2(pcFF, 1, 6), RAT2(pcFF, 1, 7), RAT2(pcFF, 1, 8), RAT2(pcFF, 1, 9),
00076             RAT2(pcFF, 1, 10), RAT2(pcFF, 1, 11), RAT2(pcFF, 1, 12), RAT2(pcFF, 1, 13), RAT2(pcFF, 1,
00077 14),
00078             RAT2(pcFF, 1, 15), RAT2(pcFF, 1, 16), RAT2(pcFF, 1, 17), RAT2(pcFF, 1, 18),
00079             RAT2(pcFF, 1, 19), RAT2(pcFF, 1, 20), RAT2(pcFF, 1, 21), RAT2(pcFF, 1, 22), RAT2(pcFF, 1,
00080 23),
00081             RAT2(pcFF, 1, 24), RAT2(pcFF, 1, 25), RAT2(pcFF, 1, 26), RAT2(pcFF, 1, 27),
00082             RAT2(acFF, 1, 1),
00083             RAT2(ac, 1, 1), RAT2(ac, 1, 2), RAT2(ac, 1, 3),
00084             RAT2(ac, 1, 4),
00085             RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00086             RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1, 10),
00087             RAT2(ac, 1, 11), RAT2(ac, 1, 12), RAT2(ac, 1, 13), RAT2(ac, 1, 14)
00088         );
00089
00090     } else if (*numdia == 7) {
00091
00092         VbuildG_7(
00093
00094             nxf, nyf, nzf,
00095             nxc, nyc, nzc,
00096
00097             RAT2(pcFF, 1, 1), RAT2(pcFF, 1, 2), RAT2(pcFF, 1, 3), RAT2(pcFF, 1, 4), RAT2(pcFF, 1,
00098 5),
00099             RAT2(pcFF, 1, 6), RAT2(pcFF, 1, 7), RAT2(pcFF, 1, 8), RAT2(pcFF, 1, 9),
00100             RAT2(pcFF, 1, 10), RAT2(pcFF, 1, 11), RAT2(pcFF, 1, 12), RAT2(pcFF, 1, 13), RAT2(pcFF, 1,
00101 14),
00102             RAT2(pcFF, 1, 15), RAT2(pcFF, 1, 16), RAT2(pcFF, 1, 17), RAT2(pcFF, 1, 18),
00103             RAT2(pcFF, 1, 19), RAT2(pcFF, 1, 20), RAT2(pcFF, 1, 21), RAT2(pcFF, 1, 22), RAT2(pcFF, 1,
00104 23),
00105             RAT2(pcFF, 1, 24), RAT2(pcFF, 1, 25), RAT2(pcFF, 1, 26), RAT2(pcFF, 1, 27),
00106             RAT2(acFF, 1, 1), RAT2(acFF, 1, 2), RAT2(acFF, 1, 3), RAT2(acFF, 1, 4),
00107             RAT2(ac, 1, 1), RAT2(ac, 1, 2), RAT2(ac, 1, 3),
00108             RAT2(ac, 1, 4),
00109             RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00110             RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1, 10),
00111             RAT2(ac, 1, 11), RAT2(ac, 1, 12), RAT2(ac, 1, 13), RAT2(ac, 1, 14)
00112         );
00113
00114     } else if (*numdia == 27) {
00115
00116         VbuildG_27(
00117
00118             nxf, nyf, nzf,
00119             nxc, nyc, nzc,
00120
00121             RAT2(pcFF, 1, 1), RAT2(pcFF, 1, 2), RAT2(pcFF, 1, 3), RAT2(pcFF, 1, 4), RAT2(pcFF, 1,
00122 5),
00123             RAT2(pcFF, 1, 6), RAT2(pcFF, 1, 7), RAT2(pcFF, 1, 8), RAT2(pcFF, 1, 9),
00124             RAT2(pcFF, 1, 10), RAT2(pcFF, 1, 11), RAT2(pcFF, 1, 12), RAT2(pcFF, 1, 13), RAT2(pcFF, 1,
00125 14),
00126             RAT2(pcFF, 1, 15), RAT2(pcFF, 1, 16), RAT2(pcFF, 1, 17), RAT2(pcFF, 1, 18),
00127             RAT2(pcFF, 1, 19), RAT2(pcFF, 1, 20), RAT2(pcFF, 1, 21), RAT2(pcFF, 1, 22), RAT2(pcFF, 1,
00128 23),
00129             RAT2(pcFF, 1, 24), RAT2(pcFF, 1, 25), RAT2(pcFF, 1, 26), RAT2(pcFF, 1, 27),

```

```

00127
00128         RAT2(acFF, 1, 1), RAT2(acFF, 1, 2), RAT2(acFF, 1, 3), RAT2(acFF, 1, 4),
00129         RAT2(acFF, 1, 5), RAT2(acFF, 1, 6), RAT2(acFF, 1, 7), RAT2(acFF, 1, 8), RAT2(acFF, 1,
9),
00130         RAT2(acFF, 1, 10), RAT2(acFF, 1, 11), RAT2(acFF, 1, 12), RAT2(acFF, 1, 13), RAT2(acFF, 1,
14),
00131
00132         RAT2(ac, 1, 1), RAT2(ac, 1, 2), RAT2(ac, 1, 3),
00133         RAT2(ac, 1, 4),
00134         RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00135         RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1, 10),
00136         RAT2(ac, 1, 11), RAT2(ac, 1, 12), RAT2(ac, 1, 13), RAT2(ac, 1, 14)
00137     );
00138 }
00139
00140 } else {
00141     Vnm_print(2, "BUILDG: invalid stencil type given...\n");
00142 }
00143 }
00144
00145 VPUBLIC void VbuildG_1(int *nxf, int *nyf, int *nzf,
00146     int *nx, int *ny, int *nz,
00147     double *oPC, double *oPN, double *oPS, double *oPE, double *oPW,
00148     double *oPNE, double *oPNW, double *oPSE, double *oPSW,
00149     double *uPC, double *uPN, double *uPS, double *uPE, double *uPW,
00150     double *uPNE, double *uPNW, double *uPSE, double *uPSW,
00151     double *dPC, double *dPN, double *dPS, double *dPE, double *dPW,
00152     double *dPNE, double *dPNW, double *dPSE, double *dPSW,
00153     double *oC,
00154     double *XoC, double *XoE, double *XoN,
00155     double *XuC,
00156     double *XoNE, double *XoNW,
00157     double *XuE, double *XuW, double *XuN, double *XuS,
00158     double *XuNE, double *XuNW, double *XuSE, double *XuSW
00159 ) {
00160
00161     int i, j, k, ii, jj, kk;
00162     int iml, ipl, jml, jpl, kml, kpl;
00163     int iiml, iipl, jjml, jjpl, kkml, kkpl;
00164     int nxml, nym1, nzml;
00165
00166     double TMP1_XOC, TMP2_XOC, TMP3_XOC;
00167
00168     MAT3( oC, *nxf, *nyf, *nzf);
00169
00170     MAT3( XoC, *nx, *ny, *nz);
00171     MAT3( XoE, *nx, *ny, *nz);
00172     MAT3( XoN, *nx, *ny, *nz);
00173
00174     MAT3( XuC, *nx, *ny, *nz);
00175
00176     MAT3(XoNE, *nx, *ny, *nz);
00177     MAT3(XoNW, *nx, *ny, *nz);
00178
00179     MAT3( XuE, *nx, *ny, *nz);
00180     MAT3( XuW, *nx, *ny, *nz);
00181     MAT3( XuN, *nx, *ny, *nz);
00182     MAT3( XuS, *nx, *ny, *nz);
00183     MAT3(XuNE, *nx, *ny, *nz);
00184     MAT3(XuNW, *nx, *ny, *nz);
00185     MAT3(XuSE, *nx, *ny, *nz);
00186     MAT3(XuSW, *nx, *ny, *nz);
00187
00188     MAT3( oPC, *nx, *ny, *nz);
00189     MAT3( oPN, *nx, *ny, *nz);
00190     MAT3( oPS, *nx, *ny, *nz);
00191     MAT3( oPE, *nx, *ny, *nz);
00192     MAT3( oPW, *nx, *ny, *nz);
00193     MAT3( oPNE, *nx, *ny, *nz);
00194     MAT3( oPNW, *nx, *ny, *nz);
00195     MAT3( oPSE, *nx, *ny, *nz);
00196     MAT3( oPSW, *nx, *ny, *nz);
00197
00198     MAT3( uPC, *nx, *ny, *nz);
00199     MAT3( uPN, *nx, *ny, *nz);
00200     MAT3( uPS, *nx, *ny, *nz);
00201     MAT3( uPE, *nx, *ny, *nz);
00202     MAT3( uPW, *nx, *ny, *nz);
00203     MAT3( uPNE, *nx, *ny, *nz);
00204     MAT3( uPNW, *nx, *ny, *nz);
00205     MAT3( uPSE, *nx, *ny, *nz);

```

```

00206     MAT3(uPSW, *nx, *ny, *nz);
00207
00208     MAT3( dPC, *nx, *ny, *nz);
00209     MAT3( dPN, *nx, *ny, *nz);
00210     MAT3( dPS, *nx, *ny, *nz);
00211     MAT3( dPE, *nx, *ny, *nz);
00212     MAT3( dPW, *nx, *ny, *nz);
00213     MAT3(dPNE, *nx, *ny, *nz);
00214     MAT3(dPNW, *nx, *ny, *nz);
00215     MAT3(dPSE, *nx, *ny, *nz);
00216     MAT3(dPSW, *nx, *ny, *nz);
00217
00218     // Define n and determine number of mesh points
00219     nxm1 = *nx - 1;
00220     nym1 = *ny - 1;
00221     nzm1 = *nz - 1;
00222
00223     //fprintf(data, "%s\n", PRINT_FUNC);
00224
00225     // Build the operator
00226     for(kk=2; kk<=*nz-1; kk++) {
00227         k = 2 * kk - 1;
00228
00229         for(jj=2; jj<=*ny-1; jj++) {
00230             j = 2 * jj - 1;
00231
00232             for(ii=2; ii<=*nx-1; i++) {
00233                 i = 2 * ii - 1;
00234
00235                 // Index computations
00236                 im1 = i - 1;
00237                 ip1 = i + 1;
00238                 jml = j - 1;
00239                 jpl = j + 1;
00240                 kml = k - 1;
00241                 kpl = k + 1;
00242                 iim1 = ii - 1;
00243                 iip1 = ii + 1;
00244                 jjm1 = jj - 1;
00245                 jjp1 = jj + 1;
00246                 kkm1 = kk - 1;
00247                 kkp1 = kk + 1;
00248
00249                 /* *****
00250                  * oC
00251                  * *****/
00252
00253                 // XoC(ii,jj,kk) =
00254                 TMP1_XOC =
00255                     VAT3( uPS, ii, jj, kk) * VAT3( uPS, ii, jj, kk) * VAT3( oC, i, jml, kpl)
00256                     + VAT3( dPSW, ii, jj, kk) * VAT3( dPSW, ii, jj, kk) * VAT3( oC, im1, jml, kml)
00257                     + VAT3( oPSW, ii, jj, kk) * VAT3( oPSW, ii, jj, kk) * VAT3( oC, im1, jml, k)
00258                     + VAT3( uPSW, ii, jj, kk) * VAT3( uPSW, ii, jj, kk) * VAT3( oC, im1, jml, kpl)
00259                     + VAT3( dPW, ii, jj, kk) * VAT3( dPW, ii, jj, kk) * VAT3( oC, im1, j, kml)
00260                     + VAT3( oPW, ii, jj, kk) * VAT3( oPW, ii, jj, kk) * VAT3( oC, im1, j, k)
00261                     + VAT3( uPNW, ii, jj, kk) * VAT3( uPNW, ii, jj, kk) * VAT3( oC, im1, jpl, kpl)
00262                     + VAT3( dPS, ii, jj, kk) * VAT3( dPS, ii, jj, kk) * VAT3( oC, i, jml, kml)
00263                     + VAT3( oPS, ii, jj, kk) * VAT3( oPS, ii, jj, kk) * VAT3( oC, i, jml, k);
00264
00265                 TMP2_XOC =
00266                     VAT3( dPC, ii, jj, kk) * VAT3( dPC, ii, jj, kk) * VAT3( oC, i, j, kml)
00267                     + VAT3( oPC, ii, jj, kk) * VAT3( oPC, ii, jj, kk) * VAT3( oC, i, j, k)
00268                     + VAT3( uPC, ii, jj, kk) * VAT3( uPC, ii, jj, kk) * VAT3( oC, i, j, kpl)
00269                     + VAT3( dPN, ii, jj, kk) * VAT3( dPN, ii, jj, kk) * VAT3( oC, i, jpl, kml)
00270                     + VAT3( oPN, ii, jj, kk) * VAT3( oPN, ii, jj, kk) * VAT3( oC, i, jpl, k)
00271                     + VAT3( uPW, ii, jj, kk) * VAT3( uPW, ii, jj, kk) * VAT3( oC, im1, j, kpl)
00272                     + VAT3( dPNW, ii, jj, kk) * VAT3( dPNW, ii, jj, kk) * VAT3( oC, im1, jpl, kml)
00273                     + VAT3( oPNW, ii, jj, kk) * VAT3( oPNW, ii, jj, kk) * VAT3( oC, im1, jpl, k)
00274                     + VAT3( oPE, ii, jj, kk) * VAT3( oPE, ii, jj, kk) * VAT3( oC, ip1, j, k);
00275
00276                 TMP3_XOC =
00277                     VAT3( uPE, ii, jj, kk) * VAT3( uPE, ii, jj, kk) * VAT3( oC, ip1, j, kpl)
00278                     + VAT3( dPNE, ii, jj, kk) * VAT3( dPNE, ii, jj, kk) * VAT3( oC, ip1, jpl, kml)
00279                     + VAT3( oPNE, ii, jj, kk) * VAT3( oPNE, ii, jj, kk) * VAT3( oC, ip1, jpl, k)
00280                     + VAT3( uPNE, ii, jj, kk) * VAT3( uPNE, ii, jj, kk) * VAT3( oC, ip1, jpl, kpl)
00281                     + VAT3( uPN, ii, jj, kk) * VAT3( uPN, ii, jj, kk) * VAT3( oC, i, jpl, kpl)
00282                     + VAT3( dPSE, ii, jj, kk) * VAT3( dPSE, ii, jj, kk) * VAT3( oC, ip1, jml, kml)
00283                     + VAT3( oPSE, ii, jj, kk) * VAT3( oPSE, ii, jj, kk) * VAT3( oC, ip1, jml, k)
00284                     + VAT3( uPSE, ii, jj, kk) * VAT3( uPSE, ii, jj, kk) * VAT3( oC, ip1, jml, kpl)
00285                     + VAT3( dPE, ii, jj, kk) * VAT3( dPE, ii, jj, kk) * VAT3( oC, ip1, j, kml);
00286

```

```

00287     VAT3( XoC, ii,jj,kk) = TMP1_XOC + TMP2_XOC + TMP3_XOC;
00288
00289     //fprintf(data, "%19.12E\n", VAT3(XoC, ii, jj, kk));
00290
00291     /* *****
00292      * *** > oE;
00293      * *****/
00294
00295     VAT3( XoE, ii,jj,kk) =
00296         - VAT3(dPSE, ii,jj,kk) * VAT3( oC, ip1,jm1,km1) * VAT3(dPSW, iip1,jj,kk)
00297         - VAT3(oPSE, ii,jj,kk) * VAT3( oC, ip1,jm1,k) * VAT3(oPSW, iip1,jj,kk)
00298         - VAT3(uPSE, ii,jj,kk) * VAT3( oC, ip1,jm1,kp1) * VAT3(uPSW, iip1,jj,kk)
00299         - VAT3( dPE, ii,jj,kk) * VAT3( oC, ip1,j,km1) * VAT3( dPW, iip1,jj,kk)
00300         - VAT3( oPE, ii,jj,kk) * VAT3( oC, ip1,j,k) * VAT3( oPW, iip1,jj,kk)
00301         - VAT3( uPE, ii,jj,kk) * VAT3( oC, ip1,j,kp1) * VAT3( uPW, iip1,jj,kk)
00302         - VAT3(dPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,km1) * VAT3(dPNW, iip1,jj,kk)
00303         - VAT3(oPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,k) * VAT3(oPNW, iip1,jj,kk)
00304         - VAT3(uPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,kp1) * VAT3(uPNW, iip1,jj,kk);
00305
00306     //fprintf(data, "%19.12E\n", VAT3(XoE, ii, jj, kk));
00307
00308     /* *****
00309      * *** > oN;
00310      * *****/
00311
00312     VAT3( XoN, ii,jj,kk) =
00313         - VAT3(dPNW, ii,jj,kk) * VAT3( oC, im1,jp1,km1) * VAT3(dPSW, ii,jjp1,kk)
00314         - VAT3(oPNW, ii,jj,kk) * VAT3( oC, im1,jp1,k) * VAT3(oPSW, ii,jjp1,kk)
00315         - VAT3(uPNW, ii,jj,kk) * VAT3( oC, im1,jp1,kp1) * VAT3(uPSW, ii,jjp1,kk)
00316         - VAT3( dPN, ii,jj,kk) * VAT3( oC, i,jp1,km1) * VAT3( dPS, ii,jjp1,kk)
00317         - VAT3( oPN, ii,jj,kk) * VAT3( oC, i,jp1,k) * VAT3( oPS, ii,jjp1,kk)
00318         - VAT3( uPN, ii,jj,kk) * VAT3( oC, i,jp1,kp1) * VAT3( uPS, ii,jjp1,kk)
00319         - VAT3(dPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,km1) * VAT3(dPSE, ii,jjp1,kk)
00320         - VAT3(oPNE, ii,jj,kk) * VAT3( oC, ip1,jp1, k) * VAT3(oPSE, ii,jjp1,kk)
00321         - VAT3(uPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,kp1) * VAT3(uPSE, ii,jjp1,kk);
00322
00323     //fprintf(data, "%19.12E\n", VAT3(XoN, ii, jj, kk));
00324
00325     /* *****
00326      * *** > uC;
00327      * *****/
00328
00329     VAT3( XuC, ii,jj,kk) =
00330         - VAT3(dPSW, ii,jj,kkp1) * VAT3( oC, im1,jm1,kp1) * VAT3(uPSW, ii,jj,kk)
00331         - VAT3( dPW, ii,jj,kkp1) * VAT3( oC, im1,j,kp1) * VAT3( uPW, ii,jj,kk)
00332         - VAT3(dPNW, ii,jj,kkp1) * VAT3( oC, im1,jp1,kp1) * VAT3(uPNW, ii,jj,kk)
00333         - VAT3( dPS, ii,jj,kkp1) * VAT3( oC, i,jm1,kp1) * VAT3( uPS, ii,jj,kk)
00334         - VAT3( dPC, ii,jj,kkp1) * VAT3( oC, i,j,kp1) * VAT3( uPC, ii,jj,kk)
00335         - VAT3( dPN, ii,jj,kkp1) * VAT3( oC, i,jp1,kp1) * VAT3( uPN, ii,jj,kk)
00336         - VAT3(dPSE, ii,jj,kkp1) * VAT3( oC, ip1,jm1,kp1) * VAT3(uPSE, ii,jj,kk)
00337         - VAT3( dPE, ii,jj,kkp1) * VAT3( oC, ip1,j,kp1) * VAT3( uPE, ii,jj,kk)
00338         - VAT3(dPNE, ii,jj,kkp1) * VAT3( oC, ip1,jp1,kp1) * VAT3(uPNE, ii,jj,kk);
00339
00340     //fprintf(data, "%19.12E\n", VAT3(XuC, ii, jj, kk));
00341
00342     /* *****
00343      * *** > oNE;
00344      * *****/
00345
00346     VAT3(XoNE, ii,jj,kk) =
00347         - VAT3(dPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,km1) * VAT3(dPSW, iip1,jjp1,kk)
00348         - VAT3(oPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,k) * VAT3(oPSW, iip1,jjp1,kk)
00349         - VAT3(uPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,kp1) * VAT3(uPSW, iip1,jjp1,kk);
00350
00351     //fprintf(data, "%19.12E\n", VAT3(XoNE, ii, jj, kk));
00352
00353     /* *****
00354      * *** > oNW;
00355      * *****/
00356
00357     VAT3(XoNW, ii,jj,kk) =
00358         - VAT3(dPNW, ii,jj,kk) * VAT3( oC, im1,jp1,km1) * VAT3(dPSE, iim1,jjp1,kk)
00359         - VAT3(oPNW, ii,jj,kk) * VAT3( oC, im1,jp1,k) * VAT3(oPSE, iim1,jjp1,kk)
00360         - VAT3(uPNW, ii,jj,kk) * VAT3( oC, im1,jp1,kp1) * VAT3(uPSE, iim1,jjp1,kk);
00361
00362     //fprintf(data, "%19.12E\n", VAT3(XoNW, ii, jj, kk));
00363
00364     /* *****
00365      * *** > uE;
00366      * *****/
00367

```

```

00368
00369 VAT3( XuE, ii,jj,kk) =
00370     - VAT3(uPSE, ii,jj,kk) * VAT3( oC, ip1,jm1,kp1) * VAT3(dPSW, iip1,jj,kkp1)
00371     - VAT3( uPE, ii,jj,kk) * VAT3( oC, ip1,j,kp1) * VAT3( dPW, iip1,jj,kkp1)
00372     - VAT3(uPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,kp1) * VAT3(dPNW, iip1,jj,kkp1);
00373
00374 //fprintf(data, "%19.12E\n", VAT3(XuE, ii, jj, kk));
00375
00376 /* *****
00377  * *** > uW;
00378  * *****/
00379
00380 VAT3( XuW, ii,jj,kk) =
00381     - VAT3(uPSW, ii,jj,kk) * VAT3( oC, im1,jm1,kp1) * VAT3(dPSE, iim1,jj,kkp1)
00382     - VAT3( uPW, ii,jj,kk) * VAT3( oC, im1,j,kp1) * VAT3( dPE, iim1,jj,kkp1)
00383     - VAT3(uPNW, ii,jj,kk) * VAT3( oC, im1,jp1,kp1) * VAT3(dPNE, iim1,jj,kkp1);
00384
00385 //fprintf(data, "%19.12E\n", VAT3(XuW, ii, jj, kk));
00386
00387 /* *****
00388  * *** > uN;
00389  * *****/
00390
00391 VAT3( XuN, ii,jj,kk) =
00392     - VAT3(uPNW, ii,jj,kk) * VAT3( oC, im1,jp1,kp1) * VAT3(dPSW, ii,jjp1,kkp1)
00393     - VAT3( uPN, ii,jj,kk) * VAT3( oC, i,jp1,kp1) * VAT3( dPS, ii,jjp1,kkp1)
00394     - VAT3(uPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,kp1) * VAT3(dPSE, ii,jjp1,kkp1);
00395
00396 //fprintf(data, "%19.12E\n", VAT3(XuN, ii, jj, kk));
00397
00398 /* *****
00399  * *** > uS;
00400  * *****/
00401
00402 VAT3( XuS, ii,jj,kk) =
00403     - VAT3(uPSW, ii,jj,kk) * VAT3( oC, im1,jm1,kp1) * VAT3(dPNW, ii,jjml,kkp1)
00404     - VAT3( uPS, ii,jj,kk) * VAT3( oC, i,jm1,kp1) * VAT3( dPN, ii,jjml,kkp1)
00405     - VAT3(uPSE, ii,jj,kk) * VAT3( oC, ip1,jm1,kp1) * VAT3(dPNE, ii,jjml,kkp1);
00406
00407 //fprintf(data, "%19.12E\n", VAT3(XuS, ii, jj, kk));
00408
00409 /* *****
00410  * *** > uNE;
00411  * *****/
00412
00413 VAT3(XuNE, ii,jj,kk) =
00414     - VAT3(uPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,kp1) * VAT3(dPSW, iip1,jjp1,kkp1);
00415
00416 //fprintf(data, "%19.12E\n", VAT3(XuNE, ii, jj, kk));
00417
00418 /* *****
00419  * *** > uNW;
00420  * *****/
00421
00422 VAT3(XuNW, ii,jj,kk) =
00423     - VAT3(uPNW, ii,jj,kk) * VAT3( oC, im1,jp1,kp1) * VAT3(dPSE, iim1,jjp1,kkp1);
00424
00425 //fprintf(data, "%19.12E\n", VAT3(XuNW, ii, jj, kk));
00426
00427 /* *****
00428  * *** > uSE;
00429  * *****/
00430
00431 VAT3(XuSE, ii,jj,kk) =
00432     - VAT3(uPSE, ii,jj,kk) * VAT3( oC, ip1,jm1,kp1) * VAT3(dPNW, iip1,jjml,kkp1);
00433
00434 //fprintf(data, "%19.12E\n", VAT3(XuSE, ii, jj, kk));
00435
00436 /* *****
00437  * *** > uSW;
00438  * *****/
00439
00440 VAT3(XuSW, ii,jj,kk) =
00441     - VAT3(uPSW, ii,jj,kk) * VAT3( oC, im1,jm1,kp1) * VAT3(dPNE, iim1,jjml,kkp1);
00442
00443 //fprintf(data, "%19.12E\n", VAT3(XuSW, ii, jj, kk));
00444
00445 }
00446 }
00447 }
00448 }

```

```

00449
00450 VPUBLIC void VbuildG_7(int *nxf, int *nyf, int *nzf,
00451     int *nx, int *ny, int *nz,
00452     double *oPC, double *oPN, double *oPS, double *oPE, double *oPW,
00453     double *oPNE, double *oPNW, double *oPSE, double *oPSW,
00454     double *uPC, double *uPN, double *uPS, double *uPE, double *uPW,
00455     double *uPNE, double *uPNW, double *uPSE, double *uPSW,
00456     double *dPC, double *dPN, double *dPS, double *dPE, double *dPW,
00457     double *dPNE, double *dPNW, double *dPSE, double *dPSW,
00458     double *oC, double *oE, double *oN, double *uC,
00459     double *XoC, double *XoE, double *XoN,
00460     double *XuC,
00461     double *XoNE, double *XoNW,
00462     double *XuE, double *XuW, double *XuN, double *XuS,
00463     double *XuNE, double *XuNW, double *XuSE, double *XuSW) {
00464
00465     int i, j, k;
00466     int ii, jj, kk;
00467     int i1, i1, i2, ip2;
00468     int j1, j1, j2, jp2;
00469     int k1, k1, k2, kp2;
00470     int i1, i1;
00471     int j1, j1;
00472     int k1, k1;
00473     int nx1, ny1, nz1;
00474
00475     double TMP1_XOC, TMP2_XOC, TMP3_XOC, TMP4_XOC;
00476     double TMP5_XOC, TMP6_XOC, TMP7_XOC, TMP8_XOC;
00477     double TMP9_XOC;
00478     double TMP1_XOE, TMP2_XOE, TMP3_XOE, TMP4_XOE;
00479     double TMP1_XON, TMP2_XON, TMP3_XON, TMP4_XON;
00480     double TMP1_XUC, TMP2_XUC, TMP3_XUC, TMP4_XUC;
00481
00482     MAT3( oC, *nxf, *nyf, *nzf);
00483     MAT3( oE, *nxf, *nyf, *nzf);
00484     MAT3( oN, *nxf, *nyf, *nzf);
00485
00486     MAT3( uC, *nxf, *nyf, *nzf);
00487
00488     MAT3( XoC, *nx, *ny, *nz);
00489     MAT3( XoE, *nx, *ny, *nz);
00490     MAT3( XoN, *nx, *ny, *nz);
00491     MAT3(XoNE, *nx, *ny, *nz);
00492     MAT3(XoNW, *nx, *ny, *nz);
00493
00494     MAT3( XuC, *nx, *ny, *nz);
00495     MAT3( XuE, *nx, *ny, *nz);
00496     MAT3( XuW, *nx, *ny, *nz);
00497     MAT3( XuN, *nx, *ny, *nz);
00498     MAT3( XuS, *nx, *ny, *nz);
00499     MAT3(XuNE, *nx, *ny, *nz);
00500     MAT3(XuNW, *nx, *ny, *nz);
00501     MAT3(XuSE, *nx, *ny, *nz);
00502     MAT3(XuSW, *nx, *ny, *nz);
00503
00504     MAT3( oPC, *nx, *ny, *nz);
00505     MAT3( oPN, *nx, *ny, *nz);
00506     MAT3( oPS, *nx, *ny, *nz);
00507     MAT3( oPE, *nx, *ny, *nz);
00508     MAT3( oPW, *nx, *ny, *nz);
00509     MAT3(oPNE, *nx, *ny, *nz);
00510     MAT3(oPNW, *nx, *ny, *nz);
00511     MAT3(oPSE, *nx, *ny, *nz);
00512     MAT3(oPSW, *nx, *ny, *nz);
00513
00514     MAT3( uPC, *nx, *ny, *nz);
00515     MAT3( uPN, *nx, *ny, *nz);
00516     MAT3( uPS, *nx, *ny, *nz);
00517     MAT3( uPE, *nx, *ny, *nz);
00518     MAT3( uPW, *nx, *ny, *nz);
00519     MAT3(uPNE, *nx, *ny, *nz);
00520     MAT3(uPNW, *nx, *ny, *nz);
00521     MAT3(uPSE, *nx, *ny, *nz);
00522     MAT3(uPSW, *nx, *ny, *nz);
00523
00524     MAT3( dPC, *nx, *ny, *nz);
00525     MAT3( dPN, *nx, *ny, *nz);
00526     MAT3( dPS, *nx, *ny, *nz);
00527     MAT3( dPE, *nx, *ny, *nz);
00528     MAT3( dPW, *nx, *ny, *nz);
00529     MAT3(dPNE, *nx, *ny, *nz);

```

```

00530     MAT3(dPNW, *nx, *ny, *nz);
00531     MAT3(dPSE, *nx, *ny, *nz);
00532     MAT3(dPSW, *nx, *ny, *nz);
00533
00534     // Define n and determine number of mesh points
00535     nxm1 = *nx - 1;
00536     nym1 = *ny - 1;
00537     nzm1 = *nz - 1;
00538
00539     //fprintf(data, "%s\n", PRINT_FUNC);
00540
00541     // Build the operator ***
00542     for(kk=2; kk<=*nz-1; kk++) {
00543         k = 2 * kk - 1;
00544
00545         for(jj=2; jj<=*ny-1; jj++) {
00546             j = 2 * jj - 1;
00547
00548             for(ii=2; ii<=*nx-1; ii++) {
00549                 i = 2 * ii - 1;
00550
00551                 // Index computations
00552                 im1 = i - 1;
00553                 ip1 = i + 1;
00554                 im2 = i - 2;
00555                 ip2 = i + 2;
00556                 jml = j - 1;
00557                 jpl = j + 1;
00558                 jm2 = j - 2;
00559                 jp2 = j + 2;
00560                 kml = k - 1;
00561                 kp1 = k + 1;
00562                 km2 = k - 2;
00563                 kp2 = k + 2;
00564                 iim1 = ii - 1;
00565                 iip1 = ii + 1;
00566                 jjm1 = jj - 1;
00567                 jjp1 = jj + 1;
00568                 kkm1 = kk - 1;
00569                 kkp1 = kk + 1;
00570
00571                 /* *****
00572                  * *** > oC;
00573                  * *****/
00574
00575                 // XoC(ii,jj,kk) =
00576                 TMP1_XOC =
00577                     VAT3(dPSW, ii,jj,kk) * ( VAT3( oC, im1,jml,kml) * VAT3(dPSW, ii,jj,kk)
00578                         - VAT3( uC, im1,jml,kml) * VAT3(oPSW, ii,jj,kk)
00579                         - VAT3( oN, im1,jml,kml) * VAT3( dPW, ii,jj,kk)
00580                         - VAT3( oE, im1,jml,kml) * VAT3( dPS, ii,jj,kk))
00581
00582                     + VAT3(oPNE, ii,jj,kk) * (- VAT3( oE, i,jpl, k) * VAT3( oPN, ii,jj,kk)
00583                         - VAT3( oN, ip1, j, k) * VAT3( oPE, ii,jj,kk)
00584                         - VAT3( uC, ip1,jpl,kml) * VAT3(dPNE, ii,jj,kk)
00585                         + VAT3( oC, ip1,jpl, k) * VAT3(oPNE, ii,jj,kk)
00586                         - VAT3( uC, ip1,jpl, k) * VAT3(uPNE, ii,jj,kk))
00587
00588                     + VAT3(dPNE, ii,jj,kk) * (- VAT3( oE, i,jpl,kml) * VAT3( dPN, ii,jj,kk)
00589                         - VAT3( oN, ip1, j,kml) * VAT3( dPE, ii,jj,kk)
00590                         + VAT3( oC, ip1,jpl,kml) * VAT3(dPNE, ii,jj,kk)
00591                         - VAT3( uC, ip1,jpl,kml) * VAT3(oPNE, ii,jj,kk));
00592
00593                 TMP2_XOC =
00594                     VAT3(dPSE, ii,jj,kk) * (- VAT3( oE, i,jml,kml) * VAT3( dPS, ii,jj,kk)
00595                         + VAT3( oC, ip1,jml,kml) * VAT3(dPSE, ii,jj,kk)
00596                         - VAT3( uC, ip1,jml,kml) * VAT3(oPSE, ii,jj,kk)
00597                         - VAT3( oN, ip1,jml,kml) * VAT3( dPE, ii,jj,kk))
00598
00599                     + VAT3( uPE, ii,jj,kk) * (- VAT3( oE, i, j,kp1) * VAT3( uPC, ii,jj,kk)
00600                         - VAT3( oN, ip1,jml,kp1) * VAT3(uPSE, ii,jj,kk)
00601                         - VAT3( uC, ip1, j, k) * VAT3( oPE, ii,jj,kk)
00602                         + VAT3( oC, ip1, j,kp1) * VAT3( uPE, ii,jj,kk)
00603                         - VAT3( oN, ip1, j,kp1) * VAT3(uPNE, ii,jj,kk))
00604
00605                     + VAT3( oPE, ii,jj,kk) * (- VAT3( oE, i, j, k) * VAT3( oPC, ii,jj,kk)
00606                         - VAT3( oN, ip1,jml, k) * VAT3(oPSE, ii,jj,kk)
00607                         - VAT3( uC, ip1, j,kml) * VAT3( dPE, ii,jj,kk)
00608                         + VAT3( oC, ip1, j, k) * VAT3( oPE, ii,jj,kk)
00609                         - VAT3( uC, ip1, j, k) * VAT3( uPE, ii,jj,kk)
00610                         - VAT3( oN, ip1, j, k) * VAT3(oPNE, ii,jj,kk));

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00611
00612 TMP3_XOC =
00613 + VAT3( dPE, ii,jj,kk) * (- VAT3( oE, i, j,kml) * VAT3( dPC, ii,jj,kk)
00614 - VAT3( oN, ip1,jml,kml) * VAT3(dPSE, ii,jj,kk)
00615 + VAT3( oC, ip1, j,kml) * VAT3( dPE, ii,jj,kk)
00616 - VAT3( uC, ip1, j,kml) * VAT3( oPE, ii,jj,kk)
00617 - VAT3( oN, ip1, j,kml) * VAT3(dPNE, ii,jj,kk))
00618
00619 + VAT3(uPSE, ii,jj,kk) * (- VAT3( oE, i,jml,kp1) * VAT3( uPS, ii,jj,kk)
00620 - VAT3( uC, ip1,jml, k) * VAT3(oPSE, ii,jj,kk)
00621 + VAT3( oC, ip1,jml,kp1) * VAT3(uPSE, ii,jj,kk)
00622 - VAT3( oN, ip1,jml,kp1) * VAT3( uPE, ii,jj,kk))
00623
00624 + VAT3(uPNE, ii,jj,kk) * (- VAT3( oE, i,jp1,kp1) * VAT3( uPN, ii,jj,kk)
00625 - VAT3( oN, ip1, j,kp1) * VAT3( uPE, ii,jj,kk)
00626 - VAT3( uC, ip1,jp1, k) * VAT3(oPNE, ii,jj,kk)
00627 + VAT3( oC, ip1,jp1,kp1) * VAT3(uPNE, ii,jj,kk));
00628
00629 TMP4_XOC =
00630 + VAT3( oPS, ii,jj,kk) * (- VAT3( oE, im1,jml, k) * VAT3(oPSW, ii,jj,kk)
00631 - VAT3( uC, i,jml,kml) * VAT3( dPS, ii,jj,kk)
00632 + VAT3( oC, i,jml, k) * VAT3( oPS, ii,jj,kk)
00633 - VAT3( uC, i,jml, k) * VAT3( uPS, ii,jj,kk)
00634 - VAT3( oN, i,jml, k) * VAT3( oPC, ii,jj,kk)
00635 - VAT3( oE, i,jml, k) * VAT3(oPSE, ii,jj,kk))
00636
00637 + VAT3( dPS, ii,jj,kk) * (- VAT3( oE, im1,jml,kml) * VAT3(dPSW, ii,jj,kk)
00638 + VAT3( oC, i,jml,kml) * VAT3( dPS, ii,jj,kk)
00639 - VAT3( uC, i,jml,kml) * VAT3( oPS, ii,jj,kk)
00640 - VAT3( oN, i,jml,kml) * VAT3( dPC, ii,jj,kk)
00641 - VAT3( oE, i,jml,kml) * VAT3(dPSE, ii,jj,kk))
00642
00643 + VAT3(oPSE, ii,jj,kk) * (- VAT3( oE, i,jml, k) * VAT3( oPS, ii,jj,kk)
00644 - VAT3( uC, ip1,jml,kml) * VAT3(dPSE, ii,jj,kk)
00645 + VAT3( oC, ip1,jml, k) * VAT3(oPSE, ii,jj,kk)
00646 - VAT3( uC, ip1,jml, k) * VAT3(uPSE, ii,jj,kk)
00647 - VAT3( oN, ip1,jml, k) * VAT3( oPE, ii,jj,kk));
00648
00649 TMP5_XOC =
00650 + VAT3( dPN, ii,jj,kk) * (- VAT3( oE, im1,jp1,kml) * VAT3(dPNW, ii,jj,kk)
00651 - VAT3( oN, i, j,kml) * VAT3( dPC, ii,jj,kk)
00652 + VAT3( oC, i,jp1,kml) * VAT3( dPN, ii,jj,kk)
00653 - VAT3( uC, i,jp1,kml) * VAT3( oPN, ii,jj,kk)
00654 - VAT3( oE, i,jp1,kml) * VAT3(dPNE, ii,jj,kk))
00655
00656 + VAT3( uPC, ii,jj,kk) * (- VAT3( oE, im1, j,kp1) * VAT3( uPW, ii,jj,kk)
00657 - VAT3( oN, i,jml,kp1) * VAT3( uPS, ii,jj,kk)
00658 - VAT3( uC, i, j, k) * VAT3( oPC, ii,jj,kk)
00659 + VAT3( oC, i, j,kp1) * VAT3( uPC, ii,jj,kk)
00660 - VAT3( oN, i, j,kp1) * VAT3( uPN, ii,jj,kk)
00661 - VAT3( oE, i, j,kp1) * VAT3( uPE, ii,jj,kk))
00662
00663 + VAT3( oPC, ii,jj,kk) * (- VAT3( oE, im1, j, k) * VAT3( oPW, ii,jj,kk)
00664 - VAT3( oN, i,jml, k) * VAT3( oPS, ii,jj,kk)
00665 - VAT3( uC, i, j,kml) * VAT3( dPC, ii,jj,kk)
00666 + VAT3( oC, i, j, k) * VAT3( oPC, ii,jj,kk)
00667 - VAT3( uC, i, j, k) * VAT3( uPC, ii,jj,kk)
00668 - VAT3( oN, i, j, k) * VAT3( oPN, ii,jj,kk)
00669 - VAT3( oE, i, j, k) * VAT3( oPE, ii,jj,kk));
00670
00671 TMP6_XOC =
00672 + VAT3( dPC, ii,jj,kk) * (- VAT3( oE, im1, j,kml) * VAT3( dPW, ii,jj,kk)
00673 - VAT3( oN, i,jml,kml) * VAT3( dPS, ii,jj,kk)
00674 + VAT3( oC, i, j,kml) * VAT3( dPC, ii,jj,kk)
00675 - VAT3( uC, i, j,kml) * VAT3( oPC, ii,jj,kk)
00676 - VAT3( oN, i, j,kml) * VAT3( dPN, ii,jj,kk)
00677 - VAT3( oE, i, j,kml) * VAT3( dPE, ii,jj,kk))
00678
00679 + VAT3( uPS, ii,jj,kk) * (- VAT3( oE, im1,jml,kp1) * VAT3(uPSW, ii,jj,kk)
00680 - VAT3( uC, i,jml, k) * VAT3( oPS, ii,jj,kk)
00681 + VAT3( oC, i,jml,kp1) * VAT3( uPS, ii,jj,kk)
00682 - VAT3( oN, i,jml,kp1) * VAT3( uPC, ii,jj,kk)
00683 - VAT3( oE, i,jml,kp1) * VAT3(uPSE, ii,jj,kk))
00684
00685 + VAT3(uPNW, ii,jj,kk) * (- VAT3( oN, im1, j,kp1) * VAT3( uPW, ii,jj,kk)
00686 - VAT3( uC, im1,jp1, k) * VAT3(oPNW, ii,jj,kk)
00687 + VAT3( oC, im1,jp1,kp1) * VAT3(uPNW, ii,jj,kk)
00688 - VAT3( oE, im1,jp1,kp1) * VAT3( uPN, ii,jj,kk));
00689
00690 TMP7_XOC =
00691 + VAT3( dPW, ii,jj,kk) * (- VAT3( oN, im1,jml,kml) * VAT3(dPSW, ii,jj,kk)

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00692             + VAT3( oC, iml, j, kml) * VAT3( dPW, ii, jj, kk)
00693             - VAT3( uC, iml, j, kml) * VAT3( oPW, ii, jj, kk)
00694             - VAT3( oN, iml, j, kml) * VAT3( dPNW, ii, jj, kk)
00695             - VAT3( oE, iml, j, kml) * VAT3( dPC, ii, jj, kk))
00696
00697         + VAT3(uPSW, ii, jj, kk) * (- VAT3( uC, iml, jml, k) * VAT3(oPSW, ii, jj, kk)
00698             + VAT3( oC, iml, jml, kpl) * VAT3(uPSW, ii, jj, kk)
00699             - VAT3( oN, iml, jml, kpl) * VAT3( uPW, ii, jj, kk)
00700             - VAT3( oE, iml, jml, kpl) * VAT3( uPS, ii, jj, kk))
00701
00702         + VAT3(oPSW, ii, jj, kk) * (- VAT3( uC, iml, jml, kml) * VAT3(dPSW, ii, jj, kk)
00703             + VAT3( oC, iml, jml, k) * VAT3(oPSW, ii, jj, kk)
00704             - VAT3( uC, iml, jml, k) * VAT3(uPSW, ii, jj, kk)
00705             - VAT3( oN, iml, jml, k) * VAT3( oPW, ii, jj, kk)
00706             - VAT3( oE, iml, jml, k) * VAT3( oPS, ii, jj, kk));
00707
00708     TMP8_XOC =
00709         + VAT3(oPNW, ii, jj, kk) * (- VAT3( oN, iml, j, k) * VAT3( oPW, ii, jj, kk)
00710             - VAT3( uC, iml, jpl, kml) * VAT3(dPNW, ii, jj, kk)
00711             + VAT3( oC, iml, jpl, k) * VAT3(oPNW, ii, jj, kk)
00712             - VAT3( uC, iml, jpl, k) * VAT3(uPNW, ii, jj, kk)
00713             - VAT3( oE, iml, jpl, k) * VAT3( oPN, ii, jj, kk))
00714
00715         + VAT3(dPNW, ii, jj, kk) * (- VAT3( oN, iml, j, kml) * VAT3( dPW, ii, jj, kk)
00716             + VAT3( oC, iml, jpl, kml) * VAT3(dPNW, ii, jj, kk)
00717             - VAT3( uC, iml, jpl, kml) * VAT3(oPNW, ii, jj, kk)
00718             - VAT3( oE, iml, jpl, kml) * VAT3( dPN, ii, jj, kk))
00719
00720         + VAT3( oPW, ii, jj, kk) * (- VAT3( oN, iml, jml, k) * VAT3(oPSW, ii, jj, kk)
00721             - VAT3( uC, iml, j, kml) * VAT3( dPW, ii, jj, kk)
00722             + VAT3( oC, iml, j, k) * VAT3( oPW, ii, jj, kk)
00723             - VAT3( uC, iml, j, k) * VAT3( uPW, ii, jj, kk)
00724             - VAT3( oN, iml, j, k) * VAT3(oPNW, ii, jj, kk)
00725             - VAT3( oE, iml, j, k) * VAT3( oPC, ii, jj, kk));
00726
00727     TMP9_XOC =
00728         + VAT3( uPW, ii, jj, kk) * (- VAT3( oN, iml, jml, kpl) * VAT3(uPSW, ii, jj, kk)
00729             - VAT3( uC, iml, j, k) * VAT3( oPW, ii, jj, kk)
00730             + VAT3( oC, iml, j, kpl) * VAT3( uPW, ii, jj, kk)
00731             - VAT3( oN, iml, j, kpl) * VAT3(uPNW, ii, jj, kk)
00732             - VAT3( oE, iml, j, kpl) * VAT3( uPC, ii, jj, kk))
00733
00734         + VAT3( uPN, ii, jj, kk) * (- VAT3( oE, iml, jpl, kpl) * VAT3(uPNW, ii, jj, kk)
00735             - VAT3( oN, i, j, kpl) * VAT3( uPC, ii, jj, kk)
00736             - VAT3( uC, i, jpl, k) * VAT3( oPN, ii, jj, kk)
00737             + VAT3( oC, i, jpl, kpl) * VAT3( uPN, ii, jj, kk)
00738             - VAT3( oE, i, jpl, kpl) * VAT3(uPNE, ii, jj, kk))
00739
00740         + VAT3( oPN, ii, jj, kk) * (- VAT3( oE, iml, jpl, k) * VAT3(oPNW, ii, jj, kk)
00741             - VAT3( oN, i, j, k) * VAT3( oPC, ii, jj, kk)
00742             - VAT3( uC, i, jpl, kml) * VAT3( dPN, ii, jj, kk)
00743             + VAT3( oC, i, jpl, k) * VAT3( oPN, ii, jj, kk)
00744             - VAT3( uC, i, jpl, k) * VAT3( uPN, ii, jj, kk)
00745             - VAT3( oE, i, jpl, k) * VAT3(oPNE, ii, jj, kk));
00746
00747     VAT3( XoC, ii, jj, kk) = TMP1_XOC + TMP2_XOC + TMP3_XOC
00748         + TMP4_XOC + TMP5_XOC + TMP6_XOC
00749         + TMP7_XOC + TMP8_XOC + TMP9_XOC;
00750
00751     //fprintf(data, "%19.12E\n", VAT3(XoC, ii, jj, kk));
00752
00753     /* *****
00754      * *** > oE;
00755      * *****/
00756
00757     // VAT3( XoE, ii, jj, kk) =
00758     TMP1_XOE =
00759         VAT3( dPS, ii, jj, kk) * VAT3( oE, i, jml, kml) * VAT3(dPSW, iipl, jj, kk)
00760         + VAT3( oPS, ii, jj, kk) * VAT3( oE, i, jml, k) * VAT3(oPSW, iipl, jj, kk)
00761         + VAT3( uPS, ii, jj, kk) * VAT3( oE, i, jml, kpl) * VAT3(uPSW, iipl, jj, kk)
00762         + VAT3( dPC, ii, jj, kk) * VAT3( oE, i, j, kml) * VAT3( dPW, iipl, jj, kk)
00763         + VAT3( oPC, ii, jj, kk) * VAT3( oE, i, j, k) * VAT3( oPW, iipl, jj, kk)
00764         + VAT3( uPC, ii, jj, kk) * VAT3( oE, i, j, kpl) * VAT3( uPW, iipl, jj, kk)
00765         + VAT3( dPN, ii, jj, kk) * VAT3( oE, i, jpl, kml) * VAT3(dPNW, iipl, jj, kk)
00766         + VAT3( oPN, ii, jj, kk) * VAT3( oE, i, jpl, k) * VAT3(oPNW, iipl, jj, kk)
00767         + VAT3( uPN, ii, jj, kk) * VAT3( oE, i, jpl, kpl) * VAT3(uPNW, iipl, jj, kk)
00768
00769         - VAT3(dPSE, ii, jj, kk) * ( VAT3( oC, ipl, jml, kml) * VAT3(dPSW, iipl, jj, kk)
00770             - VAT3( uC, ipl, jml, kml) * VAT3(oPSW, iipl, jj, kk)
00771             - VAT3( oN, ipl, jml, kml) * VAT3( dPW, iipl, jj, kk)
00772             - VAT3( oE, ipl, jml, kml) * VAT3( dPS, iipl, jj, kk));

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00773
00774
00775     TMP2_XOE =
00776         - VAT3(oPSE, ii,jj,kk) * (- VAT3( uC, ip1,jm1,km1) * VAT3(dPSW, iip1,jj,kk)
00777             + VAT3( oC, ip1,jm1, k) * VAT3(oPSW, iip1,jj,kk)
00778             - VAT3( uC, ip1,jm1, k) * VAT3(uPSW, iip1,jj,kk)
00779             - VAT3( oN, ip1,jm1, k) * VAT3( oPW, iip1,jj,kk)
00780             - VAT3( oE, ip1,jm1, k) * VAT3( oPS, iip1,jj,kk))
00781
00782         - VAT3(uPSE, ii,jj,kk) * (- VAT3( uC, ip1,jm1, k) * VAT3(oPSW, iip1,jj,kk)
00783             + VAT3( oC, ip1,jm1,kp1) * VAT3(uPSW, iip1,jj,kk)
00784             - VAT3( oN, ip1,jm1,kp1) * VAT3( uPW, iip1,jj,kk)
00785             - VAT3( oE, ip1,jm1,kp1) * VAT3( uPS, iip1,jj,kk))
00786
00787         - VAT3( dPE, ii,jj,kk) * (- VAT3( oN, ip1,jm1,km1) * VAT3(dPSW, iip1,jj,kk)
00788             + VAT3( oC, ip1, j,km1) * VAT3( dPW, iip1,jj,kk)
00789             - VAT3( uC, ip1, j,km1) * VAT3( oPW, iip1,jj,kk)
00790             - VAT3( oN, ip1, j,km1) * VAT3(dPNW, iip1,jj,kk)
00791             - VAT3( oE, ip1, j,km1) * VAT3( dPC, iip1,jj,kk));
00792
00793     TMP3_XOE =
00794         - VAT3( oPE, ii,jj,kk) * (- VAT3( oN, ip1,jm1, k) * VAT3(oPSW, iip1,jj,kk)
00795             - VAT3( uC, ip1, j,km1) * VAT3( dPW, iip1,jj,kk)
00796             + VAT3( oC, ip1, j, k) * VAT3( oPW, iip1,jj,kk)
00797             - VAT3( uC, ip1, j, k) * VAT3( uPW, iip1,jj,kk)
00798             - VAT3( oN, ip1, j, k) * VAT3(oPNW, iip1,jj,kk)
00799             - VAT3( oE, ip1, j, k) * VAT3( oPC, iip1,jj,kk))
00800
00801         - VAT3( uPE, ii,jj,kk) * (- VAT3( oN, ip1,jm1,kp1) * VAT3(uPSW, iip1,jj,kk)
00802             - VAT3( uC, ip1, j, k) * VAT3( oPW, iip1,jj,kk)
00803             + VAT3( oC, ip1, j,kp1) * VAT3( uPW, iip1,jj,kk)
00804             - VAT3( oN, ip1, j,kp1) * VAT3(uPNW, iip1,jj,kk)
00805             - VAT3( oE, ip1, j,kp1) * VAT3( uPC, iip1,jj,kk))
00806
00807         - VAT3(dPNE, ii,jj,kk) * (- VAT3( oN, ip1, j,km1) * VAT3( dPW, iip1,jj,kk)
00808             + VAT3( oC, ip1,jp1,km1) * VAT3(dPNW, iip1,jj,kk)
00809             - VAT3( uC, ip1,jp1,km1) * VAT3(oPNW, iip1,jj,kk)
00810             - VAT3( oE, ip1,jp1,km1) * VAT3( dPN, iip1,jj,kk));
00811
00812     TMP4_XOE =
00813         - VAT3(oPNE, ii,jj,kk) * (- VAT3( oN, ip1, j, k) * VAT3( oPW, iip1,jj,kk)
00814             - VAT3( uC, ip1,jp1,km1) * VAT3(dPNW, iip1,jj,kk)
00815             + VAT3( oC, ip1,jp1, k) * VAT3(oPNW, iip1,jj,kk)
00816             - VAT3( uC, ip1,jp1, k) * VAT3(uPNW, iip1,jj,kk)
00817             - VAT3( oE, ip1,jp1, k) * VAT3( oPN, iip1,jj,kk))
00818
00819         - VAT3(uPNE, ii,jj,kk) * (- VAT3( oN, ip1, j,kp1) * VAT3( uPW, iip1,jj,kk)
00820             - VAT3( uC, ip1,jp1, k) * VAT3(oPNW, iip1,jj,kk)
00821             + VAT3( oC, ip1,jp1,kp1) * VAT3(uPNW, iip1,jj,kk)
00822             - VAT3( oE, ip1,jp1,kp1) * VAT3( uPN, iip1,jj,kk));
00823
00824     VAT3( XoE, ii,jj,kk) = TMP1_XOE + TMP2_XOE + TMP3_XOE + TMP4_XOE;
00825
00826     //fprintf(data, "%19.12E\n", VAT3(XoE, ii, jj, kk));
00827
00828
00829     /* *****
00830     * *** > oN;
00831     * *****
00832
00833     // VAT3( XoN, ii,jj,kk) =
00834     TMP1_XON =
00835         VAT3( dPW, ii,jj,kk) * VAT3( oN, im1,j,km1) * VAT3(dPSW, ii,jjp1,kk)
00836         + VAT3( oPW, ii,jj,kk) * VAT3( oN, im1,j,k) * VAT3(oPSW, ii,jjp1,kk)
00837         + VAT3( uPW, ii,jj,kk) * VAT3( oN, im1,j,kp1) * VAT3(uPSW, ii,jjp1,kk)
00838
00839         - VAT3(dPNW, ii,jj,kk) * ( VAT3( oC, im1,jp1,km1) * VAT3(dPSW, ii,jjp1,kk)
00840             - VAT3( uC, im1,jp1,km1) * VAT3(oPSW, ii,jjp1,kk)
00841             - VAT3( oN, im1,jp1,km1) * VAT3( dPW, ii,jjp1,kk)
00842             - VAT3( oE, im1,jp1,km1) * VAT3( dPS, ii,jjp1,kk))
00843
00844         - VAT3(oPNW, ii,jj,kk) * (- VAT3( uC, im1,jp1,km1) * VAT3(dPSW, ii,jjp1,kk)
00845             + VAT3( oC, im1,jp1,k) * VAT3(oPSW, ii,jjp1,kk)
00846             - VAT3( uC, im1,jp1,k) * VAT3(uPSW, ii,jjp1,kk)
00847             - VAT3( oN, im1,jp1,k) * VAT3( oPW, ii,jjp1,kk)
00848             - VAT3( oE, im1,jp1,k) * VAT3( oPS, ii,jjp1,kk));
00849
00850     TMP2_XON =
00851         - VAT3(uPNW, ii,jj,kk) * (- VAT3( uC, im1,jp1,k) * VAT3(oPSW, ii,jjp1,kk)
00852             + VAT3( oC, im1,jp1,kp1) * VAT3(uPSW, ii,jjp1,kk)
00853             - VAT3( oN, im1,jp1,kp1) * VAT3( uPW, ii,jjp1,kk)
00854             - VAT3( oE, im1,jp1,kp1) * VAT3( uPS, ii,jjp1,kk))

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00855
00856 + VAT3( dPC, ii,jj,kk) * VAT3( oN, i,j,kml) * VAT3( dPS, ii,jjp1,kk)
00857 + VAT3( oPC, ii,jj,kk) * VAT3( oN, i,j,k) * VAT3( oPS, ii,jjp1,kk)
00858 + VAT3( uPC, ii,jj,kk) * VAT3( oN, i,j,kp1) * VAT3( uPS, ii,jjp1,kk)
00859
00860 - VAT3( dPN, ii,jj,kk) * ( - VAT3( oE, im1,jp1,kml) * VAT3(dPSW, ii,jjp1,kk)
00861 + VAT3( oC, i,jp1,kml) * VAT3( dPS, ii,jjp1,kk)
00862 - VAT3( uC, i,jp1,kml) * VAT3( oPS, ii,jjp1,kk)
00863 - VAT3( oN, i,jp1,kml) * VAT3( dPC, ii,jjp1,kk)
00864 - VAT3( oE, i,jp1,kml) * VAT3(dPSE, ii,jjp1,kk));
00865
00866 TMP3_XON =
00867 - VAT3( oPN, ii,jj,kk) * ( - VAT3( oE, im1,jp1,k) * VAT3(oPSW, ii,jjp1,kk)
00868 - VAT3( uC, i,jp1,kml) * VAT3( dPS, ii,jjp1,kk)
00869 + VAT3( oC, i,jp1,k) * VAT3( oPS, ii,jjp1,kk)
00870 - VAT3( uC, i,jp1,k) * VAT3( uPS, ii,jjp1,kk)
00871 - VAT3( oN, i,jp1,k) * VAT3( oPC, ii,jjp1,kk)
00872 - VAT3( oE, i,jp1,k) * VAT3(oPSE, ii,jjp1,kk))
00873
00874 - VAT3( uPN, ii,jj,kk) * ( - VAT3( oE, im1,jp1,kp1) * VAT3(uPSW, ii,jjp1,kk)
00875 - VAT3( uC, i,jp1,k) * VAT3( oPS, ii,jjp1,kk)
00876 + VAT3( oC, i,jp1,kp1) * VAT3( uPS, ii,jjp1,kk)
00877 - VAT3( oN, i,jp1,kp1) * VAT3( uPC, ii,jjp1,kk)
00878 - VAT3( oE, i,jp1,kp1) * VAT3(uPSE, ii,jjp1,kk))
00879
00880 + VAT3( dPE, ii,jj,kk) * VAT3( oN, ip1,j,kml) * VAT3(dPSE, ii,jjp1,kk)
00881 + VAT3( oPE, ii,jj,kk) * VAT3( oN, ip1,j,k) * VAT3(oPSE, ii,jjp1,kk)
00882 + VAT3( uPE, ii,jj,kk) * VAT3( oN, ip1,j,kp1) * VAT3(uPSE, ii,jjp1,kk);
00883
00884 TMP4_XON =
00885 - VAT3(dPNE, ii,jj,kk) * ( - VAT3( oE, i,jp1,kml) * VAT3( dPS, ii,jjp1,kk)
00886 + VAT3( oC, ip1,jp1,kml) * VAT3(dPSE, ii,jjp1,kk)
00887 - VAT3( uC, ip1,jp1,kml) * VAT3(oPSE, ii,jjp1,kk)
00888 - VAT3( oN, ip1,jp1,kml) * VAT3( dPE, ii,jjp1,kk))
00889
00890 - VAT3(oPNE, ii,jj,kk) * ( - VAT3( oE, i,jp1,k) * VAT3( oPS, ii,jjp1,kk)
00891 - VAT3( uC, ip1,jp1,kml) * VAT3(dPSE, ii,jjp1,kk)
00892 + VAT3( oC, ip1,jp1,k) * VAT3(oPSE, ii,jjp1,kk)
00893 - VAT3( uC, ip1,jp1,k) * VAT3(uPSE, ii,jjp1,kk)
00894 - VAT3( oN, ip1,jp1,k) * VAT3( oPE, ii,jjp1,kk))
00895
00896 - VAT3(uPNE, ii,jj,kk) * ( - VAT3( oE, i,jp1,kp1) * VAT3( uPS, ii,jjp1,kk)
00897 - VAT3( uC, ip1,jp1,k) * VAT3(oPSE, ii,jjp1,kk)
00898 + VAT3( oC, ip1,jp1,kp1) * VAT3(uPSE, ii,jjp1,kk)
00899 - VAT3( oN, ip1,jp1,kp1) * VAT3( uPE, ii,jjp1,kk));
00900
00901 VAT3( XoN, ii,jj,kk) = TMP1_XON + TMP2_XON + TMP3_XON + TMP4_XON;
00902
00903 //fprintf(data, "%19.12E\n", VAT3(XoN, ii, jj, kk));
00904
00905 /* *****
00906 * *** > uC;
00907 * *****/
00908
00909 // VAT3( XuC, ii,jj,kk) =
00910 TMP1_XUC =
00911 VAT3(oPSW, ii,jj,kk) * VAT3( uC, im1,jml,k) * VAT3(dPSW, ii,jj,kkp1)
00912
00913 - VAT3(uPSW, ii,jj,kk) * ( VAT3( oC, im1,jml,kp1) * VAT3(dPSW, ii,jj,kkp1)
00914 - VAT3( uC, im1,jml,kp1) * VAT3(oPSW, ii,jj,kkp1)
00915 - VAT3( oN, im1,jml,kp1) * VAT3( dPW, ii,jj,kkp1)
00916 - VAT3( oE, im1,jml,kp1) * VAT3( dPS, ii,jj,kkp1))
00917
00918 + VAT3( oPW, ii,jj,kk) * VAT3( uC, im1,j,k) * VAT3( dPW, ii,jj,kkp1)
00919
00920 - VAT3( uPW, ii,jj,kk) * ( - VAT3( oN, im1,jml,kp1) * VAT3(dPSW, ii,jj,kkp1)
00921 + VAT3( oC, im1,j,kp1) * VAT3( dPW, ii,jj,kkp1)
00922 - VAT3( uC, im1,j,kp1) * VAT3( oPW, ii,jj,kkp1)
00923 - VAT3( oN, im1,j,kp1) * VAT3(dPNW, ii,jj,kkp1)
00924 - VAT3( oE, im1,j,kp1) * VAT3( dPC, ii,jj,kkp1))
00925
00926 + VAT3(oPNW, ii,jj,kk) * VAT3( uC, im1,jp1,k) * VAT3(dPNW, ii,jj,kkp1);
00927
00928 TMP2_XUC =
00929 - VAT3(uPNW, ii,jj,kk) * ( - VAT3( oN, im1,j,kp1) * VAT3( dPW, ii,jj,kkp1)
00930 + VAT3( oC, im1,jp1,kp1) * VAT3(dPNW, ii,jj,kkp1)
00931 - VAT3( uC, im1,jp1,kp1) * VAT3(oPNW, ii,jj,kkp1)
00932 - VAT3( oE, im1,jp1,kp1) * VAT3( dPN, ii,jj,kkp1))
00933
00934 + VAT3( oPS, ii,jj,kk) * VAT3( uC, i,jml,k) * VAT3( dPS, ii,jj,kkp1)
00935

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00936     - VAT3( uPS, ii,jj,kk) * ( - VAT3( oE, iml,jml,kpl) * VAT3(dPSW, ii,jj,kkpl)
00937       + VAT3( oC, i,jml,kpl) * VAT3( dPS, ii,jj,kkpl)
00938     - VAT3( uC, i,jml,kpl) * VAT3( oPS, ii,jj,kkpl)
00939     - VAT3( oN, i,jml,kpl) * VAT3( dPC, ii,jj,kkpl)
00940     - VAT3( oE, i,jml,kpl) * VAT3(dPSE, ii,jj,kkpl))
00941
00942     + VAT3( oPC, ii,jj,kk) * VAT3( uC, i,j,k) * VAT3( dPC, ii,jj,kkpl)
00943
00944     - VAT3( uPC, ii,jj,kk) * ( - VAT3( oE, iml,j,kpl) * VAT3( dPW, ii,jj,kkpl)
00945       - VAT3( oN, i,jml,kpl) * VAT3( dPS, ii,jj,kkpl)
00946       + VAT3( oC, i,j,kpl) * VAT3( dPC, ii,jj,kkpl)
00947       - VAT3( uC, i,j,kpl) * VAT3( oPC, ii,jj,kkpl)
00948       - VAT3( oN, i,j,kpl) * VAT3( dPN, ii,jj,kkpl)
00949       - VAT3( oE, i,j,kpl) * VAT3( dPE, ii,jj,kkpl));
00950
00951 TMP3_XUC =
00952     + VAT3( oPN, ii,jj,kk) * VAT3( uC, i,jpl,k) * VAT3( dPN, ii,jj,kkpl)
00953
00954     - VAT3( uPN, ii,jj,kk) * ( - VAT3( oE, iml,jpl,kpl) * VAT3(dPNW, ii,jj,kkpl)
00955       - VAT3( oN, i,j,kpl) * VAT3( dPC, ii,jj,kkpl)
00956       + VAT3( oC, i,jpl,kpl) * VAT3( dPN, ii,jj,kkpl)
00957       - VAT3( uC, i,jpl,kpl) * VAT3( oPN, ii,jj,kkpl)
00958       - VAT3( oE, i,jpl,kpl) * VAT3(dPNE, ii,jj,kkpl))
00959
00960     + VAT3(oPSE, ii,jj,kk) * VAT3( uC, ip1,jml,k) * VAT3(dPSE, ii,jj,kkpl)
00961
00962     - VAT3(uPSE, ii,jj,kk) * ( - VAT3( oE, i,jml,kpl) * VAT3( dPS, ii,jj,kkpl)
00963       + VAT3( oC, ip1,jml,kpl) * VAT3(dPSE, ii,jj,kkpl)
00964       - VAT3( uC, ip1,jml,kpl) * VAT3(oPSE, ii,jj,kkpl)
00965       - VAT3( oN, ip1,jml,kpl) * VAT3( dPE, ii,jj,kkpl));
00966
00967 TMP4_XUC =
00968     + VAT3( oPE, ii,jj,kk) * VAT3( uC, ip1,j,k) * VAT3( dPE, ii,jj,kkpl)
00969
00970     - VAT3( uPE, ii,jj,kk) * ( - VAT3( oE, i,j,kpl) * VAT3( dPC, ii,jj,kkpl)
00971       - VAT3( oN, ip1,jml,kpl) * VAT3(dPSE, ii,jj,kkpl)
00972       + VAT3( oC, ip1,j,kpl) * VAT3( dPE, ii,jj,kkpl)
00973       - VAT3( uC, ip1,j,kpl) * VAT3( oPE, ii,jj,kkpl)
00974       - VAT3( oN, ip1,j,kpl) * VAT3(dPNE, ii,jj,kkpl))
00975
00976     + VAT3(oPNE, ii,jj,kk) * VAT3( uC, ip1,jpl,k) * VAT3(dPNE, ii,jj,kkpl)
00977
00978     - VAT3(uPNE, ii,jj,kk) * ( - VAT3( oE, i,jpl,kpl) * VAT3( dPN, ii,jj,kkpl)
00979       - VAT3( oN, ip1,j,kpl) * VAT3( dPE, ii,jj,kkpl)
00980       + VAT3( oC, ip1,jpl,kpl) * VAT3(dPNE, ii,jj,kkpl)
00981       - VAT3( uC, ip1,jpl,kpl) * VAT3(oPNE, ii,jj,kkpl));
00982
00983 VAT3( XuC, ii,jj,kk) = TMP1_XUC + TMP2_XUC + TMP3_XUC + TMP4_XUC;
00984
00985     //fprintf(data, "%19.12E\n", VAT3(XuC, ii, jj, kk));
00986
00987     /* *****
00988      * *** > oNE;
00989      * *****
00990
00991 VAT3(XoNE, ii,jj,kk) =
00992     VAT3( dPN, ii,jj,kk) * VAT3( oE, i,jpl,kml) * VAT3(dPSW, iip1,jjp1,kk)
00993     + VAT3( oPN, ii,jj,kk) * VAT3( oE, i,jpl,k) * VAT3(oPSW, iip1,jjp1,kk)
00994     + VAT3( uPN, ii,jj,kk) * VAT3( oE, i,jpl,kpl) * VAT3(uPSW, iip1,jjp1,kk)
00995     + VAT3( dPE, ii,jj,kk) * VAT3( oN, ip1,j,kml) * VAT3(dPSW, iip1,jjp1,kk)
00996     + VAT3( oPE, ii,jj,kk) * VAT3( oN, ip1,j,k) * VAT3(oPSW, iip1,jjp1,kk)
00997     + VAT3( uPE, ii,jj,kk) * VAT3( oN, ip1,j,kpl) * VAT3(uPSW, iip1,jjp1,kk)
00998
00999     - VAT3(dPNE, ii,jj,kk) * ( VAT3( oC, ip1,jpl,kml) * VAT3(dPSW, iip1,jjp1,kk)
01000       - VAT3( uC, ip1,jpl,kml) * VAT3(oPSW, iip1,jjp1,kk)
01001       - VAT3( oN, ip1,jpl,kml) * VAT3( dPW, iip1,jjp1,kk)
01002       - VAT3( oE, ip1,jpl,kml) * VAT3( dPS, iip1,jjp1,kk))
01003
01004     - VAT3(oPNE, ii,jj,kk) * ( - VAT3( uC, ip1,jpl,kml) * VAT3(dPSW, iip1,jjp1,kk)
01005       + VAT3( oC, ip1,jpl,k) * VAT3(oPSW, iip1,jjp1,kk)
01006       - VAT3( uC, ip1,jpl,k) * VAT3(uPSW, iip1,jjp1,kk)
01007       - VAT3( oN, ip1,jpl,k) * VAT3( oPW, iip1,jjp1,kk)
01008       - VAT3( oE, ip1,jpl,k) * VAT3( oPS, iip1,jjp1,kk))
01009
01010     - VAT3(uPNE, ii,jj,kk) * ( - VAT3( uC, ip1,jpl,k) * VAT3(oPSW, iip1,jjp1,kk)
01011       + VAT3( oC, ip1,jpl,kpl) * VAT3(uPSW, iip1,jjp1,kk)
01012       - VAT3( oN, ip1,jpl,kpl) * VAT3( uPW, iip1,jjp1,kk)
01013       - VAT3( oE, ip1,jpl,kpl) * VAT3( uPS, iip1,jjp1,kk));
01014
01015     //fprintf(data, "%19.12E\n", VAT3(XoNE, ii, jj, kk));
01016

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01017      /* *****
01018      * *** > oNW;
01019      * *****/
01020
01021      VAT3(XoNW, ii, jj, kk) =
01022          VAT3( dPW, ii, jj, kk) * VAT3( oN, im1, j, km1) * VAT3(dPSE, iim1, jjp1, kk)
01023      + VAT3( oPW, ii, jj, kk) * VAT3( oN, im1, j, k) * VAT3(oPSE, iim1, jjp1, kk)
01024      + VAT3( uPW, ii, jj, kk) * VAT3( oN, im1, j, kp1) * VAT3(uPSE, iim1, jjp1, kk)
01025
01026      - VAT3(dPNW, ii, jj, kk) * (- VAT3( oE, im2, jp1, km1) * VAT3( dPS, iim1, jjp1, kk)
01027          + VAT3( oC, im1, jp1, km1) * VAT3(dPSE, iim1, jjp1, kk)
01028          - VAT3( uC, im1, jp1, km1) * VAT3(oPSE, iim1, jjp1, kk)
01029          - VAT3( oN, im1, jp1, km1) * VAT3( dPE, iim1, jjp1, kk))
01030
01031      - VAT3(oPNW, ii, jj, kk) * (- VAT3( oE, im2, jp1, k) * VAT3( oPS, iim1, jjp1, kk)
01032          - VAT3( uC, im1, jp1, km1) * VAT3(dPSE, iim1, jjp1, kk)
01033          + VAT3( oC, im1, jp1, k) * VAT3(oPSE, iim1, jjp1, kk)
01034          - VAT3( uC, im1, jp1, k) * VAT3(uPSE, iim1, jjp1, kk)
01035          - VAT3( oN, im1, jp1, k) * VAT3( oPE, iim1, jjp1, kk))
01036
01037      - VAT3(uPNW, ii, jj, kk) * (- VAT3( oE, im2, jp1, kp1) * VAT3( uPS, iim1, jjp1, kk)
01038          - VAT3( uC, im1, jp1, k) * VAT3(oPSE, iim1, jjp1, kk)
01039          + VAT3( oC, im1, jp1, kp1) * VAT3(uPSE, iim1, jjp1, kk)
01040          - VAT3( oN, im1, jp1, kp1) * VAT3( uPE, iim1, jjp1, kk))
01041
01042      + VAT3( dPN, ii, jj, kk) * VAT3( oE, im1, jp1, km1) * VAT3(dPSE, iim1, jjp1, kk)
01043      + VAT3( oPN, ii, jj, kk) * VAT3( oE, im1, jp1, k) * VAT3(oPSE, iim1, jjp1, kk)
01044      + VAT3( uPN, ii, jj, kk) * VAT3( oE, im1, jp1, kp1) * VAT3(uPSE, iim1, jjp1, kk);
01045
01046      //fprintf(data, "%19.12E\n", VAT3(XoNW, ii, jj, kk));
01047
01048      /* *****
01049      * *** > uE;
01050      * *****/
01051
01052      VAT3( XuE, ii, jj, kk) =
01053          VAT3( uPS, ii, jj, kk) * VAT3( oE, i, jml, kp1) * VAT3(dPSW, iip1, jj, kkp1)
01054      + VAT3( uPC, ii, jj, kk) * VAT3( oE, i, j, kp1) * VAT3( dPW, iip1, jj, kkp1)
01055      + VAT3( uPN, ii, jj, kk) * VAT3( oE, i, jp1, kp1) * VAT3(dPNW, iip1, jj, kkp1)
01056      + VAT3(oPSE, ii, jj, kk) * VAT3( uC, ip1, jml, k) * VAT3(dPSW, iip1, jj, kkp1)
01057
01058      - VAT3(uPSE, ii, jj, kk) * ( VAT3( oC, ip1, jml, kp1) * VAT3(dPSW, iip1, jj, kkp1)
01059          - VAT3( uC, ip1, jml, kp1) * VAT3(oPSW, iip1, jj, kkp1)
01060          - VAT3( oN, ip1, jml, kp1) * VAT3( dPW, iip1, jj, kkp1)
01061          - VAT3( oE, ip1, jml, kp1) * VAT3( dPS, iip1, jj, kkp1))
01062
01063      + VAT3( oPE, ii, jj, kk) * VAT3( uC, ip1, j, k) * VAT3( dPW, iip1, jj, kkp1)
01064
01065      - VAT3( uPE, ii, jj, kk) * (- VAT3( oN, ip1, jml, kp1) * VAT3(dPSW, iip1, jj, kkp1)
01066          + VAT3( oC, ip1, j, kp1) * VAT3( dPW, iip1, jj, kkp1)
01067          - VAT3( uC, ip1, j, kp1) * VAT3( oPW, iip1, jj, kkp1)
01068          - VAT3( oN, ip1, j, kp1) * VAT3(dPNW, iip1, jj, kkp1)
01069          - VAT3( oE, ip1, j, kp1) * VAT3( dPC, iip1, jj, kkp1))
01070
01071      + VAT3(oPNE, ii, jj, kk) * VAT3( uC, ip1, jp1, k) * VAT3(dPNW, iip1, jj, kkp1)
01072
01073      - VAT3(uPNE, ii, jj, kk) * (- VAT3( oN, ip1, j, kp1) * VAT3( dPW, iip1, jj, kkp1)
01074          + VAT3( oC, ip1, jp1, kp1) * VAT3(dPNW, iip1, jj, kkp1)
01075          - VAT3( uC, ip1, jp1, kp1) * VAT3(oPNW, iip1, jj, kkp1)
01076          - VAT3( oE, ip1, jp1, kp1) * VAT3( dPN, iip1, jj, kkp1));
01077
01078      //fprintf(data, "%19.12E\n", VAT3(XuE, ii, jj, kk));
01079
01080      /* *****
01081      * *** > uW;
01082      * *****/
01083
01084      VAT3( XuW, ii, jj, kk) =
01085          VAT3(oPSW, ii, jj, kk) * VAT3( uC, im1, jml, k) * VAT3(dPSE, iim1, jj, kkp1)
01086
01087      - VAT3(uPSW, ii, jj, kk) * (- VAT3( oE, im2, jml, kp1) * VAT3( dPS, iim1, jj, kkp1)
01088          + VAT3( oC, im1, jml, kp1) * VAT3(dPSE, iim1, jj, kkp1)
01089          - VAT3( uC, im1, jml, kp1) * VAT3(oPSE, iim1, jj, kkp1)
01090          - VAT3( oN, im1, jml, kp1) * VAT3( dPE, iim1, jj, kkp1))
01091
01092      + VAT3( oPW, ii, jj, kk) * VAT3( uC, im1, j, k) * VAT3( dPE, iim1, jj, kkp1)
01093
01094      - VAT3( uPW, ii, jj, kk) * (- VAT3( oE, im2, j, kp1) * VAT3( dPC, iim1, jj, kkp1)
01095          - VAT3( oN, im1, jml, kp1) * VAT3(dPSE, iim1, jj, kkp1)
01096          + VAT3( oC, im1, j, kp1) * VAT3( dPE, iim1, jj, kkp1)
01097          - VAT3( uC, im1, j, kp1) * VAT3( oPE, iim1, jj, kkp1)

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01098             - VAT3( oN, iM1,j,kp1) * VAT3(dPNE, iim1,jj,kkp1))
01099
01100 + VAT3(oPNW, ii,jj,kk) * VAT3( uC, iM1,jp1,k) * VAT3(dPNE, iim1,jj,kkp1)
01101
01102 - VAT3(uPNW, ii,jj,kk) * ( - VAT3( oE, iM2,jp1,kp1) * VAT3( dPN, iim1,jj,kkp1)
01103             - VAT3( oN, iM1,j,kp1) * VAT3( dPE, iim1,jj,kkp1)
01104             + VAT3( oC, iM1,jp1,kp1) * VAT3(dPNE, iim1,jj,kkp1)
01105             - VAT3( uC, iM1,jp1,kp1) * VAT3(oPNE, iim1,jj,kkp1))
01106
01107 + VAT3( uPS, ii,jj,kk) * VAT3( oE, iM1,jM1,kp1) * VAT3(dPSE, iim1,jj,kkp1)
01108 + VAT3( uPC, ii,jj,kk) * VAT3( oE, iM1,j,kp1) * VAT3( dPE, iim1,jj,kkp1)
01109 + VAT3( uPN, ii,jj,kk) * VAT3( oE, iM1,jp1,kp1) * VAT3(dPNE, iim1,jj,kkp1);
01110
01111 //fprintf(data, "%19.12E\n", VAT3(XuW, ii, jj, kk));
01112
01113 /* *****
01114  * *** > uN;
01115  * *****/
01116
01117 VAT3( XuN, ii,jj,kk) =
01118     VAT3( uPW, ii,jj,kk) * VAT3( oN, iM1,j,kp1) * VAT3(dPSW, ii,jjp1,kkp1)
01119 + VAT3(oPNW, ii,jj,kk) * VAT3( uC, iM1,jp1,k) * VAT3(dPSW, ii,jjp1,kkp1)
01120
01121 - VAT3(uPNW, ii,jj,kk) * ( VAT3( oC, iM1,jp1,kp1) * VAT3(dPSW, ii,jjp1,kkp1)
01122             - VAT3( uC, iM1,jp1,kp1) * VAT3(oPSW, ii,jjp1,kkp1)
01123             - VAT3( oN, iM1,jp1,kp1) * VAT3( dPW, ii,jjp1,kkp1)
01124             - VAT3( oE, iM1,jp1,kp1) * VAT3( dPS, ii,jjp1,kkp1))
01125
01126 + VAT3( uPC, ii,jj,kk) * VAT3( oN, i,j,kp1) * VAT3( dPS, ii,jjp1,kkp1)
01127 + VAT3( oPN, ii,jj,kk) * VAT3( uC, i,jp1,k) * VAT3( dPS, ii,jjp1,kkp1)
01128
01129 - VAT3( uPN, ii,jj,kk) * ( - VAT3( oE, iM1,jp1,kp1) * VAT3(dPSW, ii,jjp1,kkp1)
01130             + VAT3( oC, i,jp1,kp1) * VAT3( dPS, ii,jjp1,kkp1)
01131             - VAT3( uC, i,jp1,kp1) * VAT3( oPS, ii,jjp1,kkp1)
01132             - VAT3( oN, i,jp1,kp1) * VAT3( dPC, ii,jjp1,kkp1)
01133             - VAT3( oE, i,jp1,kp1) * VAT3(dPSE, ii,jjp1,kkp1))
01134
01135 + VAT3( uPE, ii,jj,kk) * VAT3( oN, iM1,j,kp1) * VAT3(dPSE, ii,jjp1,kkp1)
01136 + VAT3(oPNE, ii,jj,kk) * VAT3( uC, iM1,jp1,k) * VAT3(dPSE, ii,jjp1,kkp1)
01137
01138 - VAT3(uPNE, ii,jj,kk) * ( - VAT3( oE, i,jp1,kp1) * VAT3( dPS, ii,jjp1,kkp1)
01139             + VAT3( oC, iM1,jp1,kp1) * VAT3(dPSE, ii,jjp1,kkp1)
01140             - VAT3( uC, iM1,jp1,kp1) * VAT3(oPSE, ii,jjp1,kkp1)
01141             - VAT3( oN, iM1,jp1,kp1) * VAT3( dPE, ii,jjp1,kkp1));
01142
01143 //fprintf(data, "%19.12E\n", VAT3(XuN, ii, jj, kk));
01144
01145 /* *****
01146  * *** > uS;
01147  * *****/
01148
01149 VAT3( XuS, ii,jj,kk) =
01150     VAT3(oPSW, ii,jj,kk) * VAT3( uC, iM1,jM1,k) * VAT3(dPNW, ii,jjM1,kkp1)
01151
01152 - VAT3(uPSW, ii,jj,kk) * ( - VAT3( oN, iM1,jM2,kp1) * VAT3( dPW, ii,jjM1,kkp1)
01153             + VAT3( oC, iM1,jM1,kp1) * VAT3(dPNW, ii,jjM1,kkp1)
01154             - VAT3( uC, iM1,jM1,kp1) * VAT3(oPNW, ii,jjM1,kkp1)
01155             - VAT3( oE, iM1,jM1,kp1) * VAT3( dPN, ii,jjM1,kkp1))
01156
01157 + VAT3( uPW, ii,jj,kk) * VAT3( oN, iM1,jM1,kp1) * VAT3(dPNW, ii,jjM1,kkp1)
01158 + VAT3( oPS, ii,jj,kk) * VAT3( uC, i,jM1,k) * VAT3( dPN, ii,jjM1,kkp1)
01159
01160 - VAT3( uPS, ii,jj,kk) * ( - VAT3( oE, iM1,jM1,kp1) * VAT3(dPNW, ii,jjM1,kkp1)
01161             - VAT3( oN, i,jM2,kp1) * VAT3( dPC, ii,jjM1,kkp1)
01162             + VAT3( oC, i,jM1,kp1) * VAT3( dPN, ii,jjM1,kkp1)
01163             - VAT3( uC, i,jM1,kp1) * VAT3( oPN, ii,jjM1,kkp1)
01164             - VAT3( oE, i,jM1,kp1) * VAT3(dPNE, ii,jjM1,kkp1))
01165
01166 + VAT3( uPC, ii,jj,kk) * VAT3( oN, i,jM1,kp1) * VAT3( dPN, ii,jjM1,kkp1)
01167 + VAT3(oPSE, ii,jj,kk) * VAT3( uC, iM1,jM1,k) * VAT3(dPNE, ii,jjM1,kkp1)
01168
01169 - VAT3(uPSE, ii,jj,kk) * ( - VAT3( oE, i,jM1,kp1) * VAT3( dPN, ii,jjM1,kkp1)
01170             - VAT3( oN, iM1,jM2,kp1) * VAT3( dPE, ii,jjM1,kkp1)
01171             + VAT3( oC, iM1,jM1,kp1) * VAT3(dPNE, ii,jjM1,kkp1)
01172             - VAT3( uC, iM1,jM1,kp1) * VAT3(oPNE, ii,jjM1,kkp1))
01173
01174 + VAT3( uPE, ii,jj,kk) * VAT3( oN, iM1,jM1,kp1) * VAT3(dPNE, ii,jjM1,kkp1);
01175
01176 //fprintf(data, "%19.12E\n", VAT3(XuS, ii, jj, kk));
01177
01178 /* *****

```

```

01179         * *** > uNE;
01180         * *****/
01181
01182     VAT3(XuNE, ii, jj, kk) =
01183         VAT3( uPN, ii, jj, kk) * VAT3( oE, i, jpl, kpl) * VAT3(dPSW, iip1, jjp1, kkp1)
01184     + VAT3( uPE, ii, jj, kk) * VAT3( oN, ip1, j, kpl) * VAT3(dPSW, iip1, jjp1, kkp1)
01185     + VAT3(oPNE, ii, jj, kk) * VAT3( uC, ip1, jpl, k) * VAT3(dPSW, iip1, jjp1, kkp1)
01186
01187     - VAT3(uPNE, ii, jj, kk) * ( VAT3( oC, ip1, jpl, kpl) * VAT3(dPSW, iip1, jjp1, kkp1)
01188         - VAT3( uC, ip1, jpl, kpl) * VAT3(oPSW, iip1, jjp1, kkp1)
01189         - VAT3( oN, ip1, jpl, kpl) * VAT3( dPW, iip1, jjp1, kkp1)
01190         - VAT3( oE, ip1, jpl, kpl) * VAT3( dPS, iip1, jjp1, kkp1));
01191
01192     //fprintf(data, "%19.12E\n", VAT3(XuNE, ii, jj, kk));
01193
01194     /* *****/
01195     * *** > uNW;
01196     * *****/
01197
01198     VAT3(XuNW, ii, jj, kk) =
01199         VAT3( uPW, ii, jj, kk) * VAT3( oN, im1, j, kpl) * VAT3(dPSE, iim1, jjp1, kkp1)
01200     + VAT3(oPNW, ii, jj, kk) * VAT3( uC, im1, jpl, k) * VAT3(dPSE, iim1, jjp1, kkp1)
01201
01202     - VAT3(uPNW, ii, jj, kk) * ( - VAT3( oE, im2, jpl, kpl) * VAT3( dPS, iim1, jjp1, kkp1)
01203         + VAT3( oC, im1, jpl, kpl) * VAT3(dPSE, iim1, jjp1, kkp1)
01204         - VAT3( uC, im1, jpl, kpl) * VAT3(oPSE, iim1, jjp1, kkp1)
01205         - VAT3( oN, im1, jpl, kpl) * VAT3( dPE, iim1, jjp1, kkp1))
01206
01207     + VAT3( uPN, ii, jj, kk) * VAT3( oE, im1, jpl, kpl) * VAT3(dPSE, iim1, jjp1, kkp1);
01208
01209     //fprintf(data, "%19.12E\n", VAT3(XuNW, ii, jj, kk));
01210
01211     /* *****/
01212     * *** > uSE;
01213     * *****/
01214
01215     VAT3(XuSE, ii, jj, kk) =
01216         VAT3( uPS, ii, jj, kk) * VAT3( oE, i, jml, kpl) * VAT3(dPNW, iip1, jjml, kkp1)
01217     + VAT3(oPSE, ii, jj, kk) * VAT3( uC, ip1, jml, k) * VAT3(dPNW, iip1, jjml, kkp1)
01218
01219     - VAT3(uPSE, ii, jj, kk) * ( - VAT3( oN, ip1, jml, kpl) * VAT3( dPW, iip1, jjml, kkp1)
01220         + VAT3( oC, ip1, jml, kpl) * VAT3(dPNW, iip1, jjml, kkp1)
01221         - VAT3( uC, ip1, jml, kpl) * VAT3(oPNW, iip1, jjml, kkp1)
01222         - VAT3( oE, ip1, jml, kpl) * VAT3( dPN, iip1, jjml, kkp1))
01223
01224     + VAT3( uPE, ii, jj, kk) * VAT3( oN, ip1, jml, kpl) * VAT3(dPNW, iip1, jjml, kkp1);
01225
01226     //fprintf(data, "%19.12E\n", VAT3(XuSE, ii, jj, kk));
01227
01228     /* *****/
01229     * *** > uSW;
01230     * *****/
01231
01232     VAT3(XuSW, ii, jj, kk) =
01233         VAT3(oPSW, ii, jj, kk) * VAT3( uC, im1, jml, k) * VAT3(dPNE, iim1, jjml, kkp1)
01234
01235     - VAT3(uPSW, ii, jj, kk) * ( - VAT3( oE, im2, jml, kpl) * VAT3( dPN, iim1, jjml, kkp1)
01236         - VAT3( oN, im1, jml, kpl) * VAT3( dPE, iim1, jjml, kkp1)
01237         + VAT3( oC, im1, jml, kpl) * VAT3(dPNE, iim1, jjml, kkp1)
01238         - VAT3( uC, im1, jml, kpl) * VAT3(oPNE, iim1, jjml, kkp1))
01239
01240     + VAT3( uPW, ii, jj, kk) * VAT3( oN, im1, jml, kpl) * VAT3(dPNE, iim1, jjml, kkp1)
01241     + VAT3( uPS, ii, jj, kk) * VAT3( oE, im1, jml, kpl) * VAT3(dPNE, iim1, jjml, kkp1);
01242
01243     //fprintf(data, "%19.12E\n", VAT3(XuSW, ii, jj, kk));
01244
01245     }
01246 }
01247 }
01248 }
01249
01250
01251
01252 VPUBLIC void VbuildG_27(int *nxf, int *nyf, int *nzf,
01253     int *nx, int *ny, int *nz,
01254     double *oPC, double *oPN, double *oPS, double *oPE, double *oPW,
01255     double *oPNE, double *oPNW, double *oPSE, double *oPSW,
01256     double *uPC, double *uPN, double *uPS, double *uPE, double *uPW,
01257     double *uPNE, double *uPNW, double *uPSE, double *uPSW,
01258     double *dPC, double *dPN, double *dPS, double *dPE, double *dPW,
01259     double *dPNE, double *dPNW, double *dPSE, double *dPSW,

```

```

01260         double *oC,    double *oE,    double *oN,    double *uC,
01261         double *oNE,    double *oNW,    double *uE,    double *uW,    double *uN,
01262         double *uS,     double *uNE,    double *uNW,    double *uSE,    double *uSW,
01263         double *XoC,    double *XoE,    double *XoN,
01264         double *XuC,
01265         double *XoNE,    double *XoNW,
01266         double *XuE,    double *XuW,    double *XuN,    double *XuS,
01267         double *XuNE,    double *XuNW,    double *XuSE,    double *XuSW) {
01268
01269     int    i,      j,      k;
01270     int    ii,     jj,     kk;
01271     int    im1,    ip1,    im2,    ip2;
01272     int    jm1,    jp1,    jm2,    jp2;
01273     int    km1,    kp1,    km2,    kp2;
01274     int    iim1,   iip1;
01275     int    jjm1,   jjp1;
01276     int    kkm1,   kkp1;
01277     int    nxm1,   nym1,   nzm1;
01278
01279     double  TMP1_XOC,  TMP2_XOC,  TMP3_XOC,  TMP4_XOC;
01280     double  TMP5_XOC,  TMP6_XOC,  TMP7_XOC,  TMP8_XOC;
01281     double  TMP9_XOC,  TMP10_XOC, TMP11_XOC, TMP12_XOC;
01282     double  TMP13_XOC, TMP14_XOC, TMP15_XOC, TMP16_XOC;
01283     double  TMP17_XOC, TMP18_XOC, TMP19_XOC, TMP20_XOC;
01284     double  TMP21_XOC, TMP22_XOC, TMP23_XOC, TMP24_XOC;
01285     double  TMP25_XOC, TMP26_XOC, TMP27_XOC;
01286
01287     double  TMP1_XOE,  TMP2_XOE,  TMP3_XOE,  TMP4_XOE;
01288     double  TMP5_XOE,  TMP6_XOE,  TMP7_XOE,  TMP8_XOE;
01289     double  TMP9_XOE,  TMP10_XOE, TMP11_XOE, TMP12_XOE;
01290
01291     double  TMP1_XON,  TMP2_XON,  TMP3_XON,  TMP4_XON;
01292     double  TMP5_XON,  TMP6_XON,  TMP7_XON,  TMP8_XON;
01293     double  TMP9_XON,  TMP10_XON, TMP11_XON, TMP12_XON;
01294
01295     double  TMP1_XUC,  TMP2_XUC,  TMP3_XUC,  TMP4_XUC;
01296     double  TMP5_XUC,  TMP6_XUC,  TMP7_XUC,  TMP8_XUC;
01297     double  TMP9_XUC,  TMP10_XUC, TMP11_XUC, TMP12_XUC;
01298
01299     double  TMP1_XONE, TMP2_XONE, TMP3_XONE, TMP4_XONE;
01300     double  TMP5_XONE, TMP6_XONE;
01301
01302     double  TMP1_XONW, TMP2_XONW, TMP3_XONW, TMP4_XONW;
01303     double  TMP5_XONW, TMP6_XONW;
01304
01305     double  TMP1_XUE,  TMP2_XUE,  TMP3_XUE,  TMP4_XUE;
01306     double  TMP5_XUE,  TMP6_XUE;
01307
01308     double  TMP1_XUW,  TMP2_XUW,  TMP3_XUW,  TMP4_XUW;
01309     double  TMP5_XUW,  TMP6_XUW;
01310
01311     double  TMP1_XUN,  TMP2_XUN,  TMP3_XUN,  TMP4_XUN;
01312     double  TMP5_XUN,  TMP6_XUN;
01313
01314     double  TMP1_XUS,  TMP2_XUS,  TMP3_XUS,  TMP4_XUS;
01315     double  TMP5_XUS,  TMP6_XUS;
01316
01317     double  TMP1_XUNE, TMP2_XUNE, TMP1_XUNW, TMP2_XUNW;
01318     double  TMP1_XUSE, TMP2_XUSE, TMP1_XUSW, TMP2_XUSW;
01319
01320     MAT3( oC, *nxf, *nyf, *nzf);
01321     MAT3( oE, *nxf, *nyf, *nzf);
01322     MAT3( oN, *nxf, *nyf, *nzf);
01323     MAT3( oNE, *nxf, *nyf, *nzf);
01324     MAT3( oNW, *nxf, *nyf, *nzf);
01325
01326     MAT3( uC, *nxf, *nyf, *nzf);
01327     MAT3( uE, *nxf, *nyf, *nzf);
01328     MAT3( uW, *nxf, *nyf, *nzf);
01329     MAT3( uN, *nxf, *nyf, *nzf);
01330     MAT3( uS, *nxf, *nyf, *nzf);
01331     MAT3( uNE, *nxf, *nyf, *nzf);
01332     MAT3( uNW, *nxf, *nyf, *nzf);
01333     MAT3( uSE, *nxf, *nyf, *nzf);
01334     MAT3( uSW, *nxf, *nyf, *nzf);
01335
01336     MAT3( XoC, *nx, *ny, *nz);
01337     MAT3( XoE, *nx, *ny, *nz);
01338     MAT3( XoN, *nx, *ny, *nz);
01339     MAT3( XoNE, *nx, *ny, *nz);
01340     MAT3( XoNW, *nx, *ny, *nz);

```



```

01341
01342     MAT3( XuC, *nx, *ny, *nz);
01343     MAT3( XuE, *nx, *ny, *nz);
01344     MAT3( XuW, *nx, *ny, *nz);
01345     MAT3( XuN, *nx, *ny, *nz);
01346     MAT3( XuS, *nx, *ny, *nz);
01347     MAT3( XuNE, *nx, *ny, *nz);
01348     MAT3( XuNW, *nx, *ny, *nz);
01349     MAT3( XuSE, *nx, *ny, *nz);
01350     MAT3( XuSW, *nx, *ny, *nz);
01351
01352     MAT3( oPC, *nx, *ny, *nz);
01353     MAT3( oPN, *nx, *ny, *nz);
01354     MAT3( oPS, *nx, *ny, *nz);
01355     MAT3( oPE, *nx, *ny, *nz);
01356     MAT3( oPW, *nx, *ny, *nz);
01357     MAT3( oPNE, *nx, *ny, *nz);
01358     MAT3( oPNW, *nx, *ny, *nz);
01359     MAT3( oPSE, *nx, *ny, *nz);
01360     MAT3( oPSW, *nx, *ny, *nz);
01361
01362     MAT3( uPC, *nx, *ny, *nz);
01363     MAT3( uPN, *nx, *ny, *nz);
01364     MAT3( uPS, *nx, *ny, *nz);
01365     MAT3( uPE, *nx, *ny, *nz);
01366     MAT3( uPW, *nx, *ny, *nz);
01367     MAT3( uPNE, *nx, *ny, *nz);
01368     MAT3( uPNW, *nx, *ny, *nz);
01369     MAT3( uPSE, *nx, *ny, *nz);
01370     MAT3( uPSW, *nx, *ny, *nz);
01371
01372     MAT3( dPC, *nx, *ny, *nz);
01373     MAT3( dPN, *nx, *ny, *nz);
01374     MAT3( dPS, *nx, *ny, *nz);
01375     MAT3( dPE, *nx, *ny, *nz);
01376     MAT3( dPW, *nx, *ny, *nz);
01377     MAT3( dPNE, *nx, *ny, *nz);
01378     MAT3( dPNW, *nx, *ny, *nz);
01379     MAT3( dPSE, *nx, *ny, *nz);
01380     MAT3( dPSW, *nx, *ny, *nz);
01381
01382     // define n and determine number of mesh points ***
01383     nxm1 = *nx - 1;
01384     nym1 = *ny - 1;
01385     nzm1 = *nz - 1;
01386
01387     //fprintf(data, "%s\n", PRINT_FUNC);
01388
01389     // Build the operator ***
01390     for(kk=2; kk<=*nz-1; kk++) {
01391         k = 2 * kk - 1;
01392
01393         for(jj=2; jj<=*ny-1; jj++) {
01394             j = 2 * jj - 1;
01395
01396             for(ii=2; ii<=*nx-1; ii++) {
01397                 i = 2 * ii - 1;
01398
01399                 // Index computations
01400                 im1 = i - 1;
01401                 ip1 = i + 1;
01402                 im2 = i - 2;
01403                 ip2 = i + 2;
01404                 jm1 = j - 1;
01405                 jp1 = j + 1;
01406                 jm2 = j - 2;
01407                 jp2 = j + 2;
01408                 km1 = k - 1;
01409                 kp1 = k + 1;
01410                 km2 = k - 2;
01411                 kp2 = k + 2;
01412                 iim1 = ii - 1;
01413                 iip1 = ii + 1;
01414                 jjm1 = jj - 1;
01415                 jjp1 = jj + 1;
01416                 kkm1 = kk - 1;
01417                 kkp1 = kk + 1;
01418
01419
01420
01421         /* *****

```

```

01422      * *** > oC;
01423      * *****/
01424
01425      // VAT3( XoC, ii,jj,kk) =
01426      TMP1_XOC =
01427          VAT3( oPN, ii,jj,kk) * (- VAT3( uNE, im1,j,km1) * VAT3( dPW, ii,jj,kk)
01428              - VAT3( oNE, im1,j,k) * VAT3( oPW, ii,jj,kk)
01429              - VAT3( uSW, i,jp1,k) * VAT3( uPW, ii,jj,kk)
01430              - VAT3( uE, im1,jp1,km1) * VAT3( dPNW, ii,jj,kk)
01431              - VAT3( oE, im1,jp1,k) * VAT3( oPNW, ii,jj,kk)
01432              - VAT3( uW, i,jp1,k) * VAT3( uPNW, ii,jj,kk)
01433              - VAT3( uN, i,j,km1) * VAT3( dPC, ii,jj,kk)
01434              - VAT3( oN, i,j,k) * VAT3( oPC, ii,jj,kk)
01435              - VAT3( uS, i,jp1,k) * VAT3( uPC, ii,jj,kk)
01436              - VAT3( uC, i,jp1,km1) * VAT3( dPN, ii,jj,kk)
01437              + VAT3( oC, i,jp1,k) * VAT3( oPN, ii,jj,kk)
01438              - VAT3( uC, i,jp1,k) * VAT3( uPN, ii,jj,kk)
01439              - VAT3( uNW, ip1,j,km1) * VAT3( dPE, ii,jj,kk)
01440              - VAT3( oNW, ip1,j,k) * VAT3( oPE, ii,jj,kk)
01441              - VAT3( uSE, i,jp1,k) * VAT3( uPE, ii,jj,kk)
01442              - VAT3( uW, ip1,jp1,km1) * VAT3( dPNE, ii,jj,kk)
01443              - VAT3( oE, i,jp1,k) * VAT3( oPNE, ii,jj,kk)
01444              - VAT3( uE, i,jp1,k) * VAT3( uPNE, ii,jj,kk));
01445
01446      TMP2_XOC =
01447          + VAT3( dPN, ii,jj,kk) * (- VAT3( oNE, im1,j,km1) * VAT3( dPW, ii,jj,kk)
01448              - VAT3( uSW, i,jp1,km1) * VAT3( oPW, ii,jj,kk)
01449              - VAT3( oE, im1,jp1,km1) * VAT3( dPNW, ii,jj,kk)
01450              - VAT3( uW, i,jp1,km1) * VAT3( oPNW, ii,jj,kk)
01451              - VAT3( oN, i,j,km1) * VAT3( dPC, ii,jj,kk)
01452              - VAT3( uS, i,jp1,km1) * VAT3( oPC, ii,jj,kk)
01453              + VAT3( oC, i,jp1,km1) * VAT3( dPN, ii,jj,kk)
01454              - VAT3( uC, i,jp1,km1) * VAT3( oPN, ii,jj,kk)
01455              - VAT3( oNW, ip1,j,km1) * VAT3( dPE, ii,jj,kk)
01456              - VAT3( uSE, i,jp1,km1) * VAT3( oPE, ii,jj,kk)
01457              - VAT3( oE, i,jp1,km1) * VAT3( dPNE, ii,jj,kk)
01458              - VAT3( uE, i,jp1,km1) * VAT3( oPNE, ii,jj,kk));
01459
01460      TMP3_XOC =
01461          + VAT3( dPC, ii,jj,kk) * (- VAT3( oNE, im1,jm1,km1) * VAT3( dPSW, ii,jj,kk)
01462              - VAT3( uSW, i,j,km1) * VAT3( oPSW, ii,jj,kk)
01463              - VAT3( oE, im1,j,km1) * VAT3( dPW, ii,jj,kk)
01464              - VAT3( uW, i,j,km1) * VAT3( oPW, ii,jj,kk)
01465              - VAT3( oNW, i,j,km1) * VAT3( dPNW, ii,jj,kk)
01466              - VAT3( uNW, i,j,km1) * VAT3( oPNW, ii,jj,kk)
01467              - VAT3( oN, i,jm1,km1) * VAT3( dPS, ii,jj,kk)
01468              - VAT3( uS, i,j,km1) * VAT3( oPS, ii,jj,kk)
01469              + VAT3( oC, i,j,km1) * VAT3( dPC, ii,jj,kk)
01470              - VAT3( uC, i,j,km1) * VAT3( oPC, ii,jj,kk)
01471              - VAT3( oN, i,j,km1) * VAT3( dPN, ii,jj,kk)
01472              - VAT3( uN, i,j,km1) * VAT3( oPN, ii,jj,kk)
01473              - VAT3( oNW, ip1,jm1,km1) * VAT3( dPSE, ii,jj,kk)
01474              - VAT3( uSE, i,j,km1) * VAT3( oPSE, ii,jj,kk)
01475              - VAT3( oE, i,j,km1) * VAT3( dPE, ii,jj,kk)
01476              - VAT3( uE, i,j,km1) * VAT3( oPE, ii,jj,kk)
01477              - VAT3( oNE, i,j,km1) * VAT3( dPNE, ii,jj,kk)
01478              - VAT3( uNE, i,j,km1) * VAT3( oPNE, ii,jj,kk));
01479
01480      TMP4_XOC =
01481          + VAT3( uPC, ii,jj,kk) * (- VAT3( uNE, im1,jm1,k) * VAT3( oPSW, ii,jj,kk)
01482              - VAT3( oNE, im1,jm1,kp1) * VAT3( uPSW, ii,jj,kk)
01483              - VAT3( uE, im1,j,k) * VAT3( oPW, ii,jj,kk)
01484              - VAT3( oE, im1,j,kp1) * VAT3( uPW, ii,jj,kk)
01485              - VAT3( uSE, im1,jp1,k) * VAT3( oPNW, ii,jj,kk)
01486              - VAT3( oNW, i,j,kp1) * VAT3( uPNW, ii,jj,kk)
01487              - VAT3( uN, i,jm1,k) * VAT3( oPS, ii,jj,kk)
01488              - VAT3( oN, i,jm1,kp1) * VAT3( uPS, ii,jj,kk)
01489              - VAT3( uC, i,j,k) * VAT3( oPC, ii,jj,kk)
01490              + VAT3( oC, i,j,kp1) * VAT3( uPC, ii,jj,kk)
01491              - VAT3( uS, i,jp1,k) * VAT3( oPN, ii,jj,kk)
01492              - VAT3( oN, i,j,kp1) * VAT3( uPN, ii,jj,kk)
01493              - VAT3( uNW, ip1,jm1,k) * VAT3( oPSE, ii,jj,kk)
01494              - VAT3( oNW, ip1,jm1,kp1) * VAT3( uPSE, ii,jj,kk)
01495              - VAT3( uW, ip1,j,k) * VAT3( oPE, ii,jj,kk)
01496              - VAT3( oE, i,j,kp1) * VAT3( uPE, ii,jj,kk)
01497              - VAT3( uSW, ip1,jp1,k) * VAT3( oPNE, ii,jj,kk)
01498              - VAT3( oNE, i,j,kp1) * VAT3( uPNE, ii,jj,kk));
01499
01500      TMP5_XOC =
01501          + VAT3( oPC, ii,jj,kk) * (- VAT3( uW, ip1,j,km1) * VAT3( dPE, ii,jj,kk)
01502              - VAT3( oE, im1,j,k) * VAT3( oPW, ii,jj,kk)

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01503         - VAT3( uSE, im1,jp1,km1) * VAT3(dPNW, ii,jj,kk)
01504         - VAT3( uNE, im1,jm1,km1) * VAT3(dPSW, ii,jj,kk)
01505         - VAT3( uN, i,jm1,km1) * VAT3( dPS, ii,jj,kk)
01506         - VAT3( oNE, im1,jm1,k) * VAT3(oPSW, ii,jj,kk)
01507         - VAT3( uE, im1,j,km1) * VAT3( dPW, ii,jj,kk)
01508         - VAT3( oNW, ip1,jm1,k) * VAT3(oPSE, ii,jj,kk)
01509         - VAT3( uC, i,j,km1) * VAT3( dPC, ii,jj,kk)
01510         - VAT3( uNW, ip1,jm1,km1) * VAT3(dPSE, ii,jj,kk)
01511         - VAT3( uSW, ip1,jp1,km1) * VAT3(dPNE, ii,jj,kk)
01512     - VAT3( uS, i,jp1,km1) * VAT3( dPN, ii,jj,kk) - VAT3( oN, i,jm1,k) * VAT3( oPS, ii,jj,kk)
01513     - VAT3( uNE, i,j,k) * VAT3(uPNE, ii,jj,kk) - VAT3( oNE, i,j,k) * VAT3(oPNE, ii,jj,kk)
01514     - VAT3( uE, i,j,k) * VAT3( uPE, ii,jj,kk) - VAT3( uSE, i,j,k) * VAT3(uPSE, ii,jj,kk)
01515     - VAT3( oN, i,j,k) * VAT3( oPN, ii,jj,kk) - VAT3( oE, i,j,k) * VAT3( oPE, ii,jj,kk)
01516     - VAT3( uS, i,j,k) * VAT3( uPS, ii,jj,kk) + VAT3( oC, i,j,k) * VAT3( oPC, ii,jj,kk)
01517     - VAT3( uSW, i,j,k) * VAT3(uPSW, ii,jj,kk) - VAT3( uN, i,j,k) * VAT3( uPN, ii,jj,kk)
01518     - VAT3( uC, i,j,k) * VAT3( uPC, ii,jj,kk) - VAT3( uW, i,j,k) * VAT3( uPW, ii,jj,kk)
01519     - VAT3( oNW, i,j,k) * VAT3(oPNW, ii,jj,kk) - VAT3( uNW, i,j,k) * VAT3(uPNW, ii,jj,kk));
01520
01521 TMP6_XOC =
01522     + VAT3( uPS, ii,jj,kk) * (- VAT3( uE, im1,jm1,k) * VAT3(oPSW, ii,jj,kk)
01523         - VAT3( oE, im1,jm1,kp1) * VAT3(uPSW, ii,jj,kk)
01524         - VAT3( uSE, im1,j,k) * VAT3( oPW, ii,jj,kk)
01525         - VAT3( oNW, i,jm1,kp1) * VAT3( uPW, ii,jj,kk)
01526         - VAT3( uC, i,jm1,k) * VAT3( oPS, ii,jj,kk)
01527         + VAT3( oC, i,jm1,kp1) * VAT3( uPS, ii,jj,kk)
01528         - VAT3( uS, i,j,k) * VAT3( oPC, ii,jj,kk)
01529         - VAT3( oN, i,jm1,kp1) * VAT3( uPC, ii,jj,kk)
01530         - VAT3( uW, ip1,jm1,k) * VAT3(oPSE, ii,jj,kk)
01531         - VAT3( oE, i,jm1,kp1) * VAT3(uPSE, ii,jj,kk)
01532         - VAT3( uSW, ip1,j,k) * VAT3( oPE, ii,jj,kk)
01533         - VAT3( oNE, i,jm1,kp1) * VAT3( uPE, ii,jj,kk));
01534
01535 TMP7_XOC =
01536     + VAT3( oPS, ii,jj,kk) * (- VAT3( uE, im1,jm1,km1) * VAT3(dPSW, ii,jj,kk)
01537         - VAT3( oE, im1,jm1,k) * VAT3(oPSW, ii,jj,kk)
01538         - VAT3( uW, i,jm1,k) * VAT3(uPSW, ii,jj,kk)
01539         - VAT3( uSE, im1,j,km1) * VAT3( dPW, ii,jj,kk)
01540         - VAT3( oNW, i,jm1,k) * VAT3( oPW, ii,jj,kk)
01541         - VAT3( uNW, i,jm1,k) * VAT3( uPW, ii,jj,kk)
01542         - VAT3( uC, i,jm1,km1) * VAT3( dPS, ii,jj,kk)
01543         + VAT3( oC, i,jm1,k) * VAT3( oPS, ii,jj,kk)
01544         - VAT3( uC, i,jm1,k) * VAT3( uPS, ii,jj,kk)
01545         - VAT3( uS, i,j,km1) * VAT3( dPC, ii,jj,kk)
01546         - VAT3( oN, i,jm1,k) * VAT3( oPC, ii,jj,kk)
01547         - VAT3( uN, i,jm1,k) * VAT3( uPC, ii,jj,kk)
01548         - VAT3( uW, ip1,jm1,km1) * VAT3(dPSE, ii,jj,kk)
01549         - VAT3( oE, i,jm1,k) * VAT3(oPSE, ii,jj,kk)
01550         - VAT3( uE, i,jm1,k) * VAT3(uPSE, ii,jj,kk)
01551         - VAT3( uSW, ip1,j,km1) * VAT3( dPE, ii,jj,kk)
01552         - VAT3( oNE, i,jm1,k) * VAT3( oPE, ii,jj,kk)
01553         - VAT3( uNE, i,jm1,k) * VAT3( uPE, ii,jj,kk));
01554
01555 TMP8_XOC =
01556     + VAT3( dPS, ii,jj,kk) * (- VAT3( oE, im1,jm1,km1) * VAT3(dPSW, ii,jj,kk)
01557         - VAT3( uW, i,jm1,km1) * VAT3(oPSW, ii,jj,kk)
01558         - VAT3( oNW, i,jm1,km1) * VAT3( dPW, ii,jj,kk)
01559         - VAT3( uNW, i,jm1,km1) * VAT3( oPW, ii,jj,kk)
01560         + VAT3( oC, i,jm1,km1) * VAT3( dPS, ii,jj,kk)
01561         - VAT3( uC, i,jm1,km1) * VAT3( oPS, ii,jj,kk)
01562         - VAT3( oN, i,jm1,km1) * VAT3( dPC, ii,jj,kk)
01563         - VAT3( uN, i,jm1,km1) * VAT3( oPC, ii,jj,kk)
01564         - VAT3( oE, i,jm1,km1) * VAT3(dPSE, ii,jj,kk)
01565         - VAT3( uE, i,jm1,km1) * VAT3(oPSE, ii,jj,kk)
01566         - VAT3( oNE, i,jm1,km1) * VAT3( dPE, ii,jj,kk)
01567         - VAT3( uNE, i,jm1,km1) * VAT3( oPE, ii,jj,kk));
01568
01569 TMP9_XOC =
01570     + VAT3(uPNW, ii,jj,kk) * (- VAT3( uN, im1,j,k) * VAT3( oPW, ii,jj,kk)
01571         - VAT3( oN, im1,j,kp1) * VAT3( uPW, ii,jj,kk)
01572         - VAT3( uC, im1,jp1,k) * VAT3(oPNW, ii,jj,kk)
01573         + VAT3( oC, im1,jp1,kp1) * VAT3(uPNW, ii,jj,kk)
01574         - VAT3( uNW, i,j,k) * VAT3( oPC, ii,jj,kk)
01575         - VAT3( oNW, i,j,kp1) * VAT3( uPC, ii,jj,kk)
01576         - VAT3( uW, i,jp1,k) * VAT3( oPN, ii,jj,kk)
01577         - VAT3( oE, im1,jp1,kp1) * VAT3( uPN, ii,jj,kk));
01578
01579 TMP10_XOC =
01580     + VAT3(oPNW, ii,jj,kk) * (- VAT3( uN, im1,j,km1) * VAT3( dPW, ii,jj,kk)
01581         - VAT3( oN, im1,j,k) * VAT3( oPW, ii,jj,kk)
01582         - VAT3( uS, im1,jp1,k) * VAT3( uPW, ii,jj,kk)
01583         - VAT3( uC, im1,jp1,km1) * VAT3(dPNW, ii,jj,kk)

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01584             + VAT3( oC, iml,jpl,k) * VAT3(oPNW, ii,jj,kk)
01585             - VAT3( uC, iml,jpl,k) * VAT3(uPNW, ii,jj,kk)
01586             - VAT3( uNW, i,j,kml) * VAT3( dPC, ii,jj,kk)
01587             - VAT3( oNW, i,j,k) * VAT3( oPC, ii,jj,kk)
01588             - VAT3( uSE, iml,jpl,k) * VAT3( uPC, ii,jj,kk)
01589             - VAT3( uW, i,jpl,kml) * VAT3( dPN, ii,jj,kk)
01590             - VAT3( oE, iml,jpl,k) * VAT3( oPN, ii,jj,kk)
01591             - VAT3( uE, iml,jpl,k) * VAT3( uPN, ii,jj,kk));
01592
01593 TMP11_XOC =
01594     + VAT3( uPW, ii,jj,kk) * (- VAT3( uN, iml,jml,k) * VAT3(oPSW, ii,jj,kk)
01595     - VAT3( oN, iml,jml,kpl) * VAT3(uPSW, ii,jj,kk)
01596     - VAT3( uC, iml,j,k) * VAT3( oPW, ii,jj,kk)
01597     + VAT3( oC, iml,j,kpl) * VAT3( uPW, ii,jj,kk)
01598     - VAT3( uS, iml,jpl,k) * VAT3(oPNW, ii,jj,kk)
01599     - VAT3( oN, iml,j,kpl) * VAT3(uPNW, ii,jj,kk)
01600     - VAT3( uNW, i,jml,k) * VAT3( oPS, ii,jj,kk)
01601     - VAT3( oNW, i,jml,kpl) * VAT3( uPS, ii,jj,kk)
01602     - VAT3( uW, i,j,k) * VAT3( oPC, ii,jj,kk)
01603     - VAT3( oE, iml,j,kpl) * VAT3( uPC, ii,jj,kk)
01604     - VAT3( uSW, i,jpl,k) * VAT3( oPN, ii,jj,kk)
01605     - VAT3( oNE, iml,j,kpl) * VAT3( uPN, ii,jj,kk));
01606
01607 TMP12_XOC =
01608     + VAT3(dPNW, ii,jj,kk) * (- VAT3( oN, iml,j,kml) * VAT3( dPW, ii,jj,kk)
01609     - VAT3( uS, iml,jpl,kml) * VAT3( oPW, ii,jj,kk)
01610     + VAT3( oC, iml,jpl,kml) * VAT3(dPNW, ii,jj,kk)
01611     - VAT3( uC, iml,jpl,kml) * VAT3(oPNW, ii,jj,kk)
01612     - VAT3( oNW, i,j,kml) * VAT3( dPC, ii,jj,kk)
01613     - VAT3( uSE, iml,jpl,kml) * VAT3( oPC, ii,jj,kk)
01614     - VAT3( oE, iml,jpl,kml) * VAT3( dPN, ii,jj,kk)
01615     - VAT3( uE, iml,jpl,kml) * VAT3( oPN, ii,jj,kk));
01616
01617 TMP13_XOC =
01618     + VAT3( oPW, ii,jj,kk) * (- VAT3( uN, iml,jml,kml) * VAT3(dPSW, ii,jj,kk)
01619     - VAT3( oN, iml,jml,k) * VAT3(oPSW, ii,jj,kk)
01620     - VAT3( uS, iml,j,k) * VAT3(uPSW, ii,jj,kk)
01621     - VAT3( uC, iml,j,kml) * VAT3( dPW, ii,jj,kk)
01622     + VAT3( oC, iml,j,k) * VAT3( oPW, ii,jj,kk)
01623     - VAT3( uC, iml,j,k) * VAT3( uPW, ii,jj,kk)
01624     - VAT3( uS, iml,jpl,kml) * VAT3(dPNW, ii,jj,kk)
01625     - VAT3( oN, iml,j,k) * VAT3(oPNW, ii,jj,kk)
01626     - VAT3( uN, iml,j,k) * VAT3(uPNW, ii,jj,kk)
01627     - VAT3( uNW, i,jml,kml) * VAT3( dPS, ii,jj,kk)
01628     - VAT3( oNW, i,jml,k) * VAT3( oPS, ii,jj,kk)
01629     - VAT3( uSE, iml,j,k) * VAT3( uPS, ii,jj,kk)
01630     - VAT3( uW, i,j,kml) * VAT3( dPC, ii,jj,kk)
01631     - VAT3( oE, iml,j,k) * VAT3( oPC, ii,jj,kk)
01632     - VAT3( uE, iml,j,k) * VAT3( uPC, ii,jj,kk)
01633     - VAT3( uSW, i,jpl,kml) * VAT3( dPN, ii,jj,kk)
01634     - VAT3( oNE, iml,j,k) * VAT3( oPN, ii,jj,kk)
01635     - VAT3( uNE, iml,j,k) * VAT3( uPN, ii,jj,kk));
01636
01637 TMP14_XOC =
01638     + VAT3(uPSW, ii,jj,kk) * (- VAT3( uC, iml,jml,k) * VAT3(oPSW, ii,jj,kk)
01639     + VAT3( oC, iml,jml,kpl) * VAT3(uPSW, ii,jj,kk)
01640     - VAT3( uS, iml,j,k) * VAT3( oPW, ii,jj,kk)
01641     - VAT3( oN, iml,jml,kpl) * VAT3( uPW, ii,jj,kk)
01642     - VAT3( uW, i,jml,k) * VAT3( oPS, ii,jj,kk)
01643     - VAT3( oE, iml,jml,kpl) * VAT3( uPS, ii,jj,kk)
01644     - VAT3( uSW, i,j,k) * VAT3( oPC, ii,jj,kk)
01645     - VAT3( oNE, iml,jml,kpl) * VAT3( uPC, ii,jj,kk));
01646
01647 TMP15_XOC =
01648     + VAT3(oPSW, ii,jj,kk) * (- VAT3( uC, iml,jml,kml) * VAT3(dPSW, ii,jj,kk)
01649     + VAT3( oC, iml,jml,k) * VAT3(oPSW, ii,jj,kk)
01650     - VAT3( uC, iml,jml,k) * VAT3(uPSW, ii,jj,kk)
01651     - VAT3( uS, iml,j,kml) * VAT3( dPW, ii,jj,kk)
01652     - VAT3( oN, iml,jml,k) * VAT3( oPW, ii,jj,kk)
01653     - VAT3( uN, iml,jml,k) * VAT3( uPW, ii,jj,kk)
01654     - VAT3( uW, i,jml,kml) * VAT3( dPS, ii,jj,kk)
01655     - VAT3( oE, iml,jml,k) * VAT3( oPS, ii,jj,kk)
01656     - VAT3( uE, iml,jml,k) * VAT3( uPS, ii,jj,kk)
01657     - VAT3( uSW, i,j,kml) * VAT3( dPC, ii,jj,kk)
01658     - VAT3( oNE, iml,jml,k) * VAT3( oPC, ii,jj,kk)
01659     - VAT3( uNE, iml,jml,k) * VAT3( uPC, ii,jj,kk));
01660
01661 TMP16_XOC =
01662     + VAT3( dPW, ii,jj,kk) * (- VAT3( oN, iml,jml,kml) * VAT3(dPSW, ii,jj,kk)
01663     - VAT3( uS, iml,j,kml) * VAT3(oPSW, ii,jj,kk)
01664     + VAT3( oC, iml,j,kml) * VAT3( dPW, ii,jj,kk)

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01665             - VAT3( uC, i, j, k) * VAT3( oPW, ii, jj, kk)
01666             - VAT3( oN, i, j, k) * VAT3( dPNW, ii, jj, kk)
01667             - VAT3( uN, i, j, k) * VAT3( oPNW, ii, jj, kk)
01668             - VAT3( oNW, i, j, k) * VAT3( dPS, ii, jj, kk)
01669             - VAT3( uSE, i, j, k) * VAT3( oPS, ii, jj, kk)
01670             - VAT3( oE, i, j, k) * VAT3( dPC, ii, jj, kk)
01671             - VAT3( uE, i, j, k) * VAT3( oPC, ii, jj, kk)
01672             - VAT3( oNE, i, j, k) * VAT3( dPN, ii, jj, kk)
01673             - VAT3( uNE, i, j, k) * VAT3( oPN, ii, jj, kk));
01674
01675     TMP17_XOC =
01676         + VAT3( uPNE, ii, jj, kk) * (- VAT3( uNE, i, j, k) * VAT3( oPC, ii, jj, kk)
01677             - VAT3( oNE, i, j, k) * VAT3( uPC, ii, jj, kk)
01678             - VAT3( uE, i, j, k) * VAT3( oPN, ii, jj, kk)
01679             - VAT3( oE, i, j, k) * VAT3( uPN, ii, jj, kk)
01680             - VAT3( uN, i, j, k) * VAT3( oPE, ii, jj, kk)
01681             - VAT3( oN, i, j, k) * VAT3( uPE, ii, jj, kk)
01682             - VAT3( uC, i, j, k) * VAT3( oPNE, ii, jj, kk)
01683             + VAT3( oC, i, j, k) * VAT3( uPNE, ii, jj, kk));
01684
01685     TMP18_XOC =
01686         + VAT3( uPE, ii, jj, kk) * (- VAT3( uNE, i, j, k) * VAT3( oPS, ii, jj, kk)
01687             - VAT3( oNE, i, j, k) * VAT3( uPS, ii, jj, kk)
01688             - VAT3( uE, i, j, k) * VAT3( oPC, ii, jj, kk)
01689             - VAT3( oE, i, j, k) * VAT3( uPC, ii, jj, kk)
01690             - VAT3( uSE, i, j, k) * VAT3( oPN, ii, jj, kk)
01691             - VAT3( oNW, i, j, k) * VAT3( uPN, ii, jj, kk)
01692             - VAT3( uN, i, j, k) * VAT3( oPSE, ii, jj, kk)
01693             - VAT3( oN, i, j, k) * VAT3( uPSE, ii, jj, kk)
01694             - VAT3( uC, i, j, k) * VAT3( oPE, ii, jj, kk)
01695             + VAT3( oC, i, j, k) * VAT3( uPE, ii, jj, kk)
01696             - VAT3( uS, i, j, k) * VAT3( oPNE, ii, jj, kk)
01697             - VAT3( oN, i, j, k) * VAT3( uPNE, ii, jj, kk));
01698
01699     TMP19_XOC =
01700         + VAT3( dPNE, ii, jj, kk) * (- VAT3( oNE, i, j, k) * VAT3( dPC, ii, jj, kk)
01701             - VAT3( uSW, i, j, k) * VAT3( oPC, ii, jj, kk)
01702             - VAT3( oE, i, j, k) * VAT3( dPN, ii, jj, kk)
01703             - VAT3( uW, i, j, k) * VAT3( oPN, ii, jj, kk)
01704             - VAT3( oN, i, j, k) * VAT3( dPE, ii, jj, kk)
01705             - VAT3( uS, i, j, k) * VAT3( oPE, ii, jj, kk)
01706             + VAT3( oC, i, j, k) * VAT3( dPNE, ii, jj, kk)
01707             - VAT3( uC, i, j, k) * VAT3( oPNE, ii, jj, kk));
01708
01709     TMP20_XOC =
01710         + VAT3( oPNE, ii, jj, kk) * (- VAT3( uNE, i, j, k) * VAT3( dPC, ii, jj, kk)
01711             - VAT3( oNE, i, j, k) * VAT3( oPC, ii, jj, kk)
01712             - VAT3( uSW, i, j, k) * VAT3( uPC, ii, jj, kk)
01713             - VAT3( uE, i, j, k) * VAT3( dPN, ii, jj, kk)
01714             - VAT3( oE, i, j, k) * VAT3( oPN, ii, jj, kk)
01715             - VAT3( uW, i, j, k) * VAT3( uPN, ii, jj, kk)
01716             - VAT3( uN, i, j, k) * VAT3( dPE, ii, jj, kk)
01717             - VAT3( oN, i, j, k) * VAT3( oPE, ii, jj, kk)
01718             - VAT3( uS, i, j, k) * VAT3( uPE, ii, jj, kk)
01719             - VAT3( uC, i, j, k) * VAT3( dPNE, ii, jj, kk)
01720             + VAT3( oC, i, j, k) * VAT3( oPNE, ii, jj, kk)
01721             - VAT3( uC, i, j, k) * VAT3( uPNE, ii, jj, kk));
01722
01723     TMP21_XOC =
01724         + VAT3( oPSE, ii, jj, kk) * (- VAT3( uE, i, j, k) * VAT3( dPS, ii, jj, kk)
01725             - VAT3( oE, i, j, k) * VAT3( oPS, ii, jj, kk)
01726             - VAT3( uW, i, j, k) * VAT3( uPS, ii, jj, kk)
01727             - VAT3( uSE, i, j, k) * VAT3( dPC, ii, jj, kk)
01728             - VAT3( oNW, i, j, k) * VAT3( oPC, ii, jj, kk)
01729             - VAT3( uNW, i, j, k) * VAT3( uPC, ii, jj, kk)
01730             - VAT3( uC, i, j, k) * VAT3( dPSE, ii, jj, kk)
01731             + VAT3( oC, i, j, k) * VAT3( oPSE, ii, jj, kk)
01732             - VAT3( uC, i, j, k) * VAT3( uPSE, ii, jj, kk)
01733             - VAT3( uS, i, j, k) * VAT3( dPE, ii, jj, kk)
01734             - VAT3( oN, i, j, k) * VAT3( oPE, ii, jj, kk)
01735             - VAT3( uN, i, j, k) * VAT3( uPE, ii, jj, kk));
01736
01737     TMP22_XOC =
01738         + VAT3( dPSE, ii, jj, kk) * (- VAT3( oE, i, j, k) * VAT3( dPS, ii, jj, kk)
01739             - VAT3( uW, i, j, k) * VAT3( oPS, ii, jj, kk)
01740             - VAT3( oNW, i, j, k) * VAT3( dPC, ii, jj, kk)
01741             - VAT3( uNW, i, j, k) * VAT3( oPC, ii, jj, kk)
01742             + VAT3( oC, i, j, k) * VAT3( dPSE, ii, jj, kk)
01743             - VAT3( uC, i, j, k) * VAT3( oPSE, ii, jj, kk)
01744             - VAT3( oN, i, j, k) * VAT3( dPE, ii, jj, kk)
01745             - VAT3( uN, i, j, k) * VAT3( oPE, ii, jj, kk));

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01746
01747     TMP23_XOC =
01748         + VAT3(uPSE, ii,jj,kk) * (- VAT3( uE, i,jm1,k) * VAT3( oPS, ii,jj,kk)
01749             - VAT3( oE, i,jm1,kp1) * VAT3( uPS, ii,jj,kk)
01750             - VAT3( uSE, i,j,k) * VAT3( oPC, ii,jj,kk)
01751             - VAT3( oNW, ip1,jm1,kp1) * VAT3( uPC, ii,jj,kk)
01752             - VAT3( uC, ip1,jm1,k) * VAT3(oPSE, ii,jj,kk)
01753             + VAT3( oC, ip1,jm1,kp1) * VAT3(uPSE, ii,jj,kk)
01754             - VAT3( uS, ip1,j,k) * VAT3( oPE, ii,jj,kk)
01755             - VAT3( oN, ip1,jm1,kp1) * VAT3( uPE, ii,jj,kk));
01756
01757     TMP24_XOC =
01758         + VAT3( oPE, ii,jj,kk) * (- VAT3( uNE, i,jm1,km1) * VAT3( dPS, ii,jj,kk)
01759             - VAT3( oNE, i,jm1,k) * VAT3( oPS, ii,jj,kk)
01760             - VAT3( uSW, ip1,j,k) * VAT3( uPS, ii,jj,kk)
01761             - VAT3( uE, i,j,km1) * VAT3( dPC, ii,jj,kk)
01762             - VAT3( oE, i,j,k) * VAT3( oPC, ii,jj,kk)
01763             - VAT3( uW, ip1,j,k) * VAT3( uPC, ii,jj,kk)
01764             - VAT3( uSE, i,jp1,km1) * VAT3( dPN, ii,jj,kk)
01765             - VAT3( oNW, ip1,j,k) * VAT3( oPN, ii,jj,kk)
01766             - VAT3( uNW, ip1,j,k) * VAT3( uPN, ii,jj,kk)
01767             - VAT3( uN, ip1,jm1,km1) * VAT3(dPSE, ii,jj,kk)
01768             - VAT3( oN, ip1,jm1,k) * VAT3(oPSE, ii,jj,kk)
01769             - VAT3( uS, ip1,j,k) * VAT3(uPSE, ii,jj,kk)
01770             - VAT3( uC, ip1,j,km1) * VAT3( dPE, ii,jj,kk)
01771             + VAT3( oC, ip1,j,k) * VAT3( oPE, ii,jj,kk)
01772             - VAT3( uC, ip1,j,k) * VAT3( uPE, ii,jj,kk)
01773             - VAT3( uS, ip1,jp1,km1) * VAT3(dPNE, ii,jj,kk)
01774             - VAT3( oN, ip1,j,k) * VAT3(oPNE, ii,jj,kk)
01775             - VAT3( uN, ip1,j,k) * VAT3(uPNE, ii,jj,kk));
01776
01777     TMP25_XOC =
01778         + VAT3( dPE, ii,jj,kk) * (- VAT3( oNE, i,jm1,km1) * VAT3( dPS, ii,jj,kk)
01779             - VAT3( uSW, ip1,j,km1) * VAT3( oPS, ii,jj,kk)
01780             - VAT3( oE, i,j,km1) * VAT3( dPC, ii,jj,kk)
01781             - VAT3( uW, ip1,j,km1) * VAT3( oPC, ii,jj,kk)
01782             - VAT3( oNW, ip1,j,km1) * VAT3( dPN, ii,jj,kk)
01783             - VAT3( uNW, ip1,j,km1) * VAT3( oPN, ii,jj,kk)
01784             - VAT3( oN, ip1,jm1,km1) * VAT3(dPSE, ii,jj,kk)
01785             - VAT3( uS, ip1,j,km1) * VAT3(oPSE, ii,jj,kk)
01786             + VAT3( oC, ip1,j,km1) * VAT3( dPE, ii,jj,kk)
01787             - VAT3( uC, ip1,j,km1) * VAT3( oPE, ii,jj,kk)
01788             - VAT3( oN, ip1,j,km1) * VAT3(dPNE, ii,jj,kk)
01789             - VAT3( uN, ip1,j,km1) * VAT3(oPNE, ii,jj,kk));
01790
01791     TMP26_XOC =
01792         + VAT3( uPN, ii,jj,kk) * (- VAT3( uNE, im1,j,k) * VAT3( oPW, ii,jj,kk)
01793             - VAT3( oNE, im1,j,kp1) * VAT3( uPW, ii,jj,kk)
01794             - VAT3( uE, im1,jp1,k) * VAT3(oPNW, ii,jj,kk)
01795             - VAT3( oE, im1,jp1,kp1) * VAT3(uPNW, ii,jj,kk)
01796             - VAT3( uN, i,j,k) * VAT3( oPC, ii,jj,kk)
01797             - VAT3( oN, i,j,kp1) * VAT3( uPC, ii,jj,kk)
01798             - VAT3( uC, i,jp1,k) * VAT3( oPN, ii,jj,kk)
01799             + VAT3( oC, i,jp1,kp1) * VAT3( uPN, ii,jj,kk)
01800             - VAT3( uNW, ip1,j,k) * VAT3( oPE, ii,jj,kk)
01801             - VAT3( oNW, ip1,j,kp1) * VAT3( uPE, ii,jj,kk)
01802             - VAT3( uW, ip1,jp1,k) * VAT3(oPNE, ii,jj,kk)
01803             - VAT3( oE, i,jp1,kp1) * VAT3(uPNE, ii,jj,kk));
01804
01805     TMP27_XOC =
01806         + VAT3(dPSW, ii,jj,kk) * ( VAT3( oC, im1,jm1,km1) * VAT3(dPSW, ii,jj,kk)
01807             - VAT3( uC, im1,jm1,km1) * VAT3(oPSW, ii,jj,kk)
01808             - VAT3( oN, im1,jm1,km1) * VAT3( dPW, ii,jj,kk)
01809             - VAT3( uN, im1,jm1,km1) * VAT3( oPW, ii,jj,kk)
01810             - VAT3( oE, im1,jm1,km1) * VAT3( dPS, ii,jj,kk)
01811             - VAT3( uE, im1,jm1,km1) * VAT3( oPS, ii,jj,kk)
01812             - VAT3( oNE, im1,jm1,km1) * VAT3( dPC, ii,jj,kk)
01813             - VAT3( uNE, im1,jm1,km1) * VAT3( oPC, ii,jj,kk));
01814
01815     VAT3( XoC, ii,jj,kk) = TMP1_XOC + TMP2_XOC + TMP3_XOC + TMP4_XOC
01816         + TMP5_XOC + TMP6_XOC + TMP7_XOC + TMP8_XOC + TMP9_XOC
01817         + TMP10_XOC + TMP11_XOC + TMP12_XOC + TMP13_XOC + TMP14_XOC
01818         + TMP15_XOC + TMP16_XOC + TMP17_XOC + TMP18_XOC + TMP19_XOC
01819         + TMP20_XOC + TMP21_XOC + TMP22_XOC + TMP23_XOC + TMP24_XOC
01820         + TMP25_XOC + TMP26_XOC + TMP27_XOC;
01821
01822     //fprintf(data, "%19.12E\n", VAT3(XoC, ii, jj, kk));
01823
01824     /* *****
01825     * *** > OE;
01826     * *****

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01827
01828 // VAT3( XoE, ii,jj,kk) =
01829 TMP1_XOE =
01830 - VAT3( dPS, ii,jj,kk) * (- VAT3( oE, i,jm1,km1) * VAT3(dPSW, iip1,jj,kk)
01831 - VAT3( uE, i,jm1,km1) * VAT3(oPSW, iip1,jj,kk)
01832 - VAT3( oNE, i,jm1,km1) * VAT3( dPW, iip1,jj,kk)
01833 - VAT3( uNE, i,jm1,km1) * VAT3( oPW, iip1,jj,kk))
01834
01835 - VAT3( oPS, ii,jj,kk) * (- VAT3( uW, ip1,jm1,km1) * VAT3(dPSW, iip1,jj,kk)
01836 - VAT3( oE, i,jm1,k) * VAT3(oPSW, iip1,jj,kk)
01837 - VAT3( uE, i,jm1,k) * VAT3(uPSW, iip1,jj,kk)
01838 - VAT3( uSW, ip1,j,km1) * VAT3( dPW, iip1,jj,kk)
01839 - VAT3( oNE, i,jm1,k) * VAT3( oPW, iip1,jj,kk)
01840 - VAT3( uNE, i,jm1,k) * VAT3( uPW, iip1,jj,kk))
01841
01842 - VAT3( uPS, ii,jj,kk) * (- VAT3( uW, ip1,jm1,k) * VAT3(oPSW, iip1,jj,kk)
01843 - VAT3( oE, i,jm1,kp1) * VAT3(uPSW, iip1,jj,kk)
01844 - VAT3( uSW, ip1,j,k) * VAT3( oPW, iip1,jj,kk)
01845 - VAT3( oNE, i,jm1,kp1) * VAT3( uPW, iip1,jj,kk));
01846
01847 TMP2_XOE =
01848 - VAT3( dPC, ii,jj,kk) * (- VAT3( oNW, ip1,jm1,km1) * VAT3(dPSW, iip1,jj,kk)
01849 - VAT3( uSE, i,j,km1) * VAT3(oPSW, iip1,jj,kk)
01850 - VAT3( oE, i,j,km1) * VAT3( dPW, iip1,jj,kk)
01851 - VAT3( uE, i,j,km1) * VAT3( oPW, iip1,jj,kk)
01852 - VAT3( oNE, i,j,km1) * VAT3(dPNW, iip1,jj,kk)
01853 - VAT3( uNE, i,j,km1) * VAT3(oPNW, iip1,jj,kk))
01854
01855 - VAT3( oPC, ii,jj,kk) * (- VAT3( uNW, ip1,jm1,km1) * VAT3(dPSW, iip1,jj,kk)
01856 - VAT3( oNW, ip1,jm1,k) * VAT3(oPSW, iip1,jj,kk)
01857 - VAT3( uSE, i,j,k) * VAT3(uPSW, iip1,jj,kk)
01858 - VAT3( uW, ip1,j,km1) * VAT3( dPW, iip1,jj,kk)
01859 - VAT3( oE, i,j,k) * VAT3( oPW, iip1,jj,kk)
01860 - VAT3( uE, i,j,k) * VAT3( uPW, iip1,jj,kk)
01861 - VAT3( uSW, ip1,jp1,km1) * VAT3(dPNW, iip1,jj,kk)
01862 - VAT3( oNE, i,j,k) * VAT3(oPNW, iip1,jj,kk)
01863 - VAT3( uNE, i,j,k) * VAT3(uPNW, iip1,jj,kk));
01864
01865 TMP3_XOE =
01866 - VAT3( uPC, ii,jj,kk) * (- VAT3( uNW, ip1,jm1,k) * VAT3(oPSW, iip1,jj,kk)
01867 - VAT3( oNW, ip1,jm1,kp1) * VAT3(uPSW, iip1,jj,kk)
01868 - VAT3( uW, ip1,j,k) * VAT3( oPW, iip1,jj,kk)
01869 - VAT3( oE, i,j,kp1) * VAT3( uPW, iip1,jj,kk)
01870 - VAT3( uSW, ip1,jp1,k) * VAT3(oPNW, iip1,jj,kk)
01871 - VAT3( oNE, i,j,kp1) * VAT3(uPNW, iip1,jj,kk))
01872
01873 - VAT3( dPN, ii,jj,kk) * (- VAT3( oNW, ip1,j,km1) * VAT3( dPW, iip1,jj,kk)
01874 - VAT3( uSE, i,jp1,km1) * VAT3( oPW, iip1,jj,kk)
01875 - VAT3( oE, i,jp1,km1) * VAT3(dPNW, iip1,jj,kk)
01876 - VAT3( uE, i,jp1,km1) * VAT3(oPNW, iip1,jj,kk))
01877
01878 - VAT3( oPN, ii,jj,kk) * (- VAT3( uNW, ip1,j,km1) * VAT3( dPW, iip1,jj,kk)
01879 - VAT3( oNW, ip1,j,k) * VAT3( oPW, iip1,jj,kk)
01880 - VAT3( uSE, i,jp1,k) * VAT3( uPW, iip1,jj,kk)
01881 - VAT3( uW, ip1,jp1,km1) * VAT3(dPNW, iip1,jj,kk)
01882 - VAT3( oE, i,jp1,k) * VAT3(oPNW, iip1,jj,kk)
01883 - VAT3( uE, i,jp1,k) * VAT3(uPNW, iip1,jj,kk));
01884
01885 TMP4_XOE =
01886 - VAT3( uPN, ii,jj,kk) * (- VAT3( uNW, ip1,j,k) * VAT3( oPW, iip1,jj,kk)
01887 - VAT3( oNW, ip1,j,kp1) * VAT3( uPW, iip1,jj,kk)
01888 - VAT3( uW, ip1,jp1,k) * VAT3(oPNW, iip1,jj,kk)
01889 - VAT3( oE, i,jp1,kp1) * VAT3(uPNW, iip1,jj,kk))
01890
01891 - VAT3(dPSE, ii,jj,kk) * ( VAT3( oC, ip1,jm1,km1) * VAT3(dPSW, iip1,jj,kk)
01892 - VAT3( uC, ip1,jm1,km1) * VAT3(oPSW, iip1,jj,kk)
01893 - VAT3( oN, ip1,jm1,km1) * VAT3( dPW, iip1,jj,kk)
01894 - VAT3( uN, ip1,jm1,km1) * VAT3( oPW, iip1,jj,kk)
01895 - VAT3( oE, ip1,jm1,km1) * VAT3( dPS, iip1,jj,kk)
01896 - VAT3( uE, ip1,jm1,km1) * VAT3( oPS, iip1,jj,kk)
01897 - VAT3( oNE, ip1,jm1,km1) * VAT3( dPC, iip1,jj,kk)
01898 - VAT3( uNE, ip1,jm1,km1) * VAT3( oPC, iip1,jj,kk));
01899
01900 TMP5_XOE =
01901 - VAT3(oPSE, ii,jj,kk) * (- VAT3( uC, ip1,jm1,km1) * VAT3(dPSW, iip1,jj,kk)
01902 + VAT3( oC, ip1,jm1,k) * VAT3(oPSW, iip1,jj,kk)
01903 - VAT3( uC, ip1,jm1,k) * VAT3(uPSW, iip1,jj,kk)
01904 - VAT3( uS, ip1,j,km1) * VAT3( dPW, iip1,jj,kk)
01905 - VAT3( oN, ip1,jm1,k) * VAT3( oPW, iip1,jj,kk)
01906 - VAT3( uN, ip1,jm1,k) * VAT3( uPW, iip1,jj,kk)
01907 - VAT3( uW, ip2,jm1,km1) * VAT3( dPS, iip1,jj,kk)

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01908             - VAT3( oE, ip1,jm1,k) * VAT3( oPS, iip1,jj,kk)
01909             - VAT3( uE, ip1,jm1,k) * VAT3( uPS, iip1,jj,kk)
01910             - VAT3( uSW, ip2,j,kml) * VAT3( dPC, iip1,jj,kk)
01911             - VAT3( oNE, ip1,jm1,k) * VAT3( oPC, iip1,jj,kk)
01912             - VAT3( uNE, ip1,jm1,k) * VAT3( uPC, iip1,jj,kk));
01913
01914 TMP6_XOE =
01915     - VAT3(uPSE, ii,jj,kk) * (- VAT3( uC, ip1,jm1,k) * VAT3(oPSW, iip1,jj,kk)
01916       + VAT3( oC, ip1,jm1,kp1) * VAT3(uPSW, iip1,jj,kk)
01917       - VAT3( uS, ip1,j,k) * VAT3( oPW, iip1,jj,kk)
01918       - VAT3( oN, ip1,jm1,kp1) * VAT3( uPW, iip1,jj,kk)
01919       - VAT3( uW, ip2,jm1,k) * VAT3( oPS, iip1,jj,kk)
01920       - VAT3( oE, ip1,jm1,kp1) * VAT3( uPS, iip1,jj,kk)
01921       - VAT3( uSW, ip2,j,k) * VAT3( oPC, iip1,jj,kk)
01922       - VAT3( oNE, ip1,jm1,kp1) * VAT3( uPC, iip1,jj,kk));
01923
01924 TMP7_XOE =
01925     - VAT3( dPE, ii,jj,kk) * (- VAT3( oN, ip1,jm1,kml) * VAT3(dPSW, iip1,jj,kk)
01926       - VAT3( uS, ip1,j,kml) * VAT3(oPSW, iip1,jj,kk)
01927       + VAT3( oC, ip1,j,kml) * VAT3( dPW, iip1,jj,kk)
01928       - VAT3( uC, ip1,j,kml) * VAT3( oPW, iip1,jj,kk)
01929       - VAT3( oN, ip1,j,kml) * VAT3(dPNW, iip1,jj,kk)
01930       - VAT3( uN, ip1,j,kml) * VAT3(oPNW, iip1,jj,kk)
01931       - VAT3( oNW, ip2,jm1,kml) * VAT3( dPS, iip1,jj,kk)
01932       - VAT3( uSE, ip1,j,kml) * VAT3( oPS, iip1,jj,kk)
01933       - VAT3( oE, ip1,j,kml) * VAT3( dPC, iip1,jj,kk)
01934       - VAT3( uE, ip1,j,kml) * VAT3( oPC, iip1,jj,kk)
01935       - VAT3( oNE, ip1,j,kml) * VAT3( dPN, iip1,jj,kk)
01936       - VAT3( uNE, ip1,j,kml) * VAT3( oPN, iip1,jj,kk));
01937
01938 TMP8_XOE =
01939     - VAT3( oPE, ii,jj,kk) * (- VAT3( uN, ip1,jm1,kml) * VAT3(dPSW, iip1,jj,kk)
01940       - VAT3( oN, ip1,jm1,k) * VAT3(oPSW, iip1,jj,kk)
01941       - VAT3( uS, ip1,j,k) * VAT3(uPSW, iip1,jj,kk)
01942       - VAT3( uC, ip1,j,kml) * VAT3( dPW, iip1,jj,kk)
01943       + VAT3( oC, ip1,j,k) * VAT3( oPW, iip1,jj,kk)
01944       - VAT3( uC, ip1,j,k) * VAT3( uPW, iip1,jj,kk)
01945       - VAT3( uS, ip1,jp1,kml) * VAT3(dPNW, iip1,jj,kk)
01946       - VAT3( oN, ip1,j,k) * VAT3(oPNW, iip1,jj,kk)
01947       - VAT3( uN, ip1,j,k) * VAT3(uPNW, iip1,jj,kk)
01948       - VAT3( uNW, ip2,jm1,kml) * VAT3( dPS, iip1,jj,kk)
01949       - VAT3( oNW, ip2,jm1,k) * VAT3( oPS, iip1,jj,kk)
01950       - VAT3( uSE, ip1,j,k) * VAT3( uPS, iip1,jj,kk)
01951       - VAT3( uW, ip2,j,kml) * VAT3( dPC, iip1,jj,kk)
01952       - VAT3( oE, ip1,j,k) * VAT3( oPC, iip1,jj,kk)
01953       - VAT3( uE, ip1,j,k) * VAT3( uPC, iip1,jj,kk)
01954       - VAT3( uSW, ip2,jp1,kml) * VAT3( dPN, iip1,jj,kk)
01955       - VAT3( oNE, ip1,j,k) * VAT3( oPN, iip1,jj,kk)
01956       - VAT3( uNE, ip1,j,k) * VAT3( uPN, iip1,jj,kk));
01957
01958 TMP9_XOE =
01959     - VAT3( uPE, ii,jj,kk) * (- VAT3( uN, ip1,jm1,k) * VAT3(oPSW, iip1,jj,kk)
01960       - VAT3( oN, ip1,jm1,kp1) * VAT3(uPSW, iip1,jj,kk)
01961       - VAT3( uC, ip1,j,k) * VAT3( oPW, iip1,jj,kk)
01962       + VAT3( oC, ip1,j,kp1) * VAT3( uPW, iip1,jj,kk)
01963       - VAT3( uS, ip1,jp1,k) * VAT3(oPNW, iip1,jj,kk)
01964       - VAT3( oN, ip1,j,kp1) * VAT3(uPNW, iip1,jj,kk)
01965       - VAT3( uNW, ip2,jm1,k) * VAT3( oPS, iip1,jj,kk)
01966       - VAT3( oNW, ip2,jm1,kp1) * VAT3( uPS, iip1,jj,kk)
01967       - VAT3( uW, ip2,j,k) * VAT3( oPC, iip1,jj,kk)
01968       - VAT3( oE, ip1,j,kp1) * VAT3( uPC, iip1,jj,kk)
01969       - VAT3( uSW, ip2,jp1,k) * VAT3( oPN, iip1,jj,kk)
01970       - VAT3( oNE, ip1,j,kp1) * VAT3( uPN, iip1,jj,kk));
01971
01972 TMP10_XOE =
01973     - VAT3(dPNE, ii,jj,kk) * (- VAT3( oN, ip1,j,kml) * VAT3( dPW, iip1,jj,kk)
01974       - VAT3( uS, ip1,jp1,kml) * VAT3( oPW, iip1,jj,kk)
01975       + VAT3( oC, ip1,jp1,kml) * VAT3(dPNW, iip1,jj,kk)
01976       - VAT3( uC, ip1,jp1,kml) * VAT3(oPNW, iip1,jj,kk)
01977       - VAT3( oNW, ip2,j,kml) * VAT3( dPC, iip1,jj,kk)
01978       - VAT3( uSE, ip1,jp1,kml) * VAT3( oPC, iip1,jj,kk)
01979       - VAT3( oE, ip1,jp1,kml) * VAT3( dPN, iip1,jj,kk)
01980       - VAT3( uE, ip1,jp1,kml) * VAT3( oPN, iip1,jj,kk));
01981
01982 TMP11_XOE =
01983     - VAT3(oPNE, ii,jj,kk) * (- VAT3( uN, ip1,j,kml) * VAT3( dPW, iip1,jj,kk)
01984       - VAT3( oN, ip1,j,k) * VAT3( oPW, iip1,jj,kk)
01985       - VAT3( uS, ip1,jp1,k) * VAT3( uPW, iip1,jj,kk)
01986       - VAT3( uC, ip1,jp1,kml) * VAT3(dPNW, iip1,jj,kk)
01987       + VAT3( oC, ip1,jp1,k) * VAT3(oPNW, iip1,jj,kk)
01988       - VAT3( uC, ip1,jp1,k) * VAT3(uPNW, iip1,jj,kk)

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01989             - VAT3( uNW, ip2,j,km1) * VAT3( dPC, iip1,jj,kk)
01990             - VAT3( oNW, ip2,j,k) * VAT3( oPC, iip1,jj,kk)
01991             - VAT3( uSE, ip1,jp1,k) * VAT3( uPC, iip1,jj,kk)
01992             - VAT3( uW, ip2,jp1,km1) * VAT3( dPN, iip1,jj,kk)
01993             - VAT3( oE, ip1,jp1,k) * VAT3( oPN, iip1,jj,kk)
01994             - VAT3( uE, ip1,jp1,k) * VAT3( uPN, iip1,jj,kk));
01995
01996 TMP12_XOE =
01997     - VAT3(uPNE, ii,jj,kk) * ( - VAT3( uN, ip1,j,k) * VAT3( oPW, iip1,jj,kk)
01998       - VAT3( oN, ip1,j,kp1) * VAT3( uPW, iip1,jj,kk)
01999       - VAT3( uC, ip1,jp1,k) * VAT3( oPNW, iip1,jj,kk)
02000       + VAT3( oC, ip1,jp1,kp1) * VAT3( uPNW, iip1,jj,kk)
02001       - VAT3( uNW, ip2,j,k) * VAT3( oPC, iip1,jj,kk)
02002       - VAT3( oNW, ip2,j,kp1) * VAT3( uPC, iip1,jj,kk)
02003       - VAT3( uW, ip2,jp1,k) * VAT3( oPN, iip1,jj,kk)
02004       - VAT3( oE, ip1,jp1,kp1) * VAT3( uPN, iip1,jj,kk));
02005
02006 VAT3( XoE, ii,jj,kk) = TMP1_XOE + TMP2_XOE + TMP3_XOE + TMP4_XOE
02007     + TMP5_XOE + TMP6_XOE + TMP7_XOE + TMP8_XOE + TMP9_XOE
02008     + TMP10_XOE + TMP11_XOE + TMP12_XOE;
02009
02010     //fprintf(data, "%19.12E\n", VAT3(XoE, ii, jj, kk));
02011
02012 /* *****
02013 * *** > ON;
02014 * *****/
02015
02016 // VAT3( XoN, ii,jj,kk) =
02017 TMP1_XON =
02018     - VAT3( dPW, ii,jj,kk) * ( - VAT3( oN, im1,j,km1) * VAT3(dPSW, ii,jjp1,kk)
02019       - VAT3( uN, im1,j,km1) * VAT3(oPSW, ii,jjp1,kk)
02020       - VAT3( oNE, im1,j,km1) * VAT3( dPS, ii,jjp1,kk)
02021       - VAT3( uNE, im1,j,km1) * VAT3( oPS, ii,jjp1,kk))
02022
02023     - VAT3( oPW, ii,jj,kk) * ( - VAT3( uS, im1,jp1,km1) * VAT3(dPSW, ii,jjp1,kk)
02024       - VAT3( oN, im1,j,k) * VAT3(oPSW, ii,jjp1,kk)
02025       - VAT3( uN, im1,j,k) * VAT3(uPSW, ii,jjp1,kk)
02026       - VAT3( uSW, i,jp1,km1) * VAT3( dPS, ii,jjp1,kk)
02027       - VAT3( oNE, im1,j,k) * VAT3( oPS, ii,jjp1,kk)
02028       - VAT3( uNE, im1,j,k) * VAT3( uPS, ii,jjp1,kk))
02029
02030     - VAT3( uPW, ii,jj,kk) * ( - VAT3( uS, im1,jp1,k) * VAT3(oPSW, ii,jjp1,kk)
02031       - VAT3( oN, im1,j,kp1) * VAT3(uPSW, ii,jjp1,kk)
02032       - VAT3( uSW, i,jp1,k) * VAT3( oPS, ii,jjp1,kk)
02033       - VAT3( oNE, im1,j,kp1) * VAT3( uPS, ii,jjp1,kk));
02034
02035 TMP2_XON =
02036     - VAT3(dPNW, ii,jj,kk) * ( VAT3( oC, im1,jp1,km1) * VAT3(dPSW, ii,jjp1,kk)
02037       - VAT3( uC, im1,jp1,km1) * VAT3(oPSW, ii,jjp1,kk)
02038       - VAT3( oN, im1,jp1,km1) * VAT3( dPW, ii,jjp1,kk)
02039       - VAT3( uN, im1,jp1,km1) * VAT3( oPW, ii,jjp1,kk)
02040       - VAT3( oE, im1,jp1,km1) * VAT3( dPS, ii,jjp1,kk)
02041       - VAT3( uE, im1,jp1,km1) * VAT3( oPS, ii,jjp1,kk)
02042       - VAT3( oNE, im1,jp1,km1) * VAT3( dPC, ii,jjp1,kk)
02043       - VAT3( uNE, im1,jp1,km1) * VAT3( oPC, ii,jjp1,kk));
02044
02045 TMP3_XON =
02046     - VAT3(oPNW, ii,jj,kk) * ( - VAT3( uC, im1,jp1,km1) * VAT3(dPSW, ii,jjp1,kk)
02047       + VAT3( oC, im1,jp1,k) * VAT3(oPSW, ii,jjp1,kk)
02048       - VAT3( uC, im1,jp1,k) * VAT3(uPSW, ii,jjp1,kk)
02049       - VAT3( uS, im1,jp2,km1) * VAT3( dPW, ii,jjp1,kk)
02050       - VAT3( oN, im1,jp1,k) * VAT3( oPW, ii,jjp1,kk)
02051       - VAT3( uN, im1,jp1,k) * VAT3( uPW, ii,jjp1,kk)
02052       - VAT3( uW, i,jp1,km1) * VAT3( dPS, ii,jjp1,kk)
02053       - VAT3( oE, im1,jp1,k) * VAT3( oPS, ii,jjp1,kk)
02054       - VAT3( uE, im1,jp1,k) * VAT3( uPS, ii,jjp1,kk)
02055       - VAT3( uSW, i,jp2,km1) * VAT3( dPC, ii,jjp1,kk)
02056       - VAT3( oNE, im1,jp1,k) * VAT3( oPC, ii,jjp1,kk)
02057       - VAT3( uNE, im1,jp1,k) * VAT3( uPC, ii,jjp1,kk));
02058
02059 TMP4_XON =
02060     - VAT3(uPNW, ii,jj,kk) * ( - VAT3( uC, im1,jp1,k) * VAT3(oPSW, ii,jjp1,kk)
02061       + VAT3( oC, im1,jp1,kp1) * VAT3(uPSW, ii,jjp1,kk)
02062       - VAT3( uS, im1,jp2,k) * VAT3( oPW, ii,jjp1,kk)
02063       - VAT3( oN, im1,jp1,kp1) * VAT3( uPW, ii,jjp1,kk)
02064       - VAT3( uW, i,jp1,k) * VAT3( oPS, ii,jjp1,kk)
02065       - VAT3( oE, im1,jp1,kp1) * VAT3( uPS, ii,jjp1,kk)
02066       - VAT3( uSW, i,jp2,k) * VAT3( oPC, ii,jjp1,kk)
02067       - VAT3( oNE, im1,jp1,kp1) * VAT3( uPC, ii,jjp1,kk))
02068
02069     - VAT3( dPC, ii,jj,kk) * ( - VAT3( oNW, i,j,km1) * VAT3(dPSW, ii,jjp1,kk)

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02070             - VAT3( uNW, i, j, km1) * VAT3( oPSW, ii, jjp1, kk)
02071             - VAT3( oN, i, j, km1) * VAT3( dPS, ii, jjp1, kk)
02072             - VAT3( uN, i, j, km1) * VAT3( oPS, ii, jjp1, kk)
02073             - VAT3( oNE, i, j, km1) * VAT3( dPSE, ii, jjp1, kk)
02074             - VAT3( uNE, i, j, km1) * VAT3( oPSE, ii, jjp1, kk));
02075
02076 TMP5_XON =
02077     - VAT3( oPC, ii, jj, kk) * (- VAT3( uSE, im1, jpl, km1) * VAT3( dPSW, ii, jjp1, kk)
02078     - VAT3( oNW, i, j, k) * VAT3( oPSW, ii, jjp1, kk)
02079     - VAT3( uNW, i, j, k) * VAT3( uPSW, ii, jjp1, kk)
02080     - VAT3( uS, i, jpl, km1) * VAT3( dPS, ii, jjp1, kk)
02081     - VAT3( oN, i, j, k) * VAT3( oPS, ii, jjp1, kk)
02082     - VAT3( uN, i, j, k) * VAT3( uPS, ii, jjp1, kk)
02083     - VAT3( uSW, ip1, jpl, km1) * VAT3( dPSE, ii, jjp1, kk)
02084     - VAT3( oNE, i, j, k) * VAT3( oPSE, ii, jjp1, kk)
02085     - VAT3( uNE, i, j, k) * VAT3( uPSE, ii, jjp1, kk))
02086
02087     - VAT3( uPC, ii, jj, kk) * (- VAT3( uSE, im1, jpl, k) * VAT3( oPSW, ii, jjp1, kk)
02088     - VAT3( oNW, i, j, kp1) * VAT3( uPSW, ii, jjp1, kk)
02089     - VAT3( uS, i, jpl, k) * VAT3( oPS, ii, jjp1, kk)
02090     - VAT3( oN, i, j, kp1) * VAT3( uPS, ii, jjp1, kk)
02091     - VAT3( uSW, ip1, jpl, k) * VAT3( oPSE, ii, jjp1, kk)
02092     - VAT3( oNE, i, j, kp1) * VAT3( uPSE, ii, jjp1, kk));
02093
02094 TMP6_XON =
02095     - VAT3( dPN, ii, jj, kk) * (- VAT3( oE, im1, jpl, km1) * VAT3( dPSW, ii, jjp1, kk)
02096     - VAT3( uW, i, jpl, km1) * VAT3( oPSW, ii, jjp1, kk)
02097     - VAT3( oNW, i, jpl, km1) * VAT3( dPW, ii, jjp1, kk)
02098     - VAT3( uNW, i, jpl, km1) * VAT3( oPW, ii, jjp1, kk)
02099     + VAT3( oC, i, jpl, km1) * VAT3( dPS, ii, jjp1, kk)
02100     - VAT3( uC, i, jpl, km1) * VAT3( oPS, ii, jjp1, kk)
02101     - VAT3( oN, i, jpl, km1) * VAT3( dPC, ii, jjp1, kk)
02102     - VAT3( uN, i, jpl, km1) * VAT3( oPC, ii, jjp1, kk)
02103     - VAT3( oE, i, jpl, km1) * VAT3( dPSE, ii, jjp1, kk)
02104     - VAT3( uE, i, jpl, km1) * VAT3( oPSE, ii, jjp1, kk)
02105     - VAT3( oNE, i, jpl, km1) * VAT3( dPE, ii, jjp1, kk)
02106     - VAT3( uNE, i, jpl, km1) * VAT3( oPE, ii, jjp1, kk));
02107
02108 TMP7_XON =
02109     - VAT3( oPN, ii, jj, kk) * (- VAT3( uE, im1, jpl, km1) * VAT3( dPSW, ii, jjp1, kk)
02110     - VAT3( oE, im1, jpl, k) * VAT3( oPSW, ii, jjp1, kk)
02111     - VAT3( uW, i, jpl, k) * VAT3( uPSW, ii, jjp1, kk)
02112     - VAT3( uSE, im1, jp2, km1) * VAT3( dPW, ii, jjp1, kk)
02113     - VAT3( oNW, i, jpl, k) * VAT3( oPW, ii, jjp1, kk)
02114     - VAT3( uNW, i, jpl, k) * VAT3( uPW, ii, jjp1, kk)
02115     - VAT3( uC, i, jpl, km1) * VAT3( dPS, ii, jjp1, kk)
02116     + VAT3( oC, i, jpl, k) * VAT3( oPS, ii, jjp1, kk)
02117     - VAT3( uC, i, jpl, k) * VAT3( uPS, ii, jjp1, kk)
02118     - VAT3( uS, i, jp2, km1) * VAT3( dPC, ii, jjp1, kk)
02119     - VAT3( oN, i, jpl, k) * VAT3( oPC, ii, jjp1, kk)
02120     - VAT3( uN, i, jpl, k) * VAT3( uPC, ii, jjp1, kk)
02121     - VAT3( uW, ip1, jpl, km1) * VAT3( dPSE, ii, jjp1, kk)
02122     - VAT3( oE, i, jpl, k) * VAT3( oPSE, ii, jjp1, kk)
02123     - VAT3( uE, i, jpl, k) * VAT3( uPSE, ii, jjp1, kk)
02124     - VAT3( uSW, ip1, jp2, km1) * VAT3( dPE, ii, jjp1, kk)
02125     - VAT3( oNE, i, jpl, k) * VAT3( oPE, ii, jjp1, kk)
02126     - VAT3( uNE, i, jpl, k) * VAT3( uPE, ii, jjp1, kk));
02127
02128 TMP8_XON =
02129     - VAT3( uPN, ii, jj, kk) * (- VAT3( uE, im1, jpl, k) * VAT3( oPSW, ii, jjp1, kk)
02130     - VAT3( oE, im1, jpl, kp1) * VAT3( uPSW, ii, jjp1, kk)
02131     - VAT3( uSE, im1, jp2, k) * VAT3( oPW, ii, jjp1, kk)
02132     - VAT3( oNW, i, jpl, kp1) * VAT3( uPW, ii, jjp1, kk)
02133     - VAT3( uC, i, jpl, k) * VAT3( oPS, ii, jjp1, kk)
02134     + VAT3( oC, i, jpl, kp1) * VAT3( uPS, ii, jjp1, kk)
02135     - VAT3( uS, i, jp2, k) * VAT3( oPC, ii, jjp1, kk)
02136     - VAT3( oN, i, jpl, kp1) * VAT3( uPC, ii, jjp1, kk)
02137     - VAT3( uW, ip1, jpl, k) * VAT3( oPSE, ii, jjp1, kk)
02138     - VAT3( oE, i, jpl, kp1) * VAT3( uPSE, ii, jjp1, kk)
02139     - VAT3( uSW, ip1, jp2, k) * VAT3( oPE, ii, jjp1, kk)
02140     - VAT3( oNE, i, jpl, kp1) * VAT3( uPE, ii, jjp1, kk))
02141
02142     - VAT3( dPE, ii, jj, kk) * (- VAT3( oNW, ip1, j, km1) * VAT3( dPS, ii, jjp1, kk)
02143     - VAT3( uNW, ip1, j, km1) * VAT3( oPS, ii, jjp1, kk)
02144     - VAT3( oN, ip1, j, km1) * VAT3( dPSE, ii, jjp1, kk)
02145     - VAT3( uN, ip1, j, km1) * VAT3( oPSE, ii, jjp1, kk));
02146
02147 TMP9_XON =
02148     - VAT3( oPE, ii, jj, kk) * (- VAT3( uSE, i, jpl, km1) * VAT3( dPS, ii, jjp1, kk)
02149     - VAT3( oNW, ip1, j, k) * VAT3( oPS, ii, jjp1, kk)
02150     - VAT3( uNW, ip1, j, k) * VAT3( uPS, ii, jjp1, kk)

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02151             - VAT3( uS, ipl,jpl,kml) * VAT3(dPSE, ii,jjp1,kk)
02152             - VAT3( oN, ipl,j,k) * VAT3(oPSE, ii,jjp1,kk)
02153             - VAT3( uN, ipl,j,k) * VAT3(uPSE, ii,jjp1,kk))
02154
02155             - VAT3( uPE, ii,jj,kk) * (- VAT3( uSE, i,jpl,k) * VAT3( oPS, ii,jjp1,kk)
02156             - VAT3( oNW, ipl,j,kpl) * VAT3( uPS, ii,jjp1,kk)
02157             - VAT3( uS, ipl,jpl,k) * VAT3(oPSE, ii,jjp1,kk)
02158             - VAT3( oN, ipl,j,kpl) * VAT3(uPSE, ii,jjp1,kk));
02159
02160 TMP10_XON =
02161     - VAT3(dPNE, ii,jj,kk) * (- VAT3( oE, i,jpl,kml) * VAT3( dPS, ii,jjp1,kk)
02162     - VAT3( uW, ipl,jpl,kml) * VAT3( oPS, ii,jjp1,kk)
02163     - VAT3( oNW, ipl,jpl,kml) * VAT3( dPC, ii,jjp1,kk)
02164     - VAT3( uNW, ipl,jpl,kml) * VAT3( oPC, ii,jjp1,kk)
02165     + VAT3( oC, ipl,jpl,kml) * VAT3(dPSE, ii,jjp1,kk)
02166     - VAT3( uC, ipl,jpl,kml) * VAT3(oPSE, ii,jjp1,kk)
02167     - VAT3( oN, ipl,jpl,kml) * VAT3( dPE, ii,jjp1,kk)
02168     - VAT3( uN, ipl,jpl,kml) * VAT3( oPE, ii,jjp1,kk));
02169
02170 TMP11_XON =
02171     - VAT3(oPNE, ii,jj,kk) * (- VAT3( uE, i,jpl,kml) * VAT3( dPS, ii,jjp1,kk)
02172     - VAT3( oE, i,jpl,k) * VAT3( oPS, ii,jjp1,kk)
02173     - VAT3( uW, ipl,jpl,k) * VAT3( uPS, ii,jjp1,kk)
02174     - VAT3( uSE, i,jp2,kml) * VAT3( dPC, ii,jjp1,kk)
02175     - VAT3( oNW, ipl,jpl,k) * VAT3( oPC, ii,jjp1,kk)
02176     - VAT3( uNW, ipl,jpl,k) * VAT3( uPC, ii,jjp1,kk)
02177     - VAT3( uC, ipl,jpl,kml) * VAT3(dPSE, ii,jjp1,kk)
02178     + VAT3( oC, ipl,jpl,k) * VAT3(oPSE, ii,jjp1,kk)
02179     - VAT3( uC, ipl,jpl,k) * VAT3(uPSE, ii,jjp1,kk)
02180     - VAT3( uS, ipl,jp2,kml) * VAT3( dPE, ii,jjp1,kk)
02181     - VAT3( oN, ipl,jpl,k) * VAT3( oPE, ii,jjp1,kk)
02182     - VAT3( uN, ipl,jpl,k) * VAT3( uPE, ii,jjp1,kk));
02183
02184 TMP12_XON =
02185     - VAT3(uPNE, ii,jj,kk) * (- VAT3( uE, i,jpl,k) * VAT3( oPS, ii,jjp1,kk)
02186     - VAT3( oE, i,jpl,kpl) * VAT3( uPS, ii,jjp1,kk)
02187     - VAT3( uSE, i,jp2,k) * VAT3( oPC, ii,jjp1,kk)
02188     - VAT3( oNW, ipl,jpl,kpl) * VAT3( uPC, ii,jjp1,kk)
02189     - VAT3( uC, ipl,jpl,k) * VAT3(oPSE, ii,jjp1,kk)
02190     + VAT3( oC, ipl,jpl,kpl) * VAT3(uPSE, ii,jjp1,kk)
02191     - VAT3( uS, ipl,jp2,k) * VAT3( oPE, ii,jjp1,kk)
02192     - VAT3( oN, ipl,jpl,kpl) * VAT3( uPE, ii,jjp1,kk));
02193
02194 VAT3( XoN, ii,jj,kk) = TMP1_XON + TMP2_XON + TMP3_XON + TMP4_XON
02195 + TMP5_XON + TMP6_XON + TMP7_XON + TMP8_XON + TMP9_XON
02196 + TMP10_XON + TMP11_XON + TMP12_XON;
02197
02198 //fprintf(data, "%19.12E\n", VAT3(XoN, ii, jj, kk));
02199
02200 /* *****
02201 * *** > UC;
02202 * *****/
02203
02204 // VAT3( XuC, ii,jj,kk) =
02205 TMP1_XUC =
02206     - VAT3(oPSW, ii,jj,kk) * (- VAT3( uC, iml,jml,k) * VAT3(dPSW, ii,jj,kkp1)
02207     - VAT3( uN, iml,jml,k) * VAT3( dPW, ii,jj,kkp1)
02208     - VAT3( uE, iml,jml,k) * VAT3( dPS, ii,jj,kkp1)
02209     - VAT3( uNE, iml,jml,k) * VAT3( dPC, ii,jj,kkp1))
02210
02211     - VAT3(uPSW, ii,jj,kk) * ( VAT3( oC, iml,jml,kpl) * VAT3(dPSW, ii,jj,kkp1)
02212     - VAT3( uC, iml,jml,kpl) * VAT3(oPSW, ii,jj,kkp1)
02213     - VAT3( oN, iml,jml,kpl) * VAT3( dPW, ii,jj,kkp1)
02214     - VAT3( uN, iml,jml,kpl) * VAT3( oPW, ii,jj,kkp1)
02215     - VAT3( oE, iml,jml,kpl) * VAT3( dPS, ii,jj,kkp1)
02216     - VAT3( uE, iml,jml,kpl) * VAT3( oPS, ii,jj,kkp1)
02217     - VAT3( oNE, iml,jml,kpl) * VAT3( dPC, ii,jj,kkp1)
02218     - VAT3( uNE, iml,jml,kpl) * VAT3( oPC, ii,jj,kkp1));
02219
02220 TMP2_XUC =
02221     - VAT3( oPW, ii,jj,kk) * (- VAT3( uS, iml,j,k) * VAT3(dPSW, ii,jj,kkp1)
02222     - VAT3( uC, iml,j,k) * VAT3( dPW, ii,jj,kkp1)
02223     - VAT3( uN, iml,j,k) * VAT3(dPNW, ii,jj,kkp1)
02224     - VAT3( uSE, iml,j,k) * VAT3( dPS, ii,jj,kkp1)
02225     - VAT3( uE, iml,j,k) * VAT3( dPC, ii,jj,kkp1)
02226     - VAT3( uNE, iml,j,k) * VAT3( dPN, ii,jj,kkp1));
02227
02228 TMP3_XUC =
02229     - VAT3( uPW, ii,jj,kk) * (- VAT3( oN, iml,jml,kpl) * VAT3(dPSW, ii,jj,kkp1)
02230     - VAT3( uS, iml,j,kpl) * VAT3(oPSW, ii,jj,kkp1)

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02232          + VAT3( oC, iml,j,kpl) * VAT3( dPW, ii,jj,kkpl)
02233          - VAT3( uC, iml,j,kpl) * VAT3( oPW, ii,jj,kkpl)
02234          - VAT3( oN, iml,j,kpl) * VAT3(dPNW, ii,jj,kkpl)
02235          - VAT3( uN, iml,j,kpl) * VAT3(oPNW, ii,jj,kkpl)
02236          - VAT3( oNW, i,jml,kpl) * VAT3( dPS, ii,jj,kkpl)
02237          - VAT3( uSE, iml,j,kpl) * VAT3( oPS, ii,jj,kkpl)
02238          - VAT3( oE, iml,j,kpl) * VAT3( dPC, ii,jj,kkpl)
02239          - VAT3( uE, iml,j,kpl) * VAT3( oPC, ii,jj,kkpl)
02240          - VAT3( oNE, iml,j,kpl) * VAT3( dPN, ii,jj,kkpl)
02241          - VAT3( uNE, iml,j,kpl) * VAT3( oPN, ii,jj,kkpl))
02242
02243          - VAT3(oPNW, ii,jj,kk) * (- VAT3( uS, iml,jpl,k) * VAT3( dPW, ii,jj,kkpl)
02244          - VAT3( uC, iml,jpl,k) * VAT3(dPNW, ii,jj,kkpl)
02245          - VAT3( uSE, iml,jpl,k) * VAT3( dPC, ii,jj,kkpl)
02246          - VAT3( uE, iml,jpl,k) * VAT3( dPN, ii,jj,kkpl));
02247
02248 TMP4_XUC =
02249          - VAT3(uPNW, ii,jj,kk) * (- VAT3( oN, iml,j,kpl) * VAT3( dPW, ii,jj,kkpl)
02250          - VAT3( uS, iml,jpl,kpl) * VAT3( oPW, ii,jj,kkpl)
02251          + VAT3( oC, iml,jpl,kpl) * VAT3(dPNW, ii,jj,kkpl)
02252          - VAT3( uC, iml,jpl,kpl) * VAT3(oPNW, ii,jj,kkpl)
02253          - VAT3( oNW, i,j,kpl) * VAT3( dPC, ii,jj,kkpl)
02254          - VAT3( uSE, iml,jpl,kpl) * VAT3( oPC, ii,jj,kkpl)
02255          - VAT3( oE, iml,jpl,kpl) * VAT3( dPN, ii,jj,kkpl)
02256          - VAT3( uE, iml,jpl,kpl) * VAT3( oPN, ii,jj,kkpl))
02257
02258          - VAT3( oPS, ii,jj,kk) * (- VAT3( uW, i,jml,k) * VAT3(dPSW, ii,jj,kkpl)
02259          - VAT3( uNW, i,jml,k) * VAT3( dPW, ii,jj,kkpl)
02260          - VAT3( uC, i,jml,k) * VAT3( dPS, ii,jj,kkpl)
02261          - VAT3( uN, i,jml,k) * VAT3( dPC, ii,jj,kkpl)
02262          - VAT3( uE, i,jml,k) * VAT3(dPSE, ii,jj,kkpl)
02263          - VAT3( uNE, i,jml,k) * VAT3( dPE, ii,jj,kkpl));
02264
02265 TMP5_XUC =
02266          - VAT3( uPS, ii,jj,kk) * (- VAT3( oE, iml,jml,kpl) * VAT3(dPSW, ii,jj,kkpl)
02267          - VAT3( uW, i,jml,kpl) * VAT3(oPSW, ii,jj,kkpl)
02268          - VAT3( oNW, i,jml,kpl) * VAT3( dPW, ii,jj,kkpl)
02269          - VAT3( uNW, i,jml,kpl) * VAT3( oPW, ii,jj,kkpl)
02270          + VAT3( oC, i,jml,kpl) * VAT3( dPS, ii,jj,kkpl)
02271          - VAT3( uC, i,jml,kpl) * VAT3( oPS, ii,jj,kkpl)
02272          - VAT3( oN, i,jml,kpl) * VAT3( dPC, ii,jj,kkpl)
02273          - VAT3( uN, i,jml,kpl) * VAT3( oPC, ii,jj,kkpl)
02274          - VAT3( oE, i,jml,kpl) * VAT3(dPSE, ii,jj,kkpl)
02275          - VAT3( uE, i,jml,kpl) * VAT3(oPSE, ii,jj,kkpl)
02276          - VAT3( oNE, i,jml,kpl) * VAT3( dPE, ii,jj,kkpl)
02277          - VAT3( uNE, i,jml,kpl) * VAT3( oPE, ii,jj,kkpl));
02278
02279 TMP6_XUC =
02280          - VAT3( oPC, ii,jj,kk) * (- VAT3( uSW, i,j,k) * VAT3(dPSW, ii,jj,kkpl)
02281          - VAT3( uW, i,j,k) * VAT3( dPW, ii,jj,kkpl)
02282          - VAT3( uNW, i,j,k) * VAT3(dPNW, ii,jj,kkpl)
02283          - VAT3( uS, i,j,k) * VAT3( dPS, ii,jj,kkpl)
02284          - VAT3( uC, i,j,k) * VAT3( dPC, ii,jj,kkpl)
02285          - VAT3( uN, i,j,k) * VAT3( dPN, ii,jj,kkpl)
02286          - VAT3( uSE, i,j,k) * VAT3(dPSE, ii,jj,kkpl)
02287          - VAT3( uE, i,j,k) * VAT3( dPE, ii,jj,kkpl)
02288          - VAT3( uNE, i,j,k) * VAT3(dPNE, ii,jj,kkpl));
02289
02290 TMP7_XUC =
02291          - VAT3( uPC, ii,jj,kk) * (- VAT3( oNE, iml,jml,kpl) * VAT3(dPSW, ii,jj,kkpl)
02292          - VAT3( uSW, i,j,kpl) * VAT3(oPSW, ii,jj,kkpl)
02293          - VAT3( oE, iml,j,kpl) * VAT3( dPW, ii,jj,kkpl)
02294          - VAT3( uW, i,j,kpl) * VAT3( oPW, ii,jj,kkpl)
02295          - VAT3( oNW, i,j,kpl) * VAT3(dPNW, ii,jj,kkpl)
02296          - VAT3( uNW, i,j,kpl) * VAT3(oPNW, ii,jj,kkpl)
02297          - VAT3( oN, i,jml,kpl) * VAT3( dPS, ii,jj,kkpl)
02298          - VAT3( uS, i,j,kpl) * VAT3( oPS, ii,jj,kkpl)
02299          + VAT3( oC, i,j,kpl) * VAT3( dPC, ii,jj,kkpl)
02300          - VAT3( uC, i,j,kpl) * VAT3( oPC, ii,jj,kkpl)
02301          - VAT3( oN, i,j,kpl) * VAT3( dPN, ii,jj,kkpl)
02302          - VAT3( uN, i,j,kpl) * VAT3( oPN, ii,jj,kkpl)
02303          - VAT3( oNW, ipl,jml,kpl) * VAT3(dPSE, ii,jj,kkpl)
02304          - VAT3( uSE, i,j,kpl) * VAT3(oPSE, ii,jj,kkpl)
02305          - VAT3( oE, i,j,kpl) * VAT3( dPE, ii,jj,kkpl)
02306          - VAT3( uE, i,j,kpl) * VAT3( oPE, ii,jj,kkpl)
02307          - VAT3( oNE, i,j,kpl) * VAT3(dPNE, ii,jj,kkpl)
02308          - VAT3( uNE, i,j,kpl) * VAT3(oPNE, ii,jj,kkpl));
02309
02310 TMP8_XUC =
02311          - VAT3( oPN, ii,jj,kk) * (- VAT3( uSW, i,jpl,k) * VAT3( dPW, ii,jj,kkpl)
02312          - VAT3( uW, i,jpl,k) * VAT3(dPNW, ii,jj,kkpl)

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02313             - VAT3( uS, i, jpl, k) * VAT3( dPC, ii, jj, kkp1)
02314             - VAT3( uC, i, jpl, k) * VAT3( dPN, ii, jj, kkp1)
02315             - VAT3( uSE, i, jpl, k) * VAT3( dPE, ii, jj, kkp1)
02316             - VAT3( uE, i, jpl, k) * VAT3( dPNE, ii, jj, kkp1));
02317
02318     TMP9_XUC =
02319     - VAT3( uPN, ii, jj, kk) * (- VAT3( oNE, im1, j, kpl) * VAT3( dPW, ii, jj, kkp1)
02320     - VAT3( uSW, i, jpl, kpl) * VAT3( oPW, ii, jj, kkp1)
02321     - VAT3( oE, im1, jpl, kpl) * VAT3( dPNW, ii, jj, kkp1)
02322     - VAT3( uW, i, jpl, kpl) * VAT3( oPNW, ii, jj, kkp1)
02323     - VAT3( oN, i, j, kpl) * VAT3( dPC, ii, jj, kkp1)
02324     - VAT3( uS, i, jpl, kpl) * VAT3( oPC, ii, jj, kkp1)
02325     + VAT3( oC, i, jpl, kpl) * VAT3( dPN, ii, jj, kkp1)
02326     - VAT3( uC, i, jpl, kpl) * VAT3( oPN, ii, jj, kkp1)
02327     - VAT3( oNW, ip1, j, kpl) * VAT3( dPE, ii, jj, kkp1)
02328     - VAT3( uSE, i, jpl, kpl) * VAT3( oPE, ii, jj, kkp1)
02329     - VAT3( oE, i, jpl, kpl) * VAT3( dPNE, ii, jj, kkp1)
02330     - VAT3( uE, i, jpl, kpl) * VAT3( oPNE, ii, jj, kkp1))
02331
02332     - VAT3( oPSE, ii, jj, kk) * (- VAT3( uW, ip1, jml, k) * VAT3( dPS, ii, jj, kkp1)
02333     - VAT3( uNW, ip1, jml, k) * VAT3( dPC, ii, jj, kkp1)
02334     - VAT3( uC, ip1, jml, k) * VAT3( dPSE, ii, jj, kkp1)
02335     - VAT3( uN, ip1, jml, k) * VAT3( dPE, ii, jj, kkp1));
02336
02337     TMP10_XUC =
02338     - VAT3( uPSE, ii, jj, kk) * (- VAT3( oE, i, jml, kpl) * VAT3( dPS, ii, jj, kkp1)
02339     - VAT3( uW, ip1, jml, kpl) * VAT3( oPS, ii, jj, kkp1)
02340     - VAT3( oNW, ip1, jml, kpl) * VAT3( dPC, ii, jj, kkp1)
02341     - VAT3( uNW, ip1, jml, kpl) * VAT3( oPC, ii, jj, kkp1)
02342     + VAT3( oC, ip1, jml, kpl) * VAT3( dPSE, ii, jj, kkp1)
02343     - VAT3( uC, ip1, jml, kpl) * VAT3( oPSE, ii, jj, kkp1)
02344     - VAT3( oN, ip1, jml, kpl) * VAT3( dPE, ii, jj, kkp1)
02345     - VAT3( uN, ip1, jml, kpl) * VAT3( oPE, ii, jj, kkp1))
02346
02347     - VAT3( oPE, ii, jj, kk) * (- VAT3( uSW, ip1, j, k) * VAT3( dPS, ii, jj, kkp1)
02348     - VAT3( uW, ip1, j, k) * VAT3( dPC, ii, jj, kkp1)
02349     - VAT3( uNW, ip1, j, k) * VAT3( dPN, ii, jj, kkp1)
02350     - VAT3( uS, ip1, j, k) * VAT3( dPSE, ii, jj, kkp1)
02351     - VAT3( uC, ip1, j, k) * VAT3( dPE, ii, jj, kkp1)
02352     - VAT3( uN, ip1, j, k) * VAT3( dPNE, ii, jj, kkp1));
02353
02354     TMP11_XUC =
02355     - VAT3( uPE, ii, jj, kk) * (- VAT3( oNE, i, jml, kpl) * VAT3( dPS, ii, jj, kkp1)
02356     - VAT3( uSW, ip1, j, kpl) * VAT3( oPS, ii, jj, kkp1)
02357     - VAT3( oE, i, j, kpl) * VAT3( dPC, ii, jj, kkp1)
02358     - VAT3( uW, ip1, j, kpl) * VAT3( oPC, ii, jj, kkp1)
02359     - VAT3( oNW, ip1, j, kpl) * VAT3( dPN, ii, jj, kkp1)
02360     - VAT3( uNW, ip1, j, kpl) * VAT3( oPN, ii, jj, kkp1)
02361     - VAT3( oN, ip1, jml, kpl) * VAT3( dPSE, ii, jj, kkp1)
02362     - VAT3( uS, ip1, j, kpl) * VAT3( oPSE, ii, jj, kkp1)
02363     + VAT3( oC, ip1, j, kpl) * VAT3( dPE, ii, jj, kkp1)
02364     - VAT3( uC, ip1, j, kpl) * VAT3( oPE, ii, jj, kkp1)
02365     - VAT3( oN, ip1, j, kpl) * VAT3( dPNE, ii, jj, kkp1)
02366     - VAT3( uN, ip1, j, kpl) * VAT3( oPNE, ii, jj, kkp1));
02367
02368     TMP12_XUC =
02369     - VAT3( oPNE, ii, jj, kk) * (- VAT3( uSW, ip1, jpl, k) * VAT3( dPC, ii, jj, kkp1)
02370     - VAT3( uW, ip1, jpl, k) * VAT3( dPN, ii, jj, kkp1)
02371     - VAT3( uS, ip1, jpl, k) * VAT3( dPE, ii, jj, kkp1)
02372     - VAT3( uC, ip1, jpl, k) * VAT3( dPNE, ii, jj, kkp1))
02373
02374     - VAT3( uPNE, ii, jj, kk) * (- VAT3( oNE, i, j, kpl) * VAT3( dPC, ii, jj, kkp1)
02375     - VAT3( uSW, ip1, jpl, kpl) * VAT3( oPC, ii, jj, kkp1)
02376     - VAT3( oE, i, jpl, kpl) * VAT3( dPN, ii, jj, kkp1)
02377     - VAT3( uW, ip1, jpl, kpl) * VAT3( oPN, ii, jj, kkp1)
02378     - VAT3( oN, ip1, j, kpl) * VAT3( dPE, ii, jj, kkp1)
02379     - VAT3( uS, ip1, jpl, kpl) * VAT3( oPE, ii, jj, kkp1)
02380     + VAT3( oC, ip1, jpl, kpl) * VAT3( dPNE, ii, jj, kkp1)
02381     - VAT3( uC, ip1, jpl, kpl) * VAT3( oPNE, ii, jj, kkp1));
02382
02383     VAT3( XuC, ii, jj, kk) = TMP1_XUC + TMP2_XUC + TMP3_XUC + TMP4_XUC
02384     + TMP5_XUC + TMP6_XUC + TMP7_XUC + TMP8_XUC + TMP9_XUC
02385     + TMP10_XUC + TMP11_XUC + TMP12_XUC;
02386
02387     //fprintf(data, "%19.12E\n", VAT3(XuC, ii, jj, kk));
02388
02389     /* *****
02390     * *** > ONE;
02391     * *****
02392
02393     // VAT3(XoNE, ii, jj, kk) =

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02394 TMP1_XONE =
02395   - VAT3( dPC, ii,jj,kk) * (- VAT3( oNE, i,j,kml) * VAT3(dPSW, iip1,jjp1,kk)
02396     - VAT3( uNE, i,j,kml) * VAT3(oPSW, iip1,jjp1,kk))
02397
02398   - VAT3( oPC, ii,jj,kk) * (- VAT3( uSW, ip1,jp1,kml) * VAT3(dPSW, iip1,jjp1,kk)
02399     - VAT3( oNE, i,j,k) * VAT3(oPSW, iip1,jjp1,kk)
02400     - VAT3( uNE, i,j,k) * VAT3(uPSW, iip1,jjp1,kk))
02401
02402   - VAT3( uPC, ii,jj,kk) * (- VAT3( uSW, ip1,jp1,k) * VAT3(oPSW, iip1,jjp1,kk)
02403     - VAT3( oNE, i,j,kp1) * VAT3(uPSW, iip1,jjp1,kk))
02404
02405   - VAT3( dPN, ii,jj,kk) * (- VAT3( oE, i,jp1,kml) * VAT3(dPSW, iip1,jjp1,kk)
02406     - VAT3( uE, i,jp1,kml) * VAT3(oPSW, iip1,jjp1,kk)
02407     - VAT3( oNE, i,jp1,kml) * VAT3( dPW, iip1,jjp1,kk)
02408     - VAT3( uNE, i,jp1,kml) * VAT3( oPW, iip1,jjp1,kk));
02409
02410 TMP2_XONE =
02411   - VAT3( oPN, ii,jj,kk) * (- VAT3( uW, ip1,jp1,kml) * VAT3(dPSW, iip1,jjp1,kk)
02412     - VAT3( oE, i,jp1,k) * VAT3(oPSW, iip1,jjp1,kk)
02413     - VAT3( uE, i,jp1,k) * VAT3(uPSW, iip1,jjp1,kk)
02414     - VAT3( uSW, ip1,jp2,kml) * VAT3( dPW, iip1,jjp1,kk)
02415     - VAT3( oNE, i,jp1,k) * VAT3( oPW, iip1,jjp1,kk)
02416     - VAT3( uNE, i,jp1,k) * VAT3( uPW, iip1,jjp1,kk))
02417
02418   - VAT3( uPN, ii,jj,kk) * (- VAT3( uW, ip1,jp1,k) * VAT3(oPSW, iip1,jjp1,kk)
02419     - VAT3( oE, i,jp1,kp1) * VAT3(uPSW, iip1,jjp1,kk)
02420     - VAT3( uSW, ip1,jp2,k) * VAT3( oPW, iip1,jjp1,kk)
02421     - VAT3( oNE, i,jp1,kp1) * VAT3( uPW, iip1,jjp1,kk))
02422
02423   - VAT3( dPE, ii,jj,kk) * (- VAT3( oN, ip1,j,kml) * VAT3(dPSW, iip1,jjp1,kk)
02424     - VAT3( uN, ip1,j,kml) * VAT3(oPSW, iip1,jjp1,kk)
02425     - VAT3( oNE, ip1,j,kml) * VAT3( dPS, iip1,jjp1,kk)
02426     - VAT3( uNE, ip1,j,kml) * VAT3( oPS, iip1,jjp1,kk));
02427
02428 TMP3_XONE =
02429   - VAT3( oPE, ii,jj,kk) * (- VAT3( uS, ip1,jp1,kml) * VAT3(dPSW, iip1,jjp1,kk)
02430     - VAT3( oN, ip1,j,k) * VAT3(oPSW, iip1,jjp1,kk)
02431     - VAT3( uN, ip1,j,k) * VAT3(uPSW, iip1,jjp1,kk)
02432     - VAT3( uSW, ip2,jp1,kml) * VAT3( dPS, iip1,jjp1,kk)
02433     - VAT3( oNE, ip1,j,k) * VAT3( oPS, iip1,jjp1,kk)
02434     - VAT3( uNE, ip1,j,k) * VAT3( uPS, iip1,jjp1,kk))
02435
02436   - VAT3( uPE, ii,jj,kk) * (- VAT3( uS, ip1,jp1,k) * VAT3(oPSW, iip1,jjp1,kk)
02437     - VAT3( oN, ip1,j,kp1) * VAT3(uPSW, iip1,jjp1,kk)
02438     - VAT3( uSW, ip2,jp1,k) * VAT3( oPS, iip1,jjp1,kk)
02439     - VAT3( oNE, ip1,j,kp1) * VAT3( uPS, iip1,jjp1,kk));
02440
02441 TMP4_XONE =
02442   - VAT3( dPNE, ii,jj,kk) * ( VAT3( oC, ip1,jp1,kml) * VAT3(dPSW, iip1,jjp1,kk)
02443     - VAT3( uC, ip1,jp1,kml) * VAT3(oPSW, iip1,jjp1,kk)
02444     - VAT3( oN, ip1,jp1,kml) * VAT3( dPW, iip1,jjp1,kk)
02445     - VAT3( uN, ip1,jp1,kml) * VAT3( oPW, iip1,jjp1,kk)
02446     - VAT3( oE, ip1,jp1,kml) * VAT3( dPS, iip1,jjp1,kk)
02447     - VAT3( uE, ip1,jp1,kml) * VAT3( oPS, iip1,jjp1,kk)
02448     - VAT3( oNE, ip1,jp1,kml) * VAT3( dPC, iip1,jjp1,kk)
02449     - VAT3( uNE, ip1,jp1,kml) * VAT3( oPC, iip1,jjp1,kk));
02450
02451 TMP5_XONE =
02452   - VAT3( oPNE, ii,jj,kk) * (- VAT3( uC, ip1,jp1,kml) * VAT3(dPSW, iip1,jjp1,kk)
02453     + VAT3( oC, ip1,jp1,k) * VAT3(oPSW, iip1,jjp1,kk)
02454     - VAT3( uC, ip1,jp1,k) * VAT3(uPSW, iip1,jjp1,kk)
02455     - VAT3( uS, ip1,jp2,kml) * VAT3( dPW, iip1,jjp1,kk)
02456     - VAT3( oN, ip1,jp1,k) * VAT3( oPW, iip1,jjp1,kk)
02457     - VAT3( uN, ip1,jp1,k) * VAT3( uPW, iip1,jjp1,kk)
02458     - VAT3( uW, ip2,jp1,kml) * VAT3( dPS, iip1,jjp1,kk)
02459     - VAT3( oE, ip1,jp1,k) * VAT3( oPS, iip1,jjp1,kk)
02460     - VAT3( uE, ip1,jp1,k) * VAT3( uPS, iip1,jjp1,kk)
02461     - VAT3( uSW, ip2,jp2,kml) * VAT3( dPC, iip1,jjp1,kk)
02462     - VAT3( oNE, ip1,jp1,k) * VAT3( oPC, iip1,jjp1,kk)
02463     - VAT3( uNE, ip1,jp1,k) * VAT3( uPC, iip1,jjp1,kk));
02464
02465 TMP6_XONE =
02466   - VAT3( uPNE, ii,jj,kk) * (- VAT3( uC, ip1,jp1,k) * VAT3(oPSW, iip1,jjp1,kk)
02467     + VAT3( oC, ip1,jp1,kp1) * VAT3(uPSW, iip1,jjp1,kk)
02468     - VAT3( uS, ip1,jp2,k) * VAT3( oPW, iip1,jjp1,kk)
02469     - VAT3( oN, ip1,jp1,kp1) * VAT3( uPW, iip1,jjp1,kk)
02470     - VAT3( uW, ip2,jp1,k) * VAT3( oPS, iip1,jjp1,kk)
02471     - VAT3( oE, ip1,jp1,kp1) * VAT3( uPS, iip1,jjp1,kk)
02472     - VAT3( uSW, ip2,jp2,k) * VAT3( oPC, iip1,jjp1,kk)
02473     - VAT3( oNE, ip1,jp1,kp1) * VAT3( uPC, iip1,jjp1,kk));
02474

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02475     VAT3(XoNE, ii,jj,kk) = TMP1_XONE + TMP2_XONE + TMP3_XONE + TMP4_XONE
02476         + TMP5_XONE + TMP6_XONE;
02477
02478     //fprintf(data, "%19.12E\n", VAT3(XoNE, ii, jj, kk));
02479
02480     /* *****
02481     * *** > ONW;
02482     * *****/
02483
02484     // VAT3(XoNW, ii,jj,kk) =
02485     TMP1_XONW =
02486         - VAT3( dPW, ii,jj,kk) * (- VAT3( oNW, im1,j,kml) * VAT3( dPS, iim1,jjp1,kk)
02487             - VAT3( uNW, im1,j,kml) * VAT3( oPS, iim1,jjp1,kk)
02488             - VAT3( oN, im1,j,kml) * VAT3( dPSE, iim1,jjp1,kk)
02489             - VAT3( uN, im1,j,kml) * VAT3( oPSE, iim1,jjp1,kk))
02490
02491         - VAT3( oPW, ii,jj,kk) * (- VAT3( uSE, im2,jp1,kml) * VAT3( dPS, iim1,jjp1,kk)
02492             - VAT3( oNW, im1,j,k) * VAT3( oPS, iim1,jjp1,kk)
02493             - VAT3( uNW, im1,j,k) * VAT3( uPS, iim1,jjp1,kk)
02494             - VAT3( uS, im1,jp1,kml) * VAT3( dPSE, iim1,jjp1,kk)
02495             - VAT3( oN, im1,j,k) * VAT3( oPSE, iim1,jjp1,kk)
02496             - VAT3( uN, im1,j,k) * VAT3( uPSE, iim1,jjp1,kk));
02497
02498     TMP2_XONW =
02499         - VAT3( uPW, ii,jj,kk) * (- VAT3( uSE, im2,jp1,k) * VAT3( oPS, iim1,jjp1,kk)
02500             - VAT3( oNW, im1,j,kp1) * VAT3( uPS, iim1,jjp1,kk)
02501             - VAT3( uS, im1,jp1,k) * VAT3( oPSE, iim1,jjp1,kk)
02502             - VAT3( oN, im1,j,kp1) * VAT3( uPSE, iim1,jjp1,kk))
02503
02504         - VAT3( dPNW, ii,jj,kk) * (- VAT3( oE, im2,jp1,kml) * VAT3( dPS, iim1,jjp1,kk)
02505             - VAT3( uW, im1,jp1,kml) * VAT3( oPS, iim1,jjp1,kk)
02506             - VAT3( oNW, im1,jp1,kml) * VAT3( dPC, iim1,jjp1,kk)
02507             - VAT3( uNW, im1,jp1,kml) * VAT3( oPC, iim1,jjp1,kk)
02508             + VAT3( oC, im1,jp1,kml) * VAT3( dPSE, iim1,jjp1,kk)
02509             - VAT3( uC, im1,jp1,kml) * VAT3( oPSE, iim1,jjp1,kk)
02510             - VAT3( oN, im1,jp1,kml) * VAT3( dPE, iim1,jjp1,kk)
02511             - VAT3( uN, im1,jp1,kml) * VAT3( oPE, iim1,jjp1,kk));
02512
02513     TMP3_XONW =
02514         - VAT3( oPNW, ii,jj,kk) * (- VAT3( uE, im2,jp1,kml) * VAT3( dPS, iim1,jjp1,kk)
02515             - VAT3( oE, im2,jp1,k) * VAT3( oPS, iim1,jjp1,kk)
02516             - VAT3( uW, im1,jp1,k) * VAT3( uPS, iim1,jjp1,kk)
02517             - VAT3( uSE, im2,jp2,kml) * VAT3( dPC, iim1,jjp1,kk)
02518             - VAT3( oNW, im1,jp1,k) * VAT3( oPC, iim1,jjp1,kk)
02519             - VAT3( uNW, im1,jp1,k) * VAT3( uPC, iim1,jjp1,kk)
02520             - VAT3( uC, im1,jp1,kml) * VAT3( dPSE, iim1,jjp1,kk)
02521             + VAT3( oC, im1,jp1,k) * VAT3( oPSE, iim1,jjp1,kk)
02522             - VAT3( uC, im1,jp1,k) * VAT3( uPSE, iim1,jjp1,kk)
02523             - VAT3( uS, im1,jp2,kml) * VAT3( dPE, iim1,jjp1,kk)
02524             - VAT3( oN, im1,jp1,k) * VAT3( oPE, iim1,jjp1,kk)
02525             - VAT3( uN, im1,jp1,k) * VAT3( uPE, iim1,jjp1,kk));
02526
02527     TMP4_XONW =
02528         - VAT3( uPNW, ii,jj,kk) * (- VAT3( uE, im2,jp1,k) * VAT3( oPS, iim1,jjp1,kk)
02529             - VAT3( oE, im2,jp1,kp1) * VAT3( uPS, iim1,jjp1,kk)
02530             - VAT3( uSE, im2,jp2,k) * VAT3( oPC, iim1,jjp1,kk)
02531             - VAT3( oNW, im1,jp1,kp1) * VAT3( uPC, iim1,jjp1,kk)
02532             - VAT3( uC, im1,jp1,k) * VAT3( oPSE, iim1,jjp1,kk)
02533             + VAT3( oC, im1,jp1,kp1) * VAT3( uPSE, iim1,jjp1,kk)
02534             - VAT3( uS, im1,jp2,k) * VAT3( oPE, iim1,jjp1,kk)
02535             - VAT3( oN, im1,jp1,kp1) * VAT3( uPE, iim1,jjp1,kk))
02536
02537         - VAT3( dPC, ii,jj,kk) * (- VAT3( oNW, i,j,kml) * VAT3( dPSE, iim1,jjp1,kk)
02538             - VAT3( uNW, i,j,kml) * VAT3( oPSE, iim1,jjp1,kk));
02539
02540     TMP5_XONW =
02541         - VAT3( oPC, ii,jj,kk) * (- VAT3( uSE, im1,jp1,kml) * VAT3( dPSE, iim1,jjp1,kk)
02542             - VAT3( oNW, i,j,k) * VAT3( oPSE, iim1,jjp1,kk)
02543             - VAT3( uNW, i,j,k) * VAT3( uPSE, iim1,jjp1,kk))
02544
02545         - VAT3( uPC, ii,jj,kk) * (- VAT3( uSE, im1,jp1,k) * VAT3( oPSE, iim1,jjp1,kk)
02546             - VAT3( oNW, i,j,kp1) * VAT3( uPSE, iim1,jjp1,kk))
02547
02548         - VAT3( dPN, ii,jj,kk) * (- VAT3( oE, im1,jp1,kml) * VAT3( dPSE, iim1,jjp1,kk)
02549             - VAT3( uW, i,jp1,kml) * VAT3( oPSE, iim1,jjp1,kk)
02550             - VAT3( oNW, i,jp1,kml) * VAT3( dPE, iim1,jjp1,kk)
02551             - VAT3( uNW, i,jp1,kml) * VAT3( oPE, iim1,jjp1,kk));
02552
02553     TMP6_XONW =
02554         - VAT3( oPN, ii,jj,kk) * (- VAT3( uE, im1,jp1,kml) * VAT3( dPSE, iim1,jjp1,kk)
02555             - VAT3( oE, im1,jp1,k) * VAT3( oPSE, iim1,jjp1,kk)

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02556             - VAT3( uW, i, jpl, k) * VAT3( uPSE, iiml, jjpl, kk)
02557             - VAT3( uSE, iml, jp2, kml) * VAT3( dPE, iiml, jjpl, kk)
02558             - VAT3( oNW, i, jpl, k) * VAT3( oPE, iiml, jjpl, kk)
02559             - VAT3( uNW, i, jpl, k) * VAT3( uPE, iiml, jjpl, kk)
02560
02561         - VAT3( uPN, ii, jj, kk) * (- VAT3( uE, iml, jpl, k) * VAT3( oPSE, iiml, jjpl, kk)
02562             - VAT3( oE, iml, jpl, kpl) * VAT3( uPSE, iiml, jjpl, kk)
02563             - VAT3( uSE, iml, jp2, k) * VAT3( oPE, iiml, jjpl, kk)
02564             - VAT3( oNW, i, jpl, kpl) * VAT3( uPE, iiml, jjpl, kk));
02565
02566     VAT3(XoNW, ii, jj, kk) = TMP1_XONW + TMP2_XONW + TMP3_XONW + TMP4_XONW
02567         + TMP5_XONW + TMP6_XONW;
02568
02569     //fprintf(data, "%19.12E\n", VAT3(XoNW, ii, jj, kk));
02570
02571     /* *****
02572     * *** > UE;
02573     * *****
02574     // VAT3( XuE, ii, jj, kk) =
02575     TMP1_XUE =
02576         - VAT3( oPS, ii, jj, kk) * (- VAT3( uE, i, jml, k) * VAT3( dPSW, iip1, jj, kkp1)
02577             - VAT3( uNE, i, jml, k) * VAT3( dPW, iip1, jj, kkp1))
02578
02579         - VAT3( uPS, ii, jj, kk) * (- VAT3( oE, i, jml, kpl) * VAT3( dPSW, iip1, jj, kkp1)
02580             - VAT3( uE, i, jml, kpl) * VAT3( oPSW, iip1, jj, kkp1)
02581             - VAT3( oNE, i, jml, kpl) * VAT3( dPW, iip1, jj, kkp1)
02582             - VAT3( uNE, i, jml, kpl) * VAT3( oPW, iip1, jj, kkp1))
02583
02584         - VAT3( oPC, ii, jj, kk) * (- VAT3( uSE, i, j, k) * VAT3( dPSW, iip1, jj, kkp1)
02585             - VAT3( uE, i, j, k) * VAT3( dPW, iip1, jj, kkp1)
02586             - VAT3( uNE, i, j, k) * VAT3( dPNW, iip1, jj, kkp1));
02587
02588     TMP2_XUE =
02589         - VAT3( uPC, ii, jj, kk) * (- VAT3( oNW, ip1, jml, kpl) * VAT3( dPSW, iip1, jj, kkp1)
02590             - VAT3( uSE, i, j, kpl) * VAT3( oPSW, iip1, jj, kkp1)
02591             - VAT3( oE, i, j, kpl) * VAT3( dPW, iip1, jj, kkp1)
02592             - VAT3( uE, i, j, kpl) * VAT3( oPW, iip1, jj, kkp1)
02593             - VAT3( oNE, i, j, kpl) * VAT3( dPNW, iip1, jj, kkp1)
02594             - VAT3( uNE, i, j, kpl) * VAT3( oPNW, iip1, jj, kkp1))
02595
02596         - VAT3( oPN, ii, jj, kk) * (- VAT3( uSE, i, jpl, k) * VAT3( dPW, iip1, jj, kkp1)
02597             - VAT3( uE, i, jpl, k) * VAT3( dPNW, iip1, jj, kkp1))
02598
02599         - VAT3( uPN, ii, jj, kk) * (- VAT3( oNW, ip1, j, kpl) * VAT3( dPW, iip1, jj, kkp1)
02600             - VAT3( uSE, i, jpl, kpl) * VAT3( oPW, iip1, jj, kkp1)
02601             - VAT3( oE, i, jpl, kpl) * VAT3( dPNW, iip1, jj, kkp1)
02602             - VAT3( uE, i, jpl, kpl) * VAT3( oPNW, iip1, jj, kkp1));
02603
02604     TMP3_XUE =
02605         - VAT3( oPSE, ii, jj, kk) * (- VAT3( uC, ip1, jml, k) * VAT3( dPSW, iip1, jj, kkp1)
02606             - VAT3( uN, ip1, jml, k) * VAT3( dPW, iip1, jj, kkp1)
02607             - VAT3( uE, ip1, jml, k) * VAT3( dPS, iip1, jj, kkp1)
02608             - VAT3( uNE, ip1, jml, k) * VAT3( dPC, iip1, jj, kkp1))
02609
02610         - VAT3( uPSE, ii, jj, kk) * ( VAT3( oC, ip1, jml, kpl) * VAT3( dPSW, iip1, jj, kkp1)
02611             - VAT3( uC, ip1, jml, kpl) * VAT3( oPSW, iip1, jj, kkp1)
02612             - VAT3( oN, ip1, jml, kpl) * VAT3( dPW, iip1, jj, kkp1)
02613             - VAT3( uN, ip1, jml, kpl) * VAT3( oPW, iip1, jj, kkp1)
02614             - VAT3( oE, ip1, jml, kpl) * VAT3( dPS, iip1, jj, kkp1)
02615             - VAT3( uE, ip1, jml, kpl) * VAT3( oPS, iip1, jj, kkp1)
02616             - VAT3( oNE, ip1, jml, kpl) * VAT3( dPC, iip1, jj, kkp1)
02617             - VAT3( uNE, ip1, jml, kpl) * VAT3( oPC, iip1, jj, kkp1));
02618
02619     TMP4_XUE =
02620         - VAT3( oPE, ii, jj, kk) * (- VAT3( uS, ip1, j, k) * VAT3( dPSW, iip1, jj, kkp1)
02621             - VAT3( uC, ip1, j, k) * VAT3( dPW, iip1, jj, kkp1)
02622             - VAT3( uN, ip1, j, k) * VAT3( dPNW, iip1, jj, kkp1)
02623             - VAT3( uSE, ip1, j, k) * VAT3( dPS, iip1, jj, kkp1)
02624             - VAT3( uE, ip1, j, k) * VAT3( dPC, iip1, jj, kkp1)
02625             - VAT3( uNE, ip1, j, k) * VAT3( dPN, iip1, jj, kkp1));
02626
02627     TMP5_XUE =
02628         - VAT3( uPE, ii, jj, kk) * (- VAT3( oN, ip1, jml, kpl) * VAT3( dPSW, iip1, jj, kkp1)
02629             - VAT3( uS, ip1, j, kpl) * VAT3( oPSW, iip1, jj, kkp1)
02630             + VAT3( oC, ip1, j, kpl) * VAT3( dPW, iip1, jj, kkp1)
02631             - VAT3( uC, ip1, j, kpl) * VAT3( oPW, iip1, jj, kkp1)
02632             - VAT3( oN, ip1, j, kpl) * VAT3( dPNW, iip1, jj, kkp1)
02633             - VAT3( uN, ip1, j, kpl) * VAT3( oPNW, iip1, jj, kkp1)
02634             - VAT3( oNW, ip2, jml, kpl) * VAT3( dPS, iip1, jj, kkp1)
02635             - VAT3( uSE, ip1, j, kpl) * VAT3( oPS, iip1, jj, kkp1)
02636             - VAT3( oE, ip1, j, kpl) * VAT3( dPC, iip1, jj, kkp1)

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02637             - VAT3( uE, ip1,j,kp1) * VAT3( oPC, iip1,jj,kkp1)
02638             - VAT3( oNE, ip1,j,kp1) * VAT3( dPN, iip1,jj,kkp1)
02639             - VAT3( uNE, ip1,j,kp1) * VAT3( oPN, iip1,jj,kkp1));
02640
02641 TMP6_XUE =
02642     - VAT3(oPNE, ii,jj,kk) * (- VAT3( uS, ip1,jp1,k) * VAT3( dPW, iip1,jj,kkp1)
02643     - VAT3( uC, ip1,jp1,k) * VAT3(dPNW, iip1,jj,kkp1)
02644     - VAT3( uSE, ip1,jp1,k) * VAT3( dPC, iip1,jj,kkp1)
02645     - VAT3( uE, ip1,jp1,k) * VAT3( dPN, iip1,jj,kkp1))
02646
02647     - VAT3(uPNE, ii,jj,kk) * (- VAT3( oN, ip1,j,kp1) * VAT3( dPW, iip1,jj,kkp1)
02648     - VAT3( uS, ip1,jp1,kp1) * VAT3( oPW, iip1,jj,kkp1)
02649     + VAT3( oC, ip1,jp1,kp1) * VAT3(dPNW, iip1,jj,kkp1)
02650     - VAT3( uC, ip1,jp1,kp1) * VAT3(oPNW, iip1,jj,kkp1)
02651     - VAT3( oNW, ip2,j,kp1) * VAT3( dPC, iip1,jj,kkp1)
02652     - VAT3( uSE, ip1,jp1,kp1) * VAT3( oPC, iip1,jj,kkp1)
02653     - VAT3( oE, ip1,jp1,kp1) * VAT3( dPN, iip1,jj,kkp1)
02654     - VAT3( uE, ip1,jp1,kp1) * VAT3( oPN, iip1,jj,kkp1));
02655
02656 VAT3( XuE, ii,jj,kk) = TMP1_XUE + TMP2_XUE + TMP3_XUE + TMP4_XUE
02657     + TMP5_XUE + TMP6_XUE;
02658
02659 //fprintf(data, "%19.12E\n", VAT3(XuE, ii, jj, kk));
02660
02661 /* *****
02662  * *** > UW;
02663  * *****
02664  // VAT3( XuW, ii,jj,kk) =
02665 TMP1_XUW =
02666     - VAT3(oPSW, ii,jj,kk) * (- VAT3( uW, im1,jm1,k) * VAT3( dPS, iim1,jj,kkp1)
02667     - VAT3( uNW, im1,jm1,k) * VAT3( dPC, iim1,jj,kkp1)
02668     - VAT3( uC, im1,jm1,k) * VAT3(dPSE, iim1,jj,kkp1)
02669     - VAT3( uN, im1,jm1,k) * VAT3( dPE, iim1,jj,kkp1))
02670
02671     - VAT3(uPSW, ii,jj,kk) * (- VAT3( oE, im2,jm1,kp1) * VAT3( dPS, iim1,jj,kkp1)
02672     - VAT3( uW, im1,jm1,kp1) * VAT3( oPS, iim1,jj,kkp1)
02673     - VAT3( oNW, im1,jm1,kp1) * VAT3( dPC, iim1,jj,kkp1)
02674     - VAT3( uNW, im1,jm1,kp1) * VAT3( oPC, iim1,jj,kkp1)
02675     + VAT3( oC, im1,jm1,kp1) * VAT3(dPSE, iim1,jj,kkp1)
02676     - VAT3( uC, im1,jm1,kp1) * VAT3(oPSE, iim1,jj,kkp1)
02677     - VAT3( oN, im1,jm1,kp1) * VAT3( dPE, iim1,jj,kkp1)
02678     - VAT3( uN, im1,jm1,kp1) * VAT3( oPE, iim1,jj,kkp1));
02679
02680 TMP2_XUW =
02681     - VAT3( oPW, ii,jj,kk) * (- VAT3( uSW, im1,j,k) * VAT3( dPS, iim1,jj,kkp1)
02682     - VAT3( uW, im1,j,k) * VAT3( dPC, iim1,jj,kkp1)
02683     - VAT3( uNW, im1,j,k) * VAT3( dPN, iim1,jj,kkp1)
02684     - VAT3( uS, im1,j,k) * VAT3(dPSE, iim1,jj,kkp1)
02685     - VAT3( uC, im1,j,k) * VAT3( dPE, iim1,jj,kkp1)
02686     - VAT3( uN, im1,j,k) * VAT3(dPNE, iim1,jj,kkp1));
02687
02688 TMP3_XUW =
02689     - VAT3( uPW, ii,jj,kk) * (- VAT3( oNE, im2,jm1,kp1) * VAT3( dPS, iim1,jj,kkp1)
02690     - VAT3( uSW, im1,j,kp1) * VAT3( oPS, iim1,jj,kkp1)
02691     - VAT3( oE, im2,j,kp1) * VAT3( dPC, iim1,jj,kkp1)
02692     - VAT3( uW, im1,j,kp1) * VAT3( oPC, iim1,jj,kkp1)
02693     - VAT3( oNW, im1,j,kp1) * VAT3( dPN, iim1,jj,kkp1)
02694     - VAT3( uNW, im1,j,kp1) * VAT3( oPN, iim1,jj,kkp1)
02695     - VAT3( oN, im1,jm1,kp1) * VAT3(dPSE, iim1,jj,kkp1)
02696     - VAT3( uS, im1,j,kp1) * VAT3(oPSE, iim1,jj,kkp1)
02697     + VAT3( oC, im1,j,kp1) * VAT3( dPE, iim1,jj,kkp1)
02698     - VAT3( uC, im1,j,kp1) * VAT3( oPE, iim1,jj,kkp1)
02699     - VAT3( oN, im1,j,kp1) * VAT3(dPNE, iim1,jj,kkp1)
02700     - VAT3( uN, im1,j,kp1) * VAT3(oPNE, iim1,jj,kkp1));
02701
02702 TMP4_XUW =
02703     - VAT3(oPNW, ii,jj,kk) * (- VAT3( uSW, im1,jp1,k) * VAT3( dPC, iim1,jj,kkp1)
02704     - VAT3( uW, im1,jp1,k) * VAT3( dPN, iim1,jj,kkp1)
02705     - VAT3( uS, im1,jp1,k) * VAT3( dPE, iim1,jj,kkp1)
02706     - VAT3( uC, im1,jp1,k) * VAT3(dPNE, iim1,jj,kkp1))
02707
02708     - VAT3(uPNW, ii,jj,kk) * (- VAT3( oNE, im2,j,kp1) * VAT3( dPC, iim1,jj,kkp1)
02709     - VAT3( uSW, im1,jp1,kp1) * VAT3( oPC, iim1,jj,kkp1)
02710     - VAT3( oE, im2,jp1,kp1) * VAT3( dPN, iim1,jj,kkp1)
02711     - VAT3( uW, im1,jp1,kp1) * VAT3( oPN, iim1,jj,kkp1)
02712     - VAT3( oN, im1,j,kp1) * VAT3( dPE, iim1,jj,kkp1)
02713     - VAT3( uS, im1,jp1,kp1) * VAT3( oPE, iim1,jj,kkp1)
02714     + VAT3( oC, im1,jp1,kp1) * VAT3(dPNE, iim1,jj,kkp1)
02715     - VAT3( uC, im1,jp1,kp1) * VAT3(oPNE, iim1,jj,kkp1));
02716
02717 TMP5_XUW =

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02718     - VAT3( oPS, ii,jj,kk) * (- VAT3( uW, i,jm1,k) * VAT3(dPSE, iim1,jj,kkp1)
02719         - VAT3( uNW, i,jm1,k) * VAT3( dPE, iim1,jj,kkp1))
02720
02721     - VAT3( oPS, ii,jj,kk) * (- VAT3( oE, im1,jm1,kp1) * VAT3(dPSE, iim1,jj,kkp1)
02722         - VAT3( uW, i,jm1,kp1) * VAT3(oPSE, iim1,jj,kkp1)
02723         - VAT3( oNW, i,jm1,kp1) * VAT3( dPE, iim1,jj,kkp1)
02724         - VAT3( uNW, i,jm1,kp1) * VAT3( oPE, iim1,jj,kkp1))
02725
02726     - VAT3( oPC, ii,jj,kk) * (- VAT3( uSW, i,j,k) * VAT3(dPSE, iim1,jj,kkp1)
02727         - VAT3( uW, i,j,k) * VAT3( dPE, iim1,jj,kkp1)
02728         - VAT3( uNW, i,j,k) * VAT3(dPNE, iim1,jj,kkp1));
02729
02730 TMP6_XUW =
02731     - VAT3( uPC, ii,jj,kk) * (- VAT3( oNE, im1,jm1,kp1) * VAT3(dPSE, iim1,jj,kkp1)
02732         - VAT3( uSW, i,j,kp1) * VAT3(oPSE, iim1,jj,kkp1)
02733         - VAT3( oE, im1,j,kp1) * VAT3( dPE, iim1,jj,kkp1)
02734         - VAT3( uW, i,j,kp1) * VAT3( oPE, iim1,jj,kkp1)
02735         - VAT3( oNW, i,j,kp1) * VAT3(dPNE, iim1,jj,kkp1)
02736         - VAT3( uNW, i,j,kp1) * VAT3(oPNE, iim1,jj,kkp1))
02737
02738     - VAT3( oPN, ii,jj,kk) * (- VAT3( uSW, i,jp1,k) * VAT3( dPE, iim1,jj,kkp1)
02739         - VAT3( uW, i,jp1,k) * VAT3(dPNE, iim1,jj,kkp1))
02740
02741     - VAT3( uPN, ii,jj,kk) * (- VAT3( oNE, im1,j,kp1) * VAT3( dPE, iim1,jj,kkp1)
02742         - VAT3( uSW, i,jp1,kp1) * VAT3( oPE, iim1,jj,kkp1)
02743         - VAT3( oE, im1,jp1,kp1) * VAT3(dPNE, iim1,jj,kkp1)
02744         - VAT3( uW, i,jp1,kp1) * VAT3(oPNE, iim1,jj,kkp1));
02745
02746 VAT3( XuW, ii,jj,kk) = TMP1_XUW + TMP2_XUW + TMP3_XUW + TMP4_XUW
02747     + TMP5_XUW + TMP6_XUW;
02748
02749     //fprintf(data, "%19.12E\n", VAT3(XuW, ii, jj, kk));
02750
02751     /* *****
02752     * *** > UN;
02753     * *****
02754     // VAT3( XuN, ii,jj,kk) =
02755 TMP1_XUN =
02756     - VAT3( oPW, ii,jj,kk) * (- VAT3( uN, im1,j,k) * VAT3(dPSW, ii,jjp1,kkp1)
02757         - VAT3( uNE, im1,j,k) * VAT3( dPS, ii,jjp1,kkp1))
02758
02759     - VAT3( uPW, ii,jj,kk) * (- VAT3( oN, im1,j,kp1) * VAT3(dPSW, ii,jjp1,kkp1)
02760         - VAT3( uN, im1,j,kp1) * VAT3(oPSW, ii,jjp1,kkp1)
02761         - VAT3( oNE, im1,j,kp1) * VAT3( dPS, ii,jjp1,kkp1)
02762         - VAT3( uNE, im1,j,kp1) * VAT3( oPS, ii,jjp1,kkp1))
02763
02764     - VAT3( oPNW, ii,jj,kk) * (- VAT3( uC, im1,jp1,k) * VAT3(dPSW, ii,jjp1,kkp1)
02765         - VAT3( uN, im1,jp1,k) * VAT3( dPW, ii,jjp1,kkp1)
02766         - VAT3( uE, im1,jp1,k) * VAT3( dPS, ii,jjp1,kkp1)
02767         - VAT3( uNE, im1,jp1,k) * VAT3( dPC, ii,jjp1,kkp1));
02768
02769 TMP2_XUN =
02770     - VAT3( uPNW, ii,jj,kk) * ( VAT3( oC, im1,jp1,kp1) * VAT3(dPSW, ii,jjp1,kkp1)
02771         - VAT3( uC, im1,jp1,kp1) * VAT3(oPSW, ii,jjp1,kkp1)
02772         - VAT3( oN, im1,jp1,kp1) * VAT3( dPW, ii,jjp1,kkp1)
02773         - VAT3( uN, im1,jp1,kp1) * VAT3( oPW, ii,jjp1,kkp1)
02774         - VAT3( oE, im1,jp1,kp1) * VAT3( dPS, ii,jjp1,kkp1)
02775         - VAT3( uE, im1,jp1,kp1) * VAT3( oPS, ii,jjp1,kkp1)
02776         - VAT3( oNE, im1,jp1,kp1) * VAT3( dPC, ii,jjp1,kkp1)
02777         - VAT3( uNE, im1,jp1,kp1) * VAT3( oPC, ii,jjp1,kkp1))
02778
02779     - VAT3( oPC, ii,jj,kk) * (- VAT3( uNW, i,j,k) * VAT3(dPSW, ii,jjp1,kkp1)
02780         - VAT3( uN, i,j,k) * VAT3( dPS, ii,jjp1,kkp1)
02781         - VAT3( uNE, i,j,k) * VAT3(dPSE, ii,jjp1,kkp1));
02782
02783 TMP3_XUN =
02784     - VAT3( uPC, ii,jj,kk) * (- VAT3( oNW, i,j,kp1) * VAT3(dPSW, ii,jjp1,kkp1)
02785         - VAT3( uNW, i,j,kp1) * VAT3(oPSW, ii,jjp1,kkp1)
02786         - VAT3( oN, i,j,kp1) * VAT3( dPS, ii,jjp1,kkp1)
02787         - VAT3( uN, i,j,kp1) * VAT3( oPS, ii,jjp1,kkp1)
02788         - VAT3( oNE, i,j,kp1) * VAT3(dPSE, ii,jjp1,kkp1)
02789         - VAT3( uNE, i,j,kp1) * VAT3(oPSE, ii,jjp1,kkp1))
02790
02791     - VAT3( oPN, ii,jj,kk) * (- VAT3( uW, i,jp1,k) * VAT3(dPSW, ii,jjp1,kkp1)
02792         - VAT3( uNW, i,jp1,k) * VAT3( dPW, ii,jjp1,kkp1)
02793         - VAT3( uC, i,jp1,k) * VAT3( dPS, ii,jjp1,kkp1)
02794         - VAT3( uN, i,jp1,k) * VAT3( dPC, ii,jjp1,kkp1)
02795         - VAT3( uE, i,jp1,k) * VAT3(dPSE, ii,jjp1,kkp1)
02796         - VAT3( uNE, i,jp1,k) * VAT3( dPE, ii,jjp1,kkp1));
02797
02798 TMP4_XUN =

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02799     - VAT3( uPN, ii,jj,kk) * (- VAT3( oE, iml,jpl,kpl) * VAT3(dPSW, ii,jjpl,kkpl)
02800         - VAT3( uW, i,jpl,kpl) * VAT3(oPSW, ii,jjpl,kkpl)
02801         - VAT3( oNW, i,jpl,kpl) * VAT3( dPW, ii,jjpl,kkpl)
02802         - VAT3( uNW, i,jpl,kpl) * VAT3( oPW, ii,jjpl,kkpl)
02803         + VAT3( oC, i,jpl,kpl) * VAT3( dPS, ii,jjpl,kkpl)
02804         - VAT3( uC, i,jpl,kpl) * VAT3( oPS, ii,jjpl,kkpl)
02805         - VAT3( oN, i,jpl,kpl) * VAT3( dPC, ii,jjpl,kkpl)
02806         - VAT3( uN, i,jpl,kpl) * VAT3( oPC, ii,jjpl,kkpl)
02807         - VAT3( oE, i,jpl,kpl) * VAT3(dPSE, ii,jjpl,kkpl)
02808         - VAT3( uE, i,jpl,kpl) * VAT3(oPSE, ii,jjpl,kkpl)
02809         - VAT3( oNE, i,jpl,kpl) * VAT3( dPE, ii,jjpl,kkpl)
02810         - VAT3( uNE, i,jpl,kpl) * VAT3( oPE, ii,jjpl,kkpl));
02811
02812 TMP5_XUN =
02813     - VAT3( oPE, ii,jj,kk) * (- VAT3( uNW, ip1,j,k) * VAT3( dPS, ii,jjpl,kkpl)
02814         - VAT3( uN, ip1,j,k) * VAT3(dPSE, ii,jjpl,kkpl))
02815
02816     - VAT3( uPE, ii,jj,kk) * (- VAT3( oNW, ip1,j,kpl) * VAT3( dPS, ii,jjpl,kkpl)
02817         - VAT3( uNW, ip1,j,kpl) * VAT3( oPS, ii,jjpl,kkpl)
02818         - VAT3( oN, ip1,j,kpl) * VAT3(dPSE, ii,jjpl,kkpl)
02819         - VAT3( uN, ip1,j,kpl) * VAT3(oPSE, ii,jjpl,kkpl))
02820
02821     - VAT3(oPNE, ii,jj,kk) * (- VAT3( uW, ip1,jpl,k) * VAT3( dPS, ii,jjpl,kkpl)
02822         - VAT3( uNW, ip1,jpl,k) * VAT3( dPC, ii,jjpl,kkpl)
02823         - VAT3( uC, ip1,jpl,k) * VAT3(dPSE, ii,jjpl,kkpl)
02824         - VAT3( uN, ip1,jpl,k) * VAT3( dPE, ii,jjpl,kkpl));
02825
02826 TMP6_XUN =
02827     - VAT3(uPNE, ii,jj,kk) * (- VAT3( oE, i,jpl,kpl) * VAT3( dPS, ii,jjpl,kkpl)
02828         - VAT3( uW, ip1,jpl,kpl) * VAT3( oPS, ii,jjpl,kkpl)
02829         - VAT3( oNW, ip1,jpl,kpl) * VAT3( dPC, ii,jjpl,kkpl)
02830         - VAT3( uNW, ip1,jpl,kpl) * VAT3( oPC, ii,jjpl,kkpl)
02831         + VAT3( oC, ip1,jpl,kpl) * VAT3(dPSE, ii,jjpl,kkpl)
02832         - VAT3( uC, ip1,jpl,kpl) * VAT3(oPSE, ii,jjpl,kkpl)
02833         - VAT3( oN, ip1,jpl,kpl) * VAT3( dPE, ii,jjpl,kkpl)
02834         - VAT3( uN, ip1,jpl,kpl) * VAT3( oPE, ii,jjpl,kkpl));
02835
02836 VAT3( XuN, ii,jj,kk) = TMP1_XUN + TMP2_XUN + TMP3_XUN + TMP4_XUN
02837     + TMP5_XUN + TMP6_XUN;
02838
02839     //fprintf(data, "%19.12E\n", VAT3(XuN, ii, jj, kk));
02840
02841     /* *****
02842      * *** > US;
02843      * *****
02844
02845     // VAT3( XuS, ii,jj,kk) =
02846 TMP1_XUS =
02847     - VAT3(oPSW, ii,jj,kk) * (- VAT3( uS, iml,jml,k) * VAT3( dPW, ii,jjml,kkpl)
02848         - VAT3( uC, iml,jml,k) * VAT3(dPNW, ii,jjml,kkpl)
02849         - VAT3( uSE, iml,jml,k) * VAT3( dPC, ii,jjml,kkpl)
02850         - VAT3( uE, iml,jml,k) * VAT3( dPN, ii,jjml,kkpl))
02851
02852     - VAT3(uPSW, ii,jj,kk) * (- VAT3( oN, iml,jm2,kpl) * VAT3( dPW, ii,jjml,kkpl)
02853         - VAT3( uS, iml,jml,kpl) * VAT3( oPW, ii,jjml,kkpl)
02854         + VAT3( oC, iml,jml,kpl) * VAT3(dPNW, ii,jjml,kkpl)
02855         - VAT3( uC, iml,jml,kpl) * VAT3(oPNW, ii,jjml,kkpl)
02856         - VAT3( oNW, i,jm2,kpl) * VAT3( dPC, ii,jjml,kkpl)
02857         - VAT3( uSE, iml,jml,kpl) * VAT3( oPC, ii,jjml,kkpl)
02858         - VAT3( oE, iml,jml,kpl) * VAT3( dPN, ii,jjml,kkpl)
02859         - VAT3( uE, iml,jml,kpl) * VAT3( oPN, ii,jjml,kkpl));
02860
02861 TMP2_XUS =
02862     - VAT3( oPW, ii,jj,kk) * (- VAT3( uS, iml,j,k) * VAT3(dPNW, ii,jjml,kkpl)
02863         - VAT3( uSE, iml,j,k) * VAT3( dPN, ii,jjml,kkpl))
02864
02865     - VAT3( uPW, ii,jj,kk) * (- VAT3( oN, iml,jml,kpl) * VAT3(dPNW, ii,jjml,kkpl)
02866         - VAT3( uS, iml,j,kpl) * VAT3(oPNW, ii,jjml,kkpl)
02867         - VAT3( oNW, i,jml,kpl) * VAT3( dPN, ii,jjml,kkpl)
02868         - VAT3( uSE, iml,j,kpl) * VAT3( oPN, ii,jjml,kkpl))
02869
02870     - VAT3( oPS, ii,jj,kk) * (- VAT3( uSW, i,jml,k) * VAT3( dPW, ii,jjml,kkpl)
02871         - VAT3( uW, i,jml,k) * VAT3(dPNW, ii,jjml,kkpl)
02872         - VAT3( uS, i,jml,k) * VAT3( dPC, ii,jjml,kkpl)
02873         - VAT3( uC, i,jml,k) * VAT3( dPN, ii,jjml,kkpl)
02874         - VAT3( uSE, i,jml,k) * VAT3( dPE, ii,jjml,kkpl)
02875         - VAT3( uE, i,jml,k) * VAT3(dPNE, ii,jjml,kkpl));
02876
02877 TMP3_XUS =
02878     - VAT3( uPS, ii,jj,kk) * (- VAT3( oNE, iml,jm2,kpl) * VAT3( dPW, ii,jjml,kkpl)
02879         - VAT3( uSW, i,jml,kpl) * VAT3( oPW, ii,jjml,kkpl)

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02880             - VAT3( oE, i, j, k) * VAT3( dPNW, ii, jj, kk)
02881             - VAT3( uW, i, j, k) * VAT3( oPNW, ii, jj, kk)
02882             - VAT3( oN, i, j, k) * VAT3( dPC, ii, jj, kk)
02883             - VAT3( uS, i, j, k) * VAT3( oPC, ii, jj, kk)
02884             + VAT3( oC, i, j, k) * VAT3( dPN, ii, jj, kk)
02885             - VAT3( uC, i, j, k) * VAT3( oPN, ii, jj, kk)
02886             - VAT3( oNW, i, j, k) * VAT3( dPE, ii, jj, kk)
02887             - VAT3( uSE, i, j, k) * VAT3( oPE, ii, jj, kk)
02888             - VAT3( oE, i, j, k) * VAT3( dPNE, ii, jj, kk)
02889             - VAT3( uE, i, j, k) * VAT3( oPNE, ii, jj, kk));
02890
02891 TMP4_XUS =
02892     - VAT3( oPC, ii, jj, kk) * (- VAT3( uSW, i, j, k) * VAT3( dPNW, ii, jj, kk)
02893       - VAT3( uS, i, j, k) * VAT3( dPN, ii, jj, kk)
02894       - VAT3( uSE, i, j, k) * VAT3( dPNE, ii, jj, kk))
02895
02896     - VAT3( uPC, ii, jj, kk) * (- VAT3( oNE, i, j, k) * VAT3( dPNW, ii, jj, kk)
02897       - VAT3( uSW, i, j, k) * VAT3( oPNW, ii, jj, kk)
02898       - VAT3( oN, i, j, k) * VAT3( dPN, ii, jj, kk)
02899       - VAT3( uS, i, j, k) * VAT3( oPN, ii, jj, kk)
02900       - VAT3( oNW, i, j, k) * VAT3( dPNE, ii, jj, kk)
02901       - VAT3( uSE, i, j, k) * VAT3( oPNE, ii, jj, kk));
02902
02903 TMP5_XUS =
02904     - VAT3( oPSE, ii, jj, kk) * (- VAT3( uSW, i, j, k) * VAT3( dPC, ii, jj, kk)
02905       - VAT3( uW, i, j, k) * VAT3( dPN, ii, jj, kk)
02906       - VAT3( uS, i, j, k) * VAT3( dPE, ii, jj, kk)
02907       - VAT3( uC, i, j, k) * VAT3( dPNE, ii, jj, kk))
02908
02909     - VAT3( uPSE, ii, jj, kk) * (- VAT3( oNE, i, j, k) * VAT3( dPC, ii, jj, kk)
02910       - VAT3( uSW, i, j, k) * VAT3( oPC, ii, jj, kk)
02911       - VAT3( oE, i, j, k) * VAT3( dPN, ii, jj, kk)
02912       - VAT3( uW, i, j, k) * VAT3( oPN, ii, jj, kk)
02913       - VAT3( oN, i, j, k) * VAT3( dPE, ii, jj, kk)
02914       - VAT3( uS, i, j, k) * VAT3( oPE, ii, jj, kk)
02915       + VAT3( oC, i, j, k) * VAT3( dPNE, ii, jj, kk)
02916       - VAT3( uC, i, j, k) * VAT3( oPNE, ii, jj, kk));
02917
02918 TMP6_XUS =
02919     - VAT3( oPE, ii, jj, kk) * (- VAT3( uSW, i, j, k) * VAT3( dPN, ii, jj, kk)
02920       - VAT3( uS, i, j, k) * VAT3( dPNE, ii, jj, kk))
02921
02922     - VAT3( uPE, ii, jj, kk) * (- VAT3( oNE, i, j, k) * VAT3( dPN, ii, jj, kk)
02923       - VAT3( uSW, i, j, k) * VAT3( oPN, ii, jj, kk)
02924       - VAT3( oN, i, j, k) * VAT3( dPNE, ii, jj, kk)
02925       - VAT3( uS, i, j, k) * VAT3( oPNE, ii, jj, kk));
02926
02927 VAT3( XuS, ii, jj, kk) = TMP1_XUS + TMP2_XUS + TMP3_XUS + TMP4_XUS
02928     + TMP5_XUS + TMP6_XUS;
02929
02930 //fprintf(data, "%19.12E\n", VAT3(XuS, ii, jj, kk));
02931
02932 /* *****
02933 * *** > UNE;
02934 * *****
02935 // VAT3(XuNE, ii, jj, kk) =
02936 TMP1_XUNE =
02937     VAT3( oPC, ii, jj, kk) * VAT3( uNE, i, j, k) * VAT3( dPSW, iip1, jjp1, kkp1)
02938
02939     - VAT3( uPC, ii, jj, kk) * (- VAT3( oNE, i, j, k) * VAT3( dPSW, iip1, jjp1, kkp1)
02940       - VAT3( uNE, i, j, k) * VAT3( oPSW, iip1, jjp1, kkp1))
02941
02942     - VAT3( oPN, ii, jj, kk) * (- VAT3( uE, i, j, k) * VAT3( dPSW, iip1, jjp1, kkp1)
02943       - VAT3( uNE, i, j, k) * VAT3( dPW, iip1, jjp1, kkp1))
02944
02945     - VAT3( uPN, ii, jj, kk) * (- VAT3( oE, i, j, k) * VAT3( dPSW, iip1, jjp1, kkp1)
02946       - VAT3( uE, i, j, k) * VAT3( oPSW, iip1, jjp1, kkp1)
02947       - VAT3( oNE, i, j, k) * VAT3( dPW, iip1, jjp1, kkp1)
02948       - VAT3( uNE, i, j, k) * VAT3( oPW, iip1, jjp1, kkp1))
02949
02950     - VAT3( oPE, ii, jj, kk) * (- VAT3( uN, i, j, k) * VAT3( dPSW, iip1, jjp1, kkp1)
02951       - VAT3( uNE, i, j, k) * VAT3( dPS, iip1, jjp1, kkp1));
02952
02953 TMP2_XUNE =
02954     - VAT3( uPE, ii, jj, kk) * (- VAT3( oN, i, j, k) * VAT3( dPSW, iip1, jjp1, kkp1)
02955       - VAT3( uN, i, j, k) * VAT3( oPSW, iip1, jjp1, kkp1)
02956       - VAT3( oNE, i, j, k) * VAT3( dPS, iip1, jjp1, kkp1)
02957       - VAT3( uNE, i, j, k) * VAT3( oPS, iip1, jjp1, kkp1))
02958
02959     - VAT3( oPNE, ii, jj, kk) * (- VAT3( uC, i, j, k) * VAT3( dPSW, iip1, jjp1, kkp1)
02960       - VAT3( uN, i, j, k) * VAT3( dPW, iip1, jjp1, kkp1))

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02961         - VAT3( uE, ip1,jp1,k) * VAT3( dPS, iip1,jjp1,kkp1)
02962         - VAT3( uNE, ip1,jp1,k) * VAT3( dPC, iip1,jjp1,kkp1))
02963
02964     - VAT3(uPNE, ii,jj,kk) * ( VAT3( oC, ip1,jp1,kp1) * VAT3(dPSW, iip1,jjp1,kkp1)
02965     - VAT3( uC, ip1,jp1,kp1) * VAT3(oPSW, iip1,jjp1,kkp1)
02966     - VAT3( oN, ip1,jp1,kp1) * VAT3( dPW, iip1,jjp1,kkp1)
02967     - VAT3( uN, ip1,jp1,kp1) * VAT3( oPW, iip1,jjp1,kkp1)
02968     - VAT3( oE, ip1,jp1,kp1) * VAT3( dPS, iip1,jjp1,kkp1)
02969     - VAT3( uE, ip1,jp1,kp1) * VAT3( oPS, iip1,jjp1,kkp1)
02970     - VAT3( oNE, ip1,jp1,kp1) * VAT3( dPC, iip1,jjp1,kkp1)
02971     - VAT3( uNE, ip1,jp1,kp1) * VAT3( oPC, iip1,jjp1,kkp1));
02972 VAT3(XuNE, ii,jj,kk) = TMP1_XUNE + TMP2_XUNE;
02973
02974     //fprintf(data, "%19.12E\n", VAT3(XuNE, ii, jj, kk));
02975
02976     /* *****
02977     * *** > UNW;
02978     * *****/
02979
02980     // VAT3(XuNW, ii,jj,kk) =
02981 TMP1_XUNW =
02982     - VAT3( oPW, ii,jj,kk) * (- VAT3( uNW, im1,j,k) * VAT3( dPS, iim1,jjp1,kkp1)
02983     - VAT3( uN, im1,j,k) * VAT3(dPSE, iim1,jjp1,kkp1))
02984
02985     - VAT3( uPW, ii,jj,kk) * (- VAT3( oNW, im1,j,kp1) * VAT3( dPS, iim1,jjp1,kkp1)
02986     - VAT3( uNW, im1,j,kp1) * VAT3( oPS, iim1,jjp1,kkp1)
02987     - VAT3( oN, im1,j,kp1) * VAT3(dPSE, iim1,jjp1,kkp1)
02988     - VAT3( uN, im1,j,kp1) * VAT3(oPSE, iim1,jjp1,kkp1))
02989
02990     - VAT3(oPNW, ii,jj,kk) * (- VAT3( uW, im1,jp1,k) * VAT3( dPS, iim1,jjp1,kkp1)
02991     - VAT3( uNW, im1,jp1,k) * VAT3( dPC, iim1,jjp1,kkp1)
02992     - VAT3( uC, im1,jp1,k) * VAT3(dPSE, iim1,jjp1,kkp1)
02993     - VAT3( uN, im1,jp1,k) * VAT3( dPE, iim1,jjp1,kkp1));
02994
02995 TMP2_XUNW =
02996     - VAT3(uPNW, ii,jj,kk) * (- VAT3( oE, im2,jp1,kp1) * VAT3( dPS, iim1,jjp1,kkp1)
02997     - VAT3( uW, im1,jp1,kp1) * VAT3( oPS, iim1,jjp1,kkp1)
02998     - VAT3( oNW, im1,jp1,kp1) * VAT3( dPC, iim1,jjp1,kkp1)
02999     - VAT3( uNW, im1,jp1,kp1) * VAT3( oPC, iim1,jjp1,kkp1)
03000     + VAT3( oC, im1,jp1,kp1) * VAT3(dPSE, iim1,jjp1,kkp1)
03001     - VAT3( uC, im1,jp1,kp1) * VAT3(oPSE, iim1,jjp1,kkp1)
03002     - VAT3( oN, im1,jp1,kp1) * VAT3( dPE, iim1,jjp1,kkp1)
03003     - VAT3( uN, im1,jp1,kp1) * VAT3( oPE, iim1,jjp1,kkp1))
03004
03005     + VAT3( oPC, ii,jj,kk) * VAT3( uNW, i,j,k) * VAT3(dPSE, iim1,jjp1,kkp1)
03006
03007     - VAT3( uPC, ii,jj,kk) * (- VAT3( oNW, i,j,kp1) * VAT3(dPSE, iim1,jjp1,kkp1)
03008     - VAT3( uNW, i,j,kp1) * VAT3(oPSE, iim1,jjp1,kkp1))
03009
03010     - VAT3( oPN, ii,jj,kk) * (- VAT3( uW, i,jp1,k) * VAT3(dPSE, iim1,jjp1,kkp1)
03011     - VAT3( uNW, i,jp1,k) * VAT3( dPE, iim1,jjp1,kkp1))
03012
03013     - VAT3( uPN, ii,jj,kk) * (- VAT3( oE, im1,jp1,kp1) * VAT3(dPSE, iim1,jjp1,kkp1)
03014     - VAT3( uW, i,jp1,kp1) * VAT3(oPSE, iim1,jjp1,kkp1)
03015     - VAT3( oNW, i,jp1,kp1) * VAT3( dPE, iim1,jjp1,kkp1)
03016     - VAT3( uNW, i,jp1,kp1) * VAT3( oPE, iim1,jjp1,kkp1));
03017
03018 VAT3(XuNW, ii,jj,kk) = TMP1_XUNW + TMP2_XUNW;
03019
03020     //fprintf(data, "%19.12E\n", VAT3(XuNW, ii, jj, kk));
03021
03022     /* *****
03023     * *** > USE;
03024     * *****/
03025
03026     // VAT3(XuSE, ii,jj,kk) =
03027 TMP1_XUSE =
03028     - VAT3( oPS, ii,jj,kk) * (- VAT3( uSE, i,jm1,k) * VAT3( dPW, iip1,jjm1,kkp1)
03029     - VAT3( uE, i,jm1,k) * VAT3(dPNW, iip1,jjm1,kkp1))
03030
03031     - VAT3( uPS, ii,jj,kk) * (- VAT3( oNW, ip1,jm2,kp1) * VAT3( dPW, iip1,jjm1,kkp1)
03032     - VAT3( uSE, i,jm1,kp1) * VAT3( oPW, iip1,jjm1,kkp1)
03033     - VAT3( oE, i,jm1,kp1) * VAT3(dPNW, iip1,jjm1,kkp1)
03034     - VAT3( uE, i,jm1,kp1) * VAT3(oPNW, iip1,jjm1,kkp1))
03035
03036     + VAT3( oPC, ii,jj,kk) * VAT3( uSE, i,j,k) * VAT3(dPNW, iip1,jjm1,kkp1)
03037
03038     - VAT3( uPC, ii,jj,kk) * (- VAT3( oNW, ip1,jm1,kp1) * VAT3(dPNW, iip1,jjm1,kkp1)
03039     - VAT3( uSE, i,j,kp1) * VAT3(oPNW, iip1,jjm1,kkp1));
03040
03041 TMP2_XUSE =

```

```

03042     - VAT3(oPSE, ii,jj,kk) * (- VAT3( uS, ip1,jm1,k) * VAT3( dPW, iip1,jjm1,kkp1)
03043       - VAT3( uC, ip1,jm1,k) * VAT3(dPNW, iip1,jjm1,kkp1)
03044       - VAT3( uSE, ip1,jm1,k) * VAT3( dPC, iip1,jjm1,kkp1)
03045       - VAT3( uE, ip1,jm1,k) * VAT3( dPN, iip1,jjm1,kkp1))
03046
03047     - VAT3(uPSE, ii,jj,kk) * (- VAT3( oN, ip1,jm2,kp1) * VAT3( dPW, iip1,jjm1,kkp1)
03048       - VAT3( uS, ip1,jm1,kp1) * VAT3( oPW, iip1,jjm1,kkp1)
03049       + VAT3( oC, ip1,jm1,kp1) * VAT3(dPNW, iip1,jjm1,kkp1)
03050       - VAT3( uC, ip1,jm1,kp1) * VAT3(oPNW, iip1,jjm1,kkp1)
03051       - VAT3( oNW, ip2,jm2,kp1) * VAT3( dPC, iip1,jjm1,kkp1)
03052       - VAT3( uSE, ip1,jm1,kp1) * VAT3( oPC, iip1,jjm1,kkp1)
03053       - VAT3( oE, ip1,jm1,kp1) * VAT3( dPN, iip1,jjm1,kkp1)
03054       - VAT3( uE, ip1,jm1,kp1) * VAT3( oPN, iip1,jjm1,kkp1))
03055
03056     - VAT3( oPE, ii,jj,kk) * (- VAT3( uS, ip1,j,k) * VAT3(dPNW, iip1,jjm1,kkp1)
03057       - VAT3( uSE, ip1,j,k) * VAT3( dPN, iip1,jjm1,kkp1))
03058
03059     - VAT3( uPE, ii,jj,kk) * (- VAT3( oN, ip1,jm1,kp1) * VAT3(dPNW, iip1,jjm1,kkp1)
03060       - VAT3( uS, ip1,j,kp1) * VAT3(oPNW, iip1,jjm1,kkp1)
03061       - VAT3( oNW, ip2,jm1,kp1) * VAT3( dPN, iip1,jjm1,kkp1)
03062       - VAT3( uSE, ip1,j,kp1) * VAT3( oPN, iip1,jjm1,kkp1));
03063 VAT3(XuSE, ii,jj,kk) = TMP1_XUSE + TMP2_XUSE;
03064
03065     //fprintf(data, "%19.12E\n", VAT3(XuSE, ii, jj, kk));
03066
03067     /* *****
03068     * *** > USW;
03069     * *****/
03070
03071     // VAT3(XuSW, ii,jj,kk) =
03072     TMP1_XUSW =
03073     - VAT3(oPSW, ii,jj,kk) * (- VAT3( uSW, im1,jm1,k) * VAT3( dPC, iim1,jjm1,kkp1)
03074       - VAT3( uW, im1,jm1,k) * VAT3( dPN, iim1,jjm1,kkp1)
03075       - VAT3( uS, im1,jm1,k) * VAT3( dPE, iim1,jjm1,kkp1)
03076       - VAT3( uC, im1,jm1,k) * VAT3(dPNE, iim1,jjm1,kkp1))
03077
03078     - VAT3(uPSW, ii,jj,kk) * (- VAT3( oNE, im2,jm2,kp1) * VAT3( dPC, iim1,jjm1,kkp1)
03079       - VAT3( uSW, im1,jm1,kp1) * VAT3( oPC, iim1,jjm1,kkp1)
03080       - VAT3( oE, im2,jm1,kp1) * VAT3( dPN, iim1,jjm1,kkp1)
03081       - VAT3( uW, im1,jm1,kp1) * VAT3( oPN, iim1,jjm1,kkp1)
03082       - VAT3( oN, im1,jm2,kp1) * VAT3( dPE, iim1,jjm1,kkp1)
03083       - VAT3( uS, im1,jm1,kp1) * VAT3( oPE, iim1,jjm1,kkp1)
03084       + VAT3( oC, im1,jm1,kp1) * VAT3(dPNE, iim1,jjm1,kkp1)
03085       - VAT3( uC, im1,jm1,kp1) * VAT3(oPNE, iim1,jjm1,kkp1))
03086
03087     - VAT3( oPW, ii,jj,kk) * (- VAT3( uSW, im1,j,k) * VAT3( dPN, iim1,jjm1,kkp1)
03088       - VAT3( uS, im1,j,k) * VAT3(dPNE, iim1,jjm1,kkp1));
03089
03090     TMP2_XUSW =
03091     - VAT3( uPW, ii,jj,kk) * (- VAT3( oNE, im2,jm1,kp1) * VAT3( dPN, iim1,jjm1,kkp1)
03092       - VAT3( uSW, im1,j,kp1) * VAT3( oPN, iim1,jjm1,kkp1)
03093       - VAT3( oN, im1,jm1,kp1) * VAT3(dPNE, iim1,jjm1,kkp1)
03094       - VAT3( uS, im1,j,kp1) * VAT3(oPNE, iim1,jjm1,kkp1))
03095
03096     - VAT3( oPS, ii,jj,kk) * (- VAT3( uSW, i,jm1,k) * VAT3( dPE, iim1,jjm1,kkp1)
03097       - VAT3( uW, i,jm1,k) * VAT3(dPNE, iim1,jjm1,kkp1))
03098
03099     - VAT3( uPS, ii,jj,kk) * (- VAT3( oNE, im1,jm2,kp1) * VAT3( dPE, iim1,jjm1,kkp1)
03100       - VAT3( uSW, i,jm1,kp1) * VAT3( oPE, iim1,jjm1,kkp1)
03101       - VAT3( oE, im1,jm1,kp1) * VAT3(dPNE, iim1,jjm1,kkp1)
03102       - VAT3( uW, i,jm1,kp1) * VAT3(oPNE, iim1,jjm1,kkp1))
03103
03104     + VAT3( oPC, ii,jj,kk) * VAT3( uSW, i,j,k) * VAT3(dPNE, iim1,jjm1,kkp1)
03105
03106     - VAT3( uPC, ii,jj,kk) * (- VAT3( oNE, im1,jm1,kp1) * VAT3(dPNE, iim1,jjm1,kkp1)
03107       - VAT3( uSW, i,j,kp1) * VAT3(oPNE, iim1,jjm1,kkp1));
03108 VAT3(XuSW, ii,jj,kk) = TMP1_XUSW + TMP2_XUSW;
03109
03110     //fprintf(data, "%19.12E\n", VAT3(XuSW, ii, jj, kk));
03111
03112     }
03113   }
03114 }
03115 }

```

9.119 buildGd.h

00001

```
00049 #ifndef _BUILGDG_H_
00050 #define _BUILGDG_H_
00051
00052 #include "malloc/malloc.h"
00053
00054 #include "apbscfg.h"
00055
00056 #include "generic/vhal.h"
00057 #include "generic/vmatrix.h"
00058
00059 VEXTERNC void VbuildG(
00060     int    *nxf,
00061     int    *nyf,
00062     int    *nzf,
00063     int    *nxc,
00064     int    *nyc,
00065     int    *nzc,
00066     int    *numdia,
00067     double *pcFF,
00068     double *acFF,
00069     double *ac
00070 );
00071
00144 VEXTERNC void VbuildG_1(
00145     int    *nxf,
00146     int    *nyf,
00147     int    *nzf,
00148     int    *nx,
00149     int    *ny,
00150     int    *nz,
00151     double *oPC,
00152     double *oPN,
00153     double *oPS,
00154     double *oPE,
00155     double *oPW,
00156     double *oPNE,
00157     double *oPNW,
00158     double *oPSE,
00159     double *oPSW,
00160     double *uPC,
00161     double *uPN,
00162     double *uPS,
00163     double *uPE,
00164     double *uPW,
00165     double *uPNE,
00166     double *uPNW,
00167     double *uPSE,
00168     double *uPSW,
00169     double *dPC,
00170     double *dPN,
00171     double *dPS,
00172     double *dPE,
00173     double *dPW,
00174     double *dPNE,
00175     double *dPNW,
00176     double *dPSE,
00177     double *dPSW,
00178     double *oC,
00179     double *XoC,
00180     double *XoE,
00181     double *XoN,
00182     double *XuC,
00183     double *XoNE,
00184     double *XoNW,
00185     double *XuE,
00186     double *XuW,
00187     double *XuN,
00188     double *XuS,
00189     double *XuNE,
00190     double *XuNW,
00191     double *XuSE,
00192     double *XuSW
00193 );
00194
00195
00196
00276 VEXTERNC void VbuildG_7(
00277     int    *nxf,
00278     int    *nyf,
00279     int    *nzf,
00280     int    *nx,
```

```
00281         int      *ny,
00282         int      *nz,
00283         double   *oPC,
00284         double   *oPN,
00285         double   *oPS,
00286         double   *oPE,
00287         double   *oPW,
00288         double   *oPNE,
00289         double   *oPNW,
00290         double   *oPSE,
00291         double   *oPSW,
00292         double   *uPC,
00293         double   *uPN,
00294         double   *uPS,
00295         double   *uPE,
00296         double   *uPW,
00297         double   *uPNE,
00298         double   *uPNW,
00299         double   *uPSE,
00300         double   *uPSW,
00301         double   *dPC,
00302         double   *dPN,
00303         double   *dPS,
00304         double   *dPE,
00305         double   *dPW,
00306         double   *dPNE,
00307         double   *dPNW,
00308         double   *dPSE,
00309         double   *dPSW,
00310         double   *oC,
00311         double   *oE,
00312         double   *oN,
00313         double   *uC,
00314         double   *XoC,
00315         double   *XoE,
00316         double   *XoN,
00317         double   *XuC,
00318         double   *XoNE,
00319         double   *XoNW,
00320         double   *XuE,
00321         double   *XuW,
00322         double   *XuN,
00323         double   *XuS,
00324         double   *XuNE,
00325         double   *XuNW,
00326         double   *XuSE,
00327         double   *XuSW
00328     );
00329
00330
00423 VEXTERNC void VbuildG_27(
00424     int *nxf,
00425     int *nyf,
00426     int *nzf,
00427     int *nx,
00428     int *ny,
00429     int *nz,
00430     double *oPC,
00431     double *oPN,
00432     double *oPS,
00433     double *oPE,
00434     double *oPW,
00435     double *oPNE,
00436     double *oPNW,
00437     double *oPSE,
00438     double *oPSW,
00439     double *uPC,
00440     double *uPN,
00441     double *uPS,
00442     double *uPE,
00443     double *uPW,
00444     double *uPNE,
00445     double *uPNW,
00446     double *uPSE,
00447     double *uPSW,
00448     double *dPC,
00449     double *dPN,
00450     double *dPS,
00451     double *dPE,
00452     double *dPW,
00453     double *dPNE,
```



```

00454     double *dPNW,
00455     double *dPSE,
00456     double *dPSW,
00457     double *oC,
00458     double *oE,
00459     double *oN,
00460     double *uC,
00461     double *oNE,
00462     double *oNW,
00463     double *uE,
00464     double *uW,
00465     double *uN,
00466     double *uS,
00467     double *uNE,
00468     double *uNW,
00469     double *uSE,
00470     double *uSW,
00471     double *XoC,
00472     double *XoE,
00473     double *XoN,
00474     double *XuC,
00475     double *XoNE,
00476     double *XoNW,
00477     double *XuE,
00478     double *XuW,
00479     double *XuN,
00480     double *XuS,
00481     double *XuNE,
00482     double *XuNW,
00483     double *XuSE,
00484     double *XuSW
00485     );
00486
00487 #endif // _BUILDDGD_H_

```

9.120 buildPd.c

```

00001
00055 #include "buildPd.h"
00056
00057 VPUBLIC void VbuildP(int *nxf, int *nyf, int *nzf,
00058     int *nxc, int *nyc, int *nzc,
00059     int *mgprol,
00060     int *ipc, double *rpc,
00061     double *pc, double *ac,
00062     double *xf, double *yf, double *zf) {
00063
00064     int numdia;
00065
00066     MAT2(pc, *nxc * *nyc * *nzc, 1);
00067     MAT2(ac, *nxf * *nyf * *nzf, 1);
00068
00069     if (*mgprol == 0) {
00070
00071         VbuildP_trilin(nxf, nyf, nzf,
00072             nxc, nyc, nzc,
00073             RAT2(pc, 1, 1),
00074             xf, yf, zf);
00075
00076     } else if (*mgprol == 1) {
00077
00078         numdia = VAT(ipc, 11);
00079
00080         if (numdia == 7) {
00081             VbuildP_op7(nxf, nyf, nzf,
00082                 nxc, nyc, nzc,
00083                 ipc, rpc,
00084                 RAT2(ac, 1, 1), RAT2(pc, 1, 1));
00085         } else if (numdia == 27) {
00086             VbuildP_op27(nxf, nyf, nzf,
00087                 nxc, nyc, nzc,
00088                 ipc, rpc,
00089                 RAT2(ac, 1, 1), RAT2(pc, 1, 1));
00090         } else {
00091             Vnm_print(2, "BUILDP: invalid stencil type given: %d\n", numdia);
00092         }
00093     }
00094 }

```

```

00095
00096 VPUBLIC void VbuildP_trilin(int *nxf, int *nyf, int *nzf,
00097     int *nxc, int *nyc, int *nzc,
00098     double *pc,
00099     double *xf, double *yf, double *zf) {
00100
00101     MAT2(pc, *nxc * *nyc * *nzc, 1);
00102
00103     VbuildPb_trilin(nxf, nyf, nzf,
00104         nxc, nyc, nzc,
00105         RAT2(pc, 1, 1),RAT2(pc, 1, 2),RAT2(pc, 1, 3),RAT2(pc, 1, 4),RAT2(pc, 1, 5),
00106         RAT2(pc, 1, 6),RAT2(pc, 1, 7),RAT2(pc, 1, 8),RAT2(pc, 1, 9),
00107         RAT2(pc, 1, 10),RAT2(pc, 1, 11),RAT2(pc, 1, 12),RAT2(pc, 1, 13),RAT2(pc, 1, 14),
00108         RAT2(pc, 1, 15),RAT2(pc, 1, 16),RAT2(pc, 1, 17),RAT2(pc, 1, 18),
00109         RAT2(pc, 1, 19),RAT2(pc, 1, 20),RAT2(pc, 1, 21),RAT2(pc, 1, 22),RAT2(pc, 1, 23),
00110         RAT2(pc, 1, 24),RAT2(pc, 1, 25),RAT2(pc, 1, 26),RAT2(pc, 1, 27),
00111         xf, yf, zf);
00112 }
00113
00114 VEXTERNC void VbuildPb_trilin(int *nxf, int *nyf, int *nzf,
00115     int *nxc, int *nyc, int *nzc,
00116     double *oPC, double *oPN, double *oPS, double *oPE, double *oPW,
00117     double *oPNE, double *oPNW, double *oPSE, double *oPSW,
00118     double *uPC, double *uPN, double *uPS, double *uPE, double *uPW,
00119     double *uPNE, double *uPNW, double *uPSE, double *uPSW,
00120     double *dPC, double *dPN, double *dPS, double *dPE, double *dPW,
00121     double *dPNE, double *dPNW, double *dPSE, double *dPSW,
00122     double *xf, double *yf, double *zf) {
00123
00124     int i, j, k;
00125
00126     double won      = 1.0;
00127     double half     = 1.0 / 2.0;
00128     double quarter  = 1.0 / 4.0;
00129     double eighth   = 1.0 / 8.0;
00130
00131
00132     MAT3( oPC, *nxc, *nyc, *nzc);
00133     MAT3( oPN, *nxc, *nyc, *nzc);
00134     MAT3( oPS, *nxc, *nyc, *nzc);
00135     MAT3( oPE, *nxc, *nyc, *nzc);
00136     MAT3( oPW, *nxc, *nyc, *nzc);
00137
00138     MAT3(oPNE, *nxc, *nyc, *nzc);
00139     MAT3(oPNW, *nxc, *nyc, *nzc);
00140     MAT3(oPSE, *nxc, *nyc, *nzc);
00141     MAT3(oPSW, *nxc, *nyc, *nzc);
00142
00143     MAT3( uPC, *nxc, *nyc, *nzc);
00144     MAT3( uPN, *nxc, *nyc, *nzc);
00145     MAT3( uPS, *nxc, *nyc, *nzc);
00146     MAT3( uPE, *nxc, *nyc, *nzc);
00147     MAT3( uPW, *nxc, *nyc, *nzc);
00148
00149     MAT3(uPNE, *nxc, *nyc, *nzc);
00150     MAT3(uPNW, *nxc, *nyc, *nzc);
00151     MAT3(uPSE, *nxc, *nyc, *nzc);
00152     MAT3(uPSW, *nxc, *nyc, *nzc);
00153
00154     MAT3( dPC, *nxc, *nyc, *nzc);
00155     MAT3( dPN, *nxc, *nyc, *nzc);
00156     MAT3( dPS, *nxc, *nyc, *nzc);
00157     MAT3( dPE, *nxc, *nyc, *nzc);
00158     MAT3( dPW, *nxc, *nyc, *nzc);
00159
00160     MAT3(dPNE, *nxc, *nyc, *nzc);
00161     MAT3(dPNW, *nxc, *nyc, *nzc);
00162     MAT3(dPSE, *nxc, *nyc, *nzc);
00163     MAT3(dPSW, *nxc, *nyc, *nzc);
00164
00165     for(k=2; k<=*nzc-1; k++) {
00166         for(j=2; j<=*nyc-1; j++) {
00167             for(i=2; i<=*nxc-1; i++) {
00168
00169                 VAT3(oPC, i,j,k)  = won;
00170
00171                 VAT3(oPN, i,j,k)  = half;
00172                 VAT3(oPS, i,j,k)  = half;
00173                 VAT3(oPE, i,j,k)  = half;
00174                 VAT3(oPW, i,j,k)  = half;
00175                 VAT3(uPC, i,j,k)  = half;
00176                 VAT3(dPC, i,j,k)  = half;

```

```

00177
00178         VAT3(oPNE, i, j, k) = quarter;
00179         VAT3(oPNW, i, j, k) = quarter;
00180         VAT3(oPSE, i, j, k) = quarter;
00181         VAT3(oPSW, i, j, k) = quarter;
00182         VAT3(dPN, i, j, k) = quarter;
00183         VAT3(dPS, i, j, k) = quarter;
00184         VAT3(dPE, i, j, k) = quarter;
00185         VAT3(dPW, i, j, k) = quarter;
00186         VAT3(uPN, i, j, k) = quarter;
00187         VAT3(uPS, i, j, k) = quarter;
00188         VAT3(uPE, i, j, k) = quarter;
00189         VAT3(uPW, i, j, k) = quarter;
00190
00191         VAT3(dPNE, i, j, k) = eighth;
00192         VAT3(dPNW, i, j, k) = eighth;
00193         VAT3(dPSE, i, j, k) = eighth;
00194         VAT3(dPSW, i, j, k) = eighth;
00195         VAT3(uPNE, i, j, k) = eighth;
00196         VAT3(uPNW, i, j, k) = eighth;
00197         VAT3(uPSE, i, j, k) = eighth;
00198         VAT3(uPSW, i, j, k) = eighth;
00199     }
00200 }
00201 }
00202 }
00203
00204
00205
00206 VPUBLIC void VbuildP_op7(int *nxf, int *nyf, int *nzf,
00207     int *nxc, int *nyc, int *nzc,
00208     int *ipc, double *rpc,
00209     double *ac, double *pc) {
00210
00211     MAT2(ac, *nxf * *nyf * *nzf, 1);
00212     MAT2(pc, *nxc * *nyc * *nzc, 1);
00213
00214     WARN_UNTESTED;
00215
00216     VbuildPb_op7(nxf, nyf, nzf,
00217         nxc, nyc, nzc,
00218         ipc, rpc,
00219         RAT2(ac, 1, 1), RAT2(ac, 1, 2), RAT2(ac, 1, 3),
00220         RAT2(ac, 1, 4),
00221         RAT2(pc, 1, 1), RAT2(pc, 1, 2), RAT2(pc, 1, 3), RAT2(pc, 1, 4), RAT2(pc, 1, 5),
00222         RAT2(pc, 1, 6), RAT2(pc, 1, 7), RAT2(pc, 1, 8), RAT2(pc, 1, 9),
00223         RAT2(pc, 1, 10), RAT2(pc, 1, 11), RAT2(pc, 1, 12), RAT2(pc, 1, 13), RAT2(pc, 1, 14),
00224         RAT2(pc, 1, 15), RAT2(pc, 1, 16), RAT2(pc, 1, 17), RAT2(pc, 1, 18),
00225         RAT2(pc, 1, 19), RAT2(pc, 1, 20), RAT2(pc, 1, 21), RAT2(pc, 1, 22), RAT2(pc, 1, 23),
00226         RAT2(pc, 1, 24), RAT2(pc, 1, 25), RAT2(pc, 1, 26), RAT2(pc, 1, 27));
00227 }
00228
00229
00230
00231 VPUBLIC void VbuildPb_op7(int *nxf, int *nyf, int *nzf,
00232     int *nxc, int *nyc, int *nzc,
00233     int *ipc, double *rpc,
00234     double *oC, double *oE, double *oN,
00235     double *uC,
00236     double *oPC, double *oPN, double *oPS, double *oPE, double *oPW,
00237     double *oPNE, double *oPNW, double *oPSE, double *oPSW,
00238     double *uPC, double *uPN, double *uPS, double *uPE, double *uPW,
00239     double *uPNE, double *uPNW, double *uPSE, double *uPSW,
00240     double *dPC, double *dPN, double *dPS, double *dPE, double *dPW,
00241     double *dPNE, double *dPNW, double *dPSE, double *dPSW) {
00242
00243     int i, j, k;
00244     int ii, jj, kk;
00245     int im1, ip1;
00246     int im2, ip2;
00247     int jm1, jp1;
00248     int jm2, jp2;
00249     int km1, kp1;
00250     int km2, kp2;
00251     int iim1, iip1;
00252     int jjm1, jjp1;
00253     int kkm1, kkp1;
00254
00255     double won, half, quarter, eighth;
00256
00257     MAT3( oC, *nxf, *nyf, *nzf);

```

```

00258     MAT3( oE, *nxf, *nyf, *nzf);
00259     MAT3( oN, *nxf, *nyf, *nzf);
00260     MAT3( uC, *nxf, *nyf, *nzf);
00261     MAT3( oPC, *nxc, *nyc, *nzc);
00262     MAT3( oPN, *nxc, *nyc, *nzc);
00263     MAT3( oPS, *nxc, *nyc, *nzc);
00264     MAT3( oPE, *nxc, *nyc, *nzc);
00265     MAT3( oPW, *nxc, *nyc, *nzc);
00266     MAT3( oPNE, *nxc, *nyc, *nzc);
00267     MAT3( oPNW, *nxc, *nyc, *nzc);
00268     MAT3( oPSE, *nxc, *nyc, *nzc);
00269     MAT3( oPSW, *nxc, *nyc, *nzc);
00270     MAT3( uPC, *nxc, *nyc, *nzc);
00271     MAT3( uPN, *nxc, *nyc, *nzc);
00272     MAT3( uPS, *nxc, *nyc, *nzc);
00273     MAT3( uPE, *nxc, *nyc, *nzc);
00274     MAT3( uPW, *nxc, *nyc, *nzc);
00275     MAT3( uPNE, *nxc, *nyc, *nzc);
00276     MAT3( uPNW, *nxc, *nyc, *nzc);
00277     MAT3( uPSE, *nxc, *nyc, *nzc);
00278     MAT3( uPSW, *nxc, *nyc, *nzc);
00279     MAT3( dPC, *nxc, *nyc, *nzc);
00280     MAT3( dPN, *nxc, *nyc, *nzc);
00281     MAT3( dPS, *nxc, *nyc, *nzc);
00282     MAT3( dPE, *nxc, *nyc, *nzc);
00283     MAT3( dPW, *nxc, *nyc, *nzc);
00284     MAT3( dPNE, *nxc, *nyc, *nzc);
00285     MAT3( dPNW, *nxc, *nyc, *nzc);
00286     MAT3( dPSE, *nxc, *nyc, *nzc);
00287     MAT3( dPSW, *nxc, *nyc, *nzc);
00288
00289     WARN_UNTESTED;
00290
00291     // interpolation stencil ***
00292     won      = 1.0;
00293     half     = 1.0 / 2.0;
00294     quarter  = 1.0 / 4.0;
00295     eighth   = 1.0 / 8.0;
00296
00297     //fprintf(data, "%s\n", PRINT_FUNC);
00298
00299     for (kk = 2; kk < *nzc - 1; kk++) {
00300         k = 2 * kk - 1;
00301
00302         for (jj = 2; jj < *nyc - 1; jj++) {
00303             j = 2 * jj - 1;
00304
00305             for (ii = 2; ii < *nxc - 1; ii++) {
00306                 i = 2 * ii - 1;
00307
00308                 // index computations ***
00309                 im1 = i - 1;
00310                 ip1 = i + 1;
00311                 im2 = i - 2;
00312                 ip2 = i + 2;
00313                 jm1 = j - 1;
00314                 jp1 = j + 1;
00315                 jm2 = j - 2;
00316                 jp2 = j + 2;
00317                 km1 = k - 1;
00318                 kp1 = k + 1;
00319                 km2 = k - 2;
00320                 kp2 = k + 2;
00321                 iim1 = ii - 1;
00322                 iip1 = ii + 1;
00323                 jjm1 = jj - 1;
00324                 jjp1 = jj + 1;
00325                 kkm1 = kk - 1;
00326                 kkp1 = kk + 1;
00327
00328                 // *****
00329                 // *** > oPC;
00330                 // *****
00331
00332                 VAT3( oPC, ii, jj, kk) = won;
00333
00334                 //fprintf(data, "%19.12E\n", VAT3(oPC, ii, jj, kk));
00335
00336                 // *****
00337                 // *** > oPN;
00338                 // *****

```

```

00339
00340 VAT3( oPN, ii, jj, kk) =
00341     VAT3( oN, i, j, k) / ( VAT3( oC, i, jpl, k)
00342         - VAT3( oE, iml, jpl, k)
00343         - VAT3( oE, i, jpl, k)
00344         - VAT3( uC, i, jpl, kml)
00345         - VAT3( uC, i, jpl, k));
00346
00347 //fprintf(data, "%19.12E\n", VAT3(oPN, ii, jj, kk));
00348
00349 // *****
00350 // *** > oPS;
00351 // *****
00352
00353 VAT3( oPS, ii, jj, kk) =
00354     VAT3( oN, i, jml, k) / ( VAT3( oC, i, jml, k)
00355         - VAT3( oE, iml, jml, k)
00356         - VAT3( oE, i, jml, k)
00357         - VAT3( uC, i, jml, kml)
00358         - VAT3( uC, i, jml, k));
00359
00360 //fprintf(data, "%19.12E\n", VAT3(oPS, ii, jj, kk));
00361
00362 // *****
00363 // *** > oPE;
00364 // *****
00365
00366 VAT3( oPE, ii, jj, kk) =
00367     VAT3( oE, i, j, k) / ( VAT3( oC, ip1, j, k)
00368         - VAT3( uC, ip1, j, kml)
00369         - VAT3( uC, ip1, j, k)
00370         - VAT3( oN, ip1, j, k)
00371         - VAT3( oN, ip1, jml, k));
00372
00373 //fprintf(data, "%19.12E\n", VAT3(oPE, ii, jj, kk));
00374
00375 // *****
00376 // *** > oPW;
00377 // *****
00378
00379 VAT3( oPW, ii, jj, kk) =
00380     VAT3( oE, iml, j, k) / ( VAT3( oC, iml, j, k)
00381         - VAT3( uC, iml, j, kml)
00382         - VAT3( uC, iml, j, k)
00383         - VAT3( oN, iml, j, k)
00384         - VAT3( oN, iml, jml, k));
00385
00386 //fprintf(data, "%19.12E\n", VAT3(oPW, ii, jj, kk));
00387
00388 // *****
00389 // *** > oPNE;
00390 // *****
00391
00392 VAT3(oPNE, ii, jj, kk) =
00393     (
00394         VAT3( oN, ip1, j, k) * VAT3( oPE, ii, jj, kk)
00395         + VAT3( oE, i, jpl, k) * VAT3( oPN, ii, jj, kk)
00396     ) / (
00397         VAT3( oC, ip1, jpl, k)
00398         - VAT3( uC, ip1, jpl, kml)
00399         - VAT3( uC, ip1, jpl, k)
00400     );
00401
00402 //fprintf(data, "%19.12E\n", VAT3(oPNE, ii, jj, kk));
00403
00404 // *****
00405 // *** > oPNW;
00406 // *****
00407
00408 VAT3(oPNW, ii, jj, kk) =
00409     (
00410         VAT3( oN, iml, j, k) * VAT3( oPW, ii, jj, kk)
00411         + VAT3( oE, iml, jpl, k) * VAT3( oPN, ii, jj, kk)
00412     ) / (
00413         VAT3( oC, iml, jpl, k)
00414         - VAT3( uC, iml, jpl, kml)
00415         - VAT3( uC, iml, jpl, k)
00416     );
00417
00418 //fprintf(data, "%19.12E\n", VAT3(oPNW, ii, jj, kk));
00419

```

```

00420 // *****
00421 // *** > oPSE;
00422 // *****
00423
00424 VAT3(oPSE, ii, jj, kk) =
00425 (
00426     VAT3( oN, ipl, jml, k) * VAT3( oPE, ii, jj, kk)
00427     + VAT3( oE, i, jml, k) * VAT3( oPS, ii, jj, kk)
00428 ) / (
00429     VAT3( oC, ipl, jml, k)
00430     - VAT3( uC, ipl, jml, kml)
00431     - VAT3( uC, ipl, jml, k)
00432 );
00433
00434 //fprintf(data, "%19.12E\n", VAT3(oPSE, ii, jj, kk));
00435
00436 // *****
00437 // *** > oPSW;
00438 // *****
00439
00440 VAT3(oPSW, ii, jj, kk) =
00441 (
00442     VAT3( oN, iml, jml, k) * VAT3( oPW, ii, jj, kk)
00443     + VAT3( oE, iml, jml, k) * VAT3( oPS, ii, jj, kk)
00444 ) / (
00445     VAT3( oC, iml, jml, k)
00446     - VAT3( uC, iml, jml, kml)
00447     - VAT3( uC, iml, jml, k)
00448 );
00449
00450 //fprintf(data, "%19.12E\n", VAT3(oPSW, ii, jj, kk));
00451
00452 // *****
00453 // *** > dPC;
00454 // *****
00455
00456 VAT3( dPC, ii, jj, kk) =
00457     VAT3( uC, i, j, kml)
00458 / (
00459     VAT3( oC, i, j, kml)
00460     - VAT3( oN, i, j, kml)
00461     - VAT3( oN, i, jml, kml)
00462     - VAT3( oE, iml, j, kml)
00463     - VAT3( oE, i, j, kml)
00464 );
00465
00466 //fprintf(data, "%19.12E\n", VAT3(dPC, ii, jj, kk));
00467
00468 // *****
00469 // *** > dPN;
00470 // *****
00471
00472 VAT3( dPN, ii, jj, kk) =
00473 (
00474     VAT3( oN, i, j, kml) * VAT3( dPC, ii, jj, kk)
00475     + VAT3( uC, i, jpl, kml) * VAT3( oPN, ii, jj, kk)
00476 ) / (
00477     VAT3( oC, i, jpl, kml)
00478     - VAT3( oE, iml, jpl, kml)
00479     - VAT3( oE, i, jpl, kml)
00480 );
00481
00482 //fprintf(data, "%19.12E\n", VAT3(dPN, ii, jj, kk));
00483
00484 // *****
00485 // *** > dPS;
00486 // *****
00487
00488 VAT3( dPS, ii, jj, kk) =
00489 (
00490     VAT3( oN, i, jml, kml) * VAT3( dPC, ii, jj, kk)
00491     + VAT3( uC, i, jml, kml) * VAT3( oPS, ii, jj, kk)
00492 ) / (
00493     VAT3( oC, i, jml, kml)
00494     - VAT3( oE, iml, jml, kml)
00495     - VAT3( oE, i, jml, kml)
00496 );
00497
00498 //fprintf(data, "%19.12E\n", VAT3(dPS, ii, jj, kk));
00499
00500 // *****

```

```

00501 // *** > dPE;
00502 // *****
00503
00504 VAT3( dPE, ii, jj, kk) =
00505 (
00506     VAT3( uC, ip1, j, km1) * VAT3( oPE, ii, jj, kk)
00507 + VAT3( oE, i, j, km1) * VAT3( dPC, ii, jj, kk)
00508 ) / (
00509     VAT3( oC, ip1, j, km1)
00510 - VAT3( oN, ip1, j, km1)
00511 - VAT3( oN, ip1, jml, km1)
00512 );
00513
00514 //fprintf(data, "%19.12E\n", VAT3(dPE, ii, jj, kk));
00515
00516 // *****
00517 // *** > dPW;
00518 // *****
00519
00520 VAT3( dPW, ii, jj, kk) =
00521 (
00522     VAT3( uC, im1, j, km1) * VAT3( oPW, ii, jj, kk)
00523 + VAT3( oE, im1, j, km1) * VAT3( dPC, ii, jj, kk)
00524 ) / (
00525     VAT3( oC, im1, j, km1)
00526 - VAT3( oN, im1, j, km1)
00527 - VAT3( oN, im1, jml, km1)
00528 );
00529
00530 //fprintf(data, "%19.12E\n", VAT3(dPW, ii, jj, kk));
00531
00532 // *****
00533 // *** > dPNE;
00534 // *****
00535
00536 VAT3(dPNE, ii, jj, kk) =
00537 (
00538     VAT3( uC, ip1, jp1, km1) * VAT3( oPNE, ii, jj, kk)
00539 + VAT3( oE, i, jp1, km1) * VAT3( dPN, ii, jj, kk)
00540 + VAT3( oN, ip1, j, km1) * VAT3( dPE, ii, jj, kk)
00541 ) / VAT3( oC, ip1, jp1, km1);
00542
00543 //fprintf(data, "%19.12E\n", VAT3(dPNE, ii, jj, kk));
00544
00545 // *****
00546 // *** > dPNW;
00547 // *****
00548
00549 VAT3(dPNW, ii, jj, kk) =
00550 (
00551     VAT3( uC, im1, jp1, km1) * VAT3( oPNW, ii, jj, kk)
00552 + VAT3( oE, im1, jp1, km1) * VAT3( dPN, ii, jj, kk)
00553 + VAT3( oN, im1, j, km1) * VAT3( dPW, ii, jj, kk)
00554 ) / VAT3( oC, im1, jp1, km1);
00555
00556 //fprintf(data, "%19.12E\n", VAT3(dPNW, ii, jj, kk));
00557
00558 // *****
00559 // *** > dPSE;
00560 // *****
00561
00562 VAT3(dPSE, ii, jj, kk) =
00563 (
00564     VAT3( uC, ip1, jml, km1) * VAT3( oPSE, ii, jj, kk)
00565 + VAT3( oE, i, jml, km1) * VAT3( dPS, ii, jj, kk)
00566 + VAT3( oN, ip1, jml, km1) * VAT3( dPE, ii, jj, kk)
00567 ) / VAT3( oC, ip1, jml, km1);
00568
00569 //fprintf(data, "%19.12E\n", VAT3(dPSE, ii, jj, kk));
00570
00571 // *****
00572 // *** > dPSW;
00573 // *****
00574
00575 VAT3(dPSW, ii, jj, kk) =
00576 (
00577     VAT3( uC, im1, jml, km1) * VAT3( oPSW, ii, jj, kk)
00578 + VAT3( oE, im1, jml, km1) * VAT3( dPS, ii, jj, kk)
00579 + VAT3( oN, im1, jml, km1) * VAT3( dPW, ii, jj, kk)
00580 ) / VAT3( oC, im1, jml, km1);
00581

```

```

00582 //fprintf(data, "%19.12E\n", VAT3(dPSW, ii, jj, kk));
00583
00584 // *****
00585 // *** > uPC;
00586 // *****
00587
00588 VAT3( uPC, ii, jj, kk) =
00589     VAT3( uC, i, j, k)
00590     / ( VAT3( oC, i, j, kp1)
00591         - VAT3( oN, i, j, kp1)
00592         - VAT3( oN, i, jml, kp1)
00593         - VAT3( oE, im1, j, kp1)
00594         - VAT3( oE, i, j, kp1)
00595     );
00596
00597 //fprintf(data, "%19.12E\n", VAT3(uPC, ii, jj, kk));
00598
00599 // *****
00600 // *** > uPN;
00601 // *****
00602
00603 VAT3( uPN, ii, jj, kk) =
00604     (
00605         VAT3( oN, i, j, kp1) * VAT3( uPC, ii, jj, kk)
00606         + VAT3( uC, i, jpl, k) * VAT3( oPN, ii, jj, kk)
00607     ) / (
00608         VAT3( oC, i, jpl, kp1)
00609         - VAT3( oE, im1, jpl, kp1)
00610         - VAT3( oE, i, jpl, kp1)
00611     );
00612
00613 //fprintf(data, "%19.12E\n", VAT3(uPN, ii, jj, kk));
00614
00615 // *****
00616 // *** > uPS;
00617 // *****
00618
00619 VAT3( uPS, ii, jj, kk) =
00620     (
00621         VAT3( oN, i, jml, kp1) * VAT3( uPC, ii, jj, kk)
00622         + VAT3( uC, i, jml, k) * VAT3( oPS, ii, jj, kk)
00623     ) / (
00624         VAT3( oC, i, jml, kp1)
00625         - VAT3( oE, im1, jml, kp1)
00626         - VAT3( oE, i, jml, kp1)
00627     );
00628
00629 //fprintf(data, "%19.12E\n", VAT3(uPS, ii, jj, kk));
00630
00631 // *****
00632 // *** > uPE;
00633 // *****
00634
00635 VAT3( uPE, ii, jj, kk) =
00636     (
00637         VAT3( uC, ipl, j, k) * VAT3( oPE, ii, jj, kk)
00638         + VAT3( oE, i, j, kp1) * VAT3( uPC, ii, jj, kk)
00639     ) / (
00640         VAT3( oC, ipl, j, kp1)
00641         - VAT3( oN, ipl, j, kp1)
00642         - VAT3( oN, ipl, jml, kp1)
00643     );
00644
00645 //fprintf(data, "%19.12E\n", VAT3(uPE, ii, jj, kk));
00646
00647 // *****
00648 // *** > uPW;
00649 // *****
00650
00651 VAT3( uPW, ii, jj, kk) =
00652     (
00653         VAT3( uC, im1, j, k) * VAT3( oPW, ii, jj, kk)
00654         + VAT3( oE, im1, j, kp1) * VAT3( uPC, ii, jj, kk)
00655     ) / (
00656         VAT3( oC, im1, j, kp1)
00657         - VAT3( oN, im1, j, kp1)
00658         - VAT3( oN, im1, jml, kp1)
00659     );
00660
00661 //fprintf(data, "%19.12E\n", VAT3(uPW, ii, jj, kk));
00662

```



```

00663 // *****
00664 // *** > uPNE;
00665 // *****
00666
00667 VAT3(uPNE, ii, jj, kk) =
00668 (
00669     VAT3( uC, ipl, jpl, k) * VAT3(oPNE, ii, jj, kk)
00670     + VAT3( oE, i, jpl, kpl) * VAT3( uPN, ii, jj, kk)
00671     + VAT3( oN, ipl, j, kpl) * VAT3( uPE, ii, jj, kk)
00672     ) / VAT3( oC, ipl, jpl, kpl);
00673
00674 //fprintf(data, "%19.12E\n", VAT3(uPNE, ii, jj, kk));
00675
00676 // *****
00677 // *** > uPNW;
00678 // *****
00679
00680 VAT3(uPNW, ii, jj, kk) =
00681 (
00682     VAT3( uC, iml, jpl, k) * VAT3(oPNW, ii, jj, kk)
00683     + VAT3( oE, iml, jpl, kpl) * VAT3( uPN, ii, jj, kk)
00684     + VAT3( oN, iml, j, kpl) * VAT3( uPW, ii, jj, kk)
00685     ) / VAT3( oC, iml, jpl, kpl);
00686
00687 //fprintf(data, "%19.12E\n", VAT3(uPNW, ii, jj, kk));
00688
00689 // *****
00690 // *** > uPSE;
00691 // *****
00692
00693 VAT3(uPSE, ii, jj, kk) =
00694 (
00695     VAT3( uC, ipl, jml, k) * VAT3(oPSE, ii, jj, kk)
00696     + VAT3( oE, i, jml, kpl) * VAT3( uPS, ii, jj, kk)
00697     + VAT3( oN, ipl, jml, kpl) * VAT3( uPE, ii, jj, kk)
00698     ) / VAT3( oC, ipl, jml, kpl);
00699
00700 //fprintf(data, "%19.12E\n", VAT3(uPSE, ii, jj, kk));
00701
00702 // *****
00703 // *** > uPSW;
00704 // *****
00705
00706 VAT3(uPSW, ii, jj, kk) =
00707 (
00708     VAT3( uC, iml, jml, k) * VAT3(oPSW, ii, jj, kk)
00709     + VAT3( oE, iml, jml, kpl) * VAT3( uPS, ii, jj, kk)
00710     + VAT3( oN, iml, jml, kpl) * VAT3( uPW, ii, jj, kk)
00711     ) / VAT3( oC, iml, jml, kpl);
00712
00713 //fprintf(data, "%19.12E\n", VAT3(uPSW, ii, jj, kk));
00714
00715     }
00716 }
00717 }
00718 }
00719
00720
00721
00722 VPUBLIC void VbuildP_op27(int *nxf, int *nyf, int *nzf,
00723     int *nxc, int *nyc, int *nzc,
00724     int *ipc, double *rpc,
00725     double *ac, double *pc) {
00726
00727     MAT2(ac, *nxf * *nyf * *nzf, 1);
00728     MAT2(pc, *nxc * *nyc * *nzc, 1);
00729
00730     WARN_UNTESTED;
00731
00732     VbuildPb_op27(nxf, nyf, nzf,
00733         nxc, nyc, nzc,
00734         ipc, rpc,
00735
00736         RAT2(ac, 1, 1), RAT2(ac, 1, 2), RAT2(ac, 1, 3),
00737         RAT2(ac, 1, 4),
00738         RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00739         RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1, 10),
00740         RAT2(ac, 1, 11), RAT2(ac, 1, 12), RAT2(ac, 1, 13), RAT2(ac, 1, 14),
00741         RAT2(pc, 1, 1), RAT2(pc, 1, 2), RAT2(pc, 1, 3), RAT2(pc, 1, 4), RAT2(pc, 1, 5),
00742         RAT2(pc, 1, 6), RAT2(pc, 1, 7), RAT2(pc, 1, 8), RAT2(pc, 1, 9),
00743         RAT2(pc, 1, 10), RAT2(pc, 1, 11), RAT2(pc, 1, 12), RAT2(pc, 1, 13), RAT2(pc, 1, 14),

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```

00744         RAT2(pc, 1, 15), RAT2(pc, 1, 16), RAT2(pc, 1, 17), RAT2(pc, 1, 18),
00745         RAT2(pc, 1, 19), RAT2(pc, 1, 20), RAT2(pc, 1, 21), RAT2(pc, 1, 22), RAT2(pc, 1, 23),
00746         RAT2(pc, 1, 24), RAT2(pc, 1, 25), RAT2(pc, 1, 26), RAT2(pc, 1, 27));
00747     }
00748
00749     VPUBLIC void VbuildPb_op27(int *nxf, int *nyf, int *nzf,
00750         int *nxc, int *nyc, int *nzc,
00751         int *ipc, double *rpc,
00752         double *oC, double *oE, double *oN,
00753         double *uC,
00754         double *oNE, double *oNW,
00755         double *uE, double *uW, double *uN, double *uS,
00756         double *uNE, double *uNW, double *uSE, double *uSW,
00757         double *oPC, double *oPN, double *oPS, double *oPE, double *oPW,
00758         double *oPNE, double *oPNW, double *oPSE, double *oPSW,
00759         double *uPC, double *uPN, double *uPS, double *uPE, double *uPW,
00760         double *uPNE, double *uPNW, double *uPSE, double *uPSW,
00761         double *dPC, double *dPN, double *dPS, double *dPE, double *dPW,
00762         double *dPNE, double *dPNW, double *dPSE, double *dPSW) {
00763
00764         int i, j, k;
00765         int ii, jj, kk;
00766         int im1, ip1;
00767         int im2, ip2;
00768         int jm1, jp1;
00769         int jm2, jp2;
00770         int km1, kp1;
00771         int km2, kp2;
00772         int iim1, iip1;
00773         int jjm1, jjp1;
00774         int kkm1, kkp1;
00775
00776         double won, half, quarter, eighth;
00777
00778         MAT3( oC, *nxf, *nyf, *nzf);
00779         MAT3( oE, *nxf, *nyf, *nzf);
00780         MAT3( oN, *nxf, *nyf, *nzf);
00781         MAT3( uC, *nxf, *nyf, *nzf);
00782         MAT3( oNE, *nxf, *nyf, *nzf);
00783         MAT3( oNW, *nxf, *nyf, *nzf);
00784         MAT3( uE, *nxf, *nyf, *nzf);
00785         MAT3( uW, *nxf, *nyf, *nzf);
00786         MAT3( uN, *nxf, *nyf, *nzf);
00787         MAT3( uS, *nxf, *nyf, *nzf);
00788         MAT3( uNE, *nxf, *nyf, *nzf);
00789         MAT3( uNW, *nxf, *nyf, *nzf);
00790         MAT3( uSE, *nxf, *nyf, *nzf);
00791         MAT3( uSW, *nxf, *nyf, *nzf);
00792         MAT3( oPC, *nxc, *nyc, *nzc);
00793         MAT3( oPN, *nxc, *nyc, *nzc);
00794         MAT3( oPS, *nxc, *nyc, *nzc);
00795         MAT3( oPE, *nxc, *nyc, *nzc);
00796         MAT3( oPW, *nxc, *nyc, *nzc);
00797         MAT3( oPNE, *nxc, *nyc, *nzc);
00798         MAT3( oPNW, *nxc, *nyc, *nzc);
00799         MAT3( oPSE, *nxc, *nyc, *nzc);
00800         MAT3( oPSW, *nxc, *nyc, *nzc);
00801         MAT3( uPC, *nxc, *nyc, *nzc);
00802         MAT3( uPN, *nxc, *nyc, *nzc);
00803         MAT3( uPS, *nxc, *nyc, *nzc);
00804         MAT3( uPE, *nxc, *nyc, *nzc);
00805         MAT3( uPW, *nxc, *nyc, *nzc);
00806         MAT3( uPNE, *nxc, *nyc, *nzc);
00807         MAT3( uPNW, *nxc, *nyc, *nzc);
00808         MAT3( uPSE, *nxc, *nyc, *nzc);
00809         MAT3( uPSW, *nxc, *nyc, *nzc);
00810         MAT3( dPC, *nxc, *nyc, *nzc);
00811         MAT3( dPN, *nxc, *nyc, *nzc);
00812         MAT3( dPS, *nxc, *nyc, *nzc);
00813         MAT3( dPE, *nxc, *nyc, *nzc);
00814         MAT3( dPW, *nxc, *nyc, *nzc);
00815         MAT3( dPNE, *nxc, *nyc, *nzc);
00816         MAT3( dPNW, *nxc, *nyc, *nzc);
00817         MAT3( dPSE, *nxc, *nyc, *nzc);
00818         MAT3( dPSW, *nxc, *nyc, *nzc);
00819
00820         WARN_UNTESTED;
00821
00822         // Interpolation Stencil
00823         won = 1.0;
00824         half = 1.0 / 2.0;

```

```

00825     quarter = 1.0 / 4.0;
00826     eighth  = 1.0 / 8.0;
00827
00828     //fprintf(data, "%s\n", PRINT_FUNC);
00829
00830     for (kk = 2; kk <= *nzc - 1; kk++) {
00831         k = 2 * kk - 1;
00832
00833         for (jj = 2; jj <= *nyc - 1; jj++) {
00834             j = 2 * jj - 1;
00835
00836             for (ii = 2; ii <= *nxc - 1; ii++) {
00837                 i = 2 * ii - 1;
00838
00839                 // Index Computations
00840                 im1 = i - 1;
00841                 ip1 = i + 1;
00842                 im2 = i - 2;
00843                 ip2 = i + 2;
00844                 jm1 = j - 1;
00845                 jp1 = j + 1;
00846                 jm2 = j - 2;
00847                 jp2 = j + 2;
00848                 km1 = k - 1;
00849                 kp1 = k + 1;
00850                 km2 = k - 2;
00851                 kp2 = k + 2;
00852                 iim1 = ii - 1;
00853                 iip1 = ii + 1;
00854                 jjm1 = jj - 1;
00855                 jjp1 = jj + 1;
00856                 kkm1 = kk - 1;
00857                 kkp1 = kk + 1;
00858
00859                 /* *****
00860                 /* *** > oPC;
00861                 /* *****
00862
00863                 VAT3( oPC, ii, jj, kk) = won;
00864
00865                 //fprintf(data, "%19.12E\n", VAT3(oPC, ii, jj, kk));
00866
00867                 /* *****
00868                 /* *** > oPN;
00869                 /* *****
00870
00871                 VAT3( oPN, ii, jj, kk) =
00872                 (
00873                     VAT3( uNE, im1, j, km1)
00874                     + VAT3( uN, i, j, km1)
00875                     + VAT3( uNW, ip1, j, km1)
00876                     + VAT3( oNE, im1, j, k)
00877                     + VAT3( oN, i, j, k)
00878                     + VAT3( oNW, ip1, j, k)
00879                     + VAT3( uSW, i, jp1, k)
00880                     + VAT3( uS, i, jp1, k)
00881                     + VAT3( uSE, i, jp1, k)
00882                 ) / (
00883                     VAT3( oC, i, jp1, k)
00884                     - VAT3( oE, im1, jp1, k)
00885                     - VAT3( oE, i, jp1, k)
00886                     - VAT3( uC, i, jp1, km1)
00887                     - VAT3( uE, im1, jp1, km1)
00888                     - VAT3( uW, ip1, jp1, km1)
00889                     - VAT3( uC, i, jp1, k)
00890                     - VAT3( uW, i, jp1, k)
00891                     - VAT3( uE, i, jp1, k)
00892                 );
00893
00894                 //fprintf(data, "%19.12E\n", VAT3(oPN, ii, jj, kk));
00895
00896                 /* *****
00897                 /* *** > oPS;
00898                 /* *****
00899
00900                 VAT3( oPS, ii, jj, kk) =
00901                 (
00902                     VAT3( uSE, im1, j, km1)
00903                     + VAT3( uS, i, j, km1)
00904                     + VAT3( uSW, ip1, j, km1)
00905                     + VAT3( oNW, i, jm1, k)

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```

00906             + VAT3( oN, i, jml, k)
00907             + VAT3( oNE, i, jml, k)
00908             + VAT3( uNW, i, jml, k)
00909             + VAT3( uN, i, jml, k)
00910             + VAT3( uNE, i, jml, k)
00911         ) / (
00912             VAT3( oC, i, jml, k)
00913             - VAT3( oE, iml, jml, k)
00914             - VAT3( oE, i, jml, k)
00915             - VAT3( uC, i, jml, kml)
00916             - VAT3( uE, iml, jml, kml)
00917             - VAT3( uW, ip1, jml, kml)
00918             - VAT3( uC, i, jml, k)
00919             - VAT3( uW, i, jml, k)
00920             - VAT3( uE, i, jml, k)
00921         );
00922
00923         //fprintf(data, "%19.12E\n", VAT3(oPS, ii, jj, kk));
00924
00925         /* *****
00926         /* *** > oPE;
00927         /* *****
00928
00929         VAT3( oPE, ii, jj, kk) =
00930         (
00931             VAT3( uSE, i, jpl, kml)
00932             + VAT3( oNW, ip1, j, k)
00933             + VAT3( uNW, ip1, j, k)
00934             + VAT3( uE, i, j, kml)
00935             + VAT3( oE, i, j, k)
00936             + VAT3( uW, ip1, j, k)
00937             + VAT3( uNE, i, jml, kml)
00938             + VAT3( oNE, i, jml, k)
00939             + VAT3( uSW, ip1, j, k)
00940         ) / (
00941             VAT3( oC, ip1, j, k)
00942             - VAT3( uC, ip1, j, kml)
00943             - VAT3( uC, ip1, j, k)
00944             - VAT3( oN, ip1, j, k)
00945             - VAT3( uS, ip1, jpl, kml)
00946             - VAT3( uN, ip1, j, k)
00947             - VAT3( oN, ip1, jml, k)
00948             - VAT3( uN, ip1, jml, kml)
00949             - VAT3( uS, ip1, j, k)
00950         );
00951
00952         //fprintf(data, "%19.12E\n", VAT3(oPE, ii, jj, kk));
00953
00954         /* *****
00955         /* *** > oPW;
00956         /* *****
00957
00958         VAT3( oPW, ii, jj, kk) =
00959         (
00960             VAT3( uSW, i, jpl, kml)
00961             + VAT3( oNE, iml, j, k)
00962             + VAT3( uNE, iml, j, k)
00963             + VAT3( uW, i, j, kml)
00964             + VAT3( oE, iml, j, k)
00965             + VAT3( uE, iml, j, k)
00966             + VAT3( uNW, i, jml, kml)
00967             + VAT3( oNW, i, jml, k)
00968             + VAT3( uSE, iml, j, k)
00969         ) / (
00970             VAT3( oC, iml, j, k)
00971             - VAT3( uC, iml, j, kml)
00972             - VAT3( uC, iml, j, k)
00973             - VAT3( oN, iml, j, k)
00974             - VAT3( uS, iml, jpl, kml)
00975             - VAT3( uN, iml, j, k)
00976             - VAT3( oN, iml, jml, k)
00977             - VAT3( uN, iml, jml, kml)
00978             - VAT3( uS, iml, j, k)
00979         );
00980
00981         //fprintf(data, "%19.12E\n", VAT3(oPW, ii, jj, kk));
00982
00983         /* *****
00984         /* *** > oPNE;
00985         /* *****
00986

```

```

00987     VAT3(oPNE, ii, jj, kk) =
00988     (
00989         VAT3(uNE, i, j, km1)
00990         + VAT3(oNE, i, j, k)
00991         + VAT3(uSW, ip1, jp1, k)
00992         + (
00993             VAT3(uN, ip1, j, km1)
00994             + VAT3(oN, ip1, j, k)
00995             + VAT3(uS, ip1, jp1, k)
00996         )
00997         * VAT3(oPE, ii, jj, kk)
00998         + (
00999             VAT3(uE, i, jp1, km1)
01000             + VAT3(oE, i, jp1, k)
01001             + VAT3(uW, ip1, jp1, k)
01002         )
01003         * VAT3(oPN, ii, jj, kk)
01004     ) / (
01005         VAT3(oC, ip1, jp1, k)
01006         - VAT3(uC, ip1, jp1, km1)
01007         - VAT3(uC, ip1, jp1, k)
01008     );
01009
01010     //fprintf(data, "%19.12E\n", VAT3(oPNE, ii, jj, kk));
01011
01012     /* *****
01013     /* *** > oPNW;
01014     /* *****
01015
01016     VAT3(oPNW, ii, jj, kk) =
01017     (
01018         VAT3(uNW, i, j, km1)
01019         + VAT3(oNW, i, j, k)
01020         + VAT3(uSE, im1, jp1, k)
01021         + (
01022             VAT3(uN, im1, j, km1)
01023             + VAT3(oN, im1, j, k)
01024             + VAT3(uS, im1, jp1, k)
01025         )
01026         * VAT3(oPW, ii, jj, kk)
01027         + (
01028             VAT3(uW, i, jp1, km1)
01029             + VAT3(oE, im1, jp1, k)
01030             + VAT3(uE, im1, jp1, k)
01031         )
01032         * VAT3(oPN, ii, jj, kk)
01033     ) / (
01034         VAT3(oC, im1, jp1, k)
01035         - VAT3(uC, im1, jp1, km1)
01036         - VAT3(uC, im1, jp1, k)
01037     );
01038
01039     //fprintf(data, "%19.12E\n", VAT3(oPNW, ii, jj, kk));
01040
01041     /* *****
01042     /* *** > oPSE;
01043     /* *****
01044
01045     VAT3(oPSE, ii, jj, kk) =
01046     (
01047         VAT3(uSE, i, j, km1)
01048         + VAT3(oNW, ip1, jml, k)
01049         + VAT3(uNW, ip1, jml, k)
01050         + (
01051             VAT3(uS, ip1, j, km1)
01052             + VAT3(oN, ip1, jml, k)
01053             + VAT3(uN, ip1, jml, k)
01054         )
01055         * VAT3(oPE, ii, jj, kk)
01056         + (
01057             VAT3(uE, i, jml, km1)
01058             + VAT3(oE, i, jml, k)
01059             + VAT3(uW, ip1, jml, k)
01060         )
01061         * VAT3(oPS, ii, jj, kk)
01062     ) / (
01063         VAT3(oC, ip1, jml, k)
01064         - VAT3(uC, ip1, jml, km1)
01065         - VAT3(uC, ip1, jml, k)
01066     );
01067

```

```

01068 //fprintf(data, "%19.12E\n", VAT3(oPSE, ii, jj, kk));
01069
01070 /* *****
01071 /** *** > oPSW;
01072 /** *****
01073
01074 VAT3(oPSW, ii, jj, kk) =
01075 (
01076     VAT3(uSW, i, j, km1)
01077 + VAT3(oNE, im1, jm1, k)
01078 + VAT3(uNE, im1, jm1, k)
01079 + (
01080     VAT3(uS, im1, j, km1)
01081 + VAT3(oN, im1, jm1, k)
01082 + VAT3(uN, im1, jm1, k)
01083 )
01084 * VAT3(oPW, ii, jj, kk)
01085 + (
01086     VAT3(uW, i, jm1, km1)
01087 + VAT3(oE, im1, jm1, k)
01088 + VAT3(uE, im1, jm1, k)
01089 )
01090 * VAT3(oPS, ii, jj, kk)
01091 ) / (
01092     VAT3(oC, im1, jm1, k)
01093 - VAT3(uC, im1, jm1, km1)
01094 - VAT3(uC, im1, jm1, k)
01095 );
01096
01097 //fprintf(data, "%19.12E\n", VAT3(oPSW, ii, jj, kk));
01098
01099 /* *****
01100 /** *** > dPC;
01101 /** *****
01102
01103 VAT3(dPC, ii, jj, kk) =
01104 (
01105     VAT3(uNW, i, j, km1)
01106 + VAT3(uW, i, j, km1)
01107 + VAT3(uSW, i, j, km1)
01108 + VAT3(uN, i, j, km1)
01109 + VAT3(uC, i, j, km1)
01110 + VAT3(uS, i, j, km1)
01111 + VAT3(uNE, i, j, km1)
01112 + VAT3(uE, i, j, km1)
01113 + VAT3(uSE, i, j, km1)
01114 ) / (
01115     VAT3(oC, i, j, km1)
01116 - VAT3(oN, i, j, km1)
01117 - VAT3(oN, i, jm1, km1)
01118 - VAT3(oNW, i, j, km1)
01119 - VAT3(oE, im1, j, km1)
01120 - VAT3(oNE, im1, jm1, km1)
01121 - VAT3(oNE, i, j, km1)
01122 - VAT3(oE, i, j, km1)
01123 - VAT3(oNW, ip1, jm1, km1)
01124 );
01125
01126 //fprintf(data, "%19.12E\n", VAT3(dPC, ii, jj, kk));
01127
01128 /* *****
01129 /** *** > dPN;
01130 /** *****
01131
01132 VAT3(dPN, ii, jj, kk) =
01133 (
01134     VAT3(uSW, i, jp1, km1)
01135 + VAT3(uS, i, jp1, km1)
01136 + VAT3(uSE, i, jp1, km1)
01137 + (
01138     VAT3(oNE, im1, j, km1)
01139 + VAT3(oN, i, j, km1)
01140 + VAT3(oNW, ip1, j, km1)
01141 )
01142 * VAT3(dPC, ii, jj, kk)
01143 + (
01144     VAT3(uW, i, jp1, km1)
01145 + VAT3(uC, i, jp1, km1)
01146 + VAT3(uE, i, jp1, km1)
01147 )
01148 * VAT3(oPN, ii, jj, kk)

```

```

01149         ) / (
01150             VAT3( oC, i, jpl, kml)
01151             - VAT3( oE, iml, jpl, kml)
01152             - VAT3( oE, i, jpl, kml)
01153         );
01154
01155         //fprintf(data, "%19.12E\n", VAT3(dPN, ii, jj, kk));
01156
01157         /* *****
01158         /* *** > dPS;
01159         /* *****
01160
01161         VAT3( dPS, ii, jj, kk) =
01162         (
01163             VAT3( uNW, i, jml, kml)
01164             + VAT3( uN, i, jml, kml)
01165             + VAT3( uNE, i, jml, kml)
01166             + (
01167                 VAT3( oNW, i, jml, kml)
01168                 + VAT3( oN, i, jml, kml)
01169                 + VAT3( oNE, i, jml, kml)
01170             )
01171             * VAT3( dPC, ii, jj, kk)
01172             + (
01173                 VAT3( uW, i, jml, kml)
01174                 + VAT3( uC, i, jml, kml)
01175                 + VAT3( uE, i, jml, kml)
01176             )
01177             * VAT3( oPS, ii, jj, kk)
01178         ) / (
01179             VAT3( oC, i, jml, kml)
01180             - VAT3( oE, iml, jml, kml)
01181             - VAT3( oE, i, jml, kml)
01182         );
01183
01184         //fprintf(data, "%19.12E\n", VAT3(dPS, ii, jj, kk));
01185
01186         /* *****
01187         /* *** > dPE;
01188         /* *****
01189
01190         VAT3( dPE, ii, jj, kk) =
01191         (
01192             VAT3( uNW, ip1, j, kml)
01193             + VAT3( uW, ip1, j, kml)
01194             + VAT3( uSW, ip1, j, kml)
01195             + (
01196                 VAT3( uN, ip1, j, kml)
01197                 + VAT3( uC, ip1, j, kml)
01198                 + VAT3( uS, ip1, j, kml)
01199             )
01200             * VAT3( oPE, ii, jj, kk)
01201             + (
01202                 VAT3( oNW, ip1, j, kml)
01203                 + VAT3( oE, i, j, kml)
01204                 + VAT3( oNE, i, jml, kml)
01205             )
01206             * VAT3( dPC, ii, jj, kk)
01207         ) / (
01208             VAT3( oC, ip1, j, kml)
01209             - VAT3( oN, ip1, j, kml)
01210             - VAT3( oN, ip1, jml, kml)
01211         );
01212
01213         //fprintf(data, "%19.12E\n", VAT3(dPE, ii, jj, kk));
01214
01215         /* *****
01216         /* *** > dPW;
01217         /* *****
01218
01219         VAT3( dPW, ii, jj, kk) =
01220         (
01221             VAT3( uNE, iml, j, kml)
01222             + VAT3( uE, iml, j, kml)
01223             + VAT3( uSE, iml, j, kml)
01224             + (
01225                 VAT3( uN, iml, j, kml)
01226                 + VAT3( uC, iml, j, kml)
01227                 + VAT3( uS, iml, j, kml)
01228             )
01229             * VAT3( oPW, ii, jj, kk)

```

```

01230             + (
01231                 VAT3( oNE, im1, j, km1)
01232                 + VAT3( oE, im1, j, km1)
01233                 + VAT3( oNW, i, jml, km1)
01234             )
01235             * VAT3( dPC, ii, jj, kk)
01236         ) / (
01237             VAT3( oC, im1, j, km1)
01238             - VAT3( oN, im1, j, km1)
01239             - VAT3( oN, im1, jml, km1)
01240         );
01241
01242         //fprintf(data, "%19.12E\n", VAT3(dPW, ii, jj, kk));
01243
01244         /* *****
01245         /* *** > dPNE;
01246         /* *****
01247
01248         VAT3(dPNE, ii, jj, kk) =
01249         (
01250             VAT3( uSW, ip1, jpl, km1)
01251             + VAT3( uW, ip1, jpl, km1)
01252             * VAT3( oPN, ii, jj, kk)
01253             + VAT3( uS, ip1, jpl, km1)
01254             * VAT3( oPE, ii, jj, kk)
01255             + VAT3( uC, ip1, jpl, km1)
01256             * VAT3(oPNE, ii, jj, kk)
01257             + VAT3( oNE, i, j, km1)
01258             * VAT3( dPC, ii, jj, kk)
01259             + VAT3( oE, i, jpl, km1)
01260             * VAT3( dPN, ii, jj, kk)
01261             + VAT3( oN, ip1, j, km1)
01262             * VAT3( dPE, ii, jj, kk)
01263         )
01264         / VAT3( oC, ip1, jpl, km1);
01265
01266         //fprintf(data, "%19.12E\n", VAT3(dPNE, ii, jj, kk));
01267
01268         /* *****
01269         /* *** > dPNW;
01270         /* *****
01271
01272         VAT3(dPNW, ii, jj, kk) =
01273         (
01274             VAT3( uSE, im1, jpl, km1)
01275             + VAT3( uE, im1, jpl, km1)
01276             * VAT3( oPN, ii, jj, kk)
01277             + VAT3( uS, im1, jpl, km1)
01278             * VAT3( oPW, ii, jj, kk)
01279             + VAT3( uC, im1, jpl, km1)
01280             * VAT3(oPNW, ii, jj, kk)
01281             + VAT3( oNW, i, j, km1)
01282             * VAT3( dPC, ii, jj, kk)
01283             + VAT3( oE, im1, jpl, km1)
01284             * VAT3( dPN, ii, jj, kk)
01285             + VAT3( oN, im1, j, km1)
01286             * VAT3( dPW, ii, jj, kk)
01287         )
01288         / VAT3( oC, im1, jpl, km1);
01289
01290         //fprintf(data, "%19.12E\n", VAT3(dPNW, ii, jj, kk));
01291
01292         /* *****
01293         /* *** > dPSE;
01294         /* *****
01295
01296         VAT3(dPSE, ii, jj, kk) =
01297         (
01298             VAT3( uNW, ip1, jml, km1)
01299             + VAT3( uW, ip1, jml, km1)
01300             * VAT3( oPS, ii, jj, kk)
01301             + VAT3( uN, ip1, jml, km1)
01302             * VAT3( oPE, ii, jj, kk)
01303             + VAT3( uC, ip1, jml, km1)
01304             * VAT3(oPSE, ii, jj, kk)
01305             + VAT3( oNW, ip1, jml, km1)
01306             * VAT3( dPC, ii, jj, kk)
01307             + VAT3( oE, i, jml, km1)
01308             * VAT3( dPS, ii, jj, kk)
01309             + VAT3( oN, ip1, jml, km1)
01310             * VAT3( dPE, ii, jj, kk)

```



```

01311         )
01312         / VAT3( oC, ip1, jml, kml);
01313
01314         //fprintf(data, "%19.12E\n", VAT3(dPSE, ii, jj, kk));
01315
01316         /* *****
01317         /* *** > dPSW;
01318         /* *****
01319
01320         VAT3(dPSW, ii, jj, kk) =
01321         (
01322             VAT3( uNE, im1, jml, kml)
01323             + VAT3( uE, im1, jml, kml)
01324             * VAT3( oPS, ii, jj, kk)
01325             + VAT3( uN, im1, jml, kml)
01326             * VAT3( oPW, ii, jj, kk)
01327             + VAT3( uC, im1, jml, kml)
01328             * VAT3( oPSW, ii, jj, kk)
01329             + VAT3( oNE, im1, jml, kml)
01330             * VAT3( dPC, ii, jj, kk)
01331             + VAT3( oE, im1, jml, kml)
01332             * VAT3( dPS, ii, jj, kk)
01333             + VAT3( oN, im1, jml, kml)
01334             * VAT3( dPW, ii, jj, kk)
01335         )
01336         / VAT3( oC, im1, jml, kml);
01337
01338         //fprintf(data, "%19.12E\n", VAT3(dPSW, ii, jj, kk));
01339
01340         /* *****
01341         /* *** > uPC;
01342         /* *****
01343
01344         VAT3( uPC, ii, jj, kk) =
01345         (
01346             VAT3( uSE, im1, jpl, k)
01347             + VAT3( uE, im1, j, k)
01348             + VAT3( uNE, im1, jml, k)
01349             + VAT3( uS, i, jpl, k)
01350             + VAT3( uC, i, j, k)
01351             + VAT3( uN, i, jml, k)
01352             + VAT3( uSW, ip1, jpl, k)
01353             + VAT3( uW, ip1, j, k)
01354             + VAT3( uNW, ip1, jml, k)
01355         ) / (
01356             VAT3( oC, i, j, kp1)
01357             - VAT3( oN, i, j, kp1)
01358             - VAT3( oN, i, jml, kp1)
01359             - VAT3( oNW, i, j, kp1)
01360             - VAT3( oE, im1, j, kp1)
01361             - VAT3( oNE, im1, jml, kp1)
01362             - VAT3( oNE, i, j, kp1)
01363             - VAT3( oE, i, j, kp1)
01364             - VAT3( oNW, ip1, jml, kp1)
01365         );
01366
01367         //fprintf(data, "%19.12E\n", VAT3(uPC, ii, jj, kk));
01368
01369         /* *****
01370         /* *** > uPN;
01371         /* *****
01372
01373         VAT3( uPN, ii, jj, kk) =
01374         (
01375             VAT3( uNE, im1, j, k)
01376             + VAT3( uN, i, j, k)
01377             + VAT3( uNW, ip1, j, k)
01378             + (
01379                 VAT3( oNE, im1, j, kp1)
01380                 + VAT3( oN, i, j, kp1)
01381                 + VAT3( oNW, ip1, j, kp1)
01382             )
01383             * VAT3( uPC, ii, jj, kk)
01384             + (
01385                 VAT3( uE, im1, jpl, k)
01386                 + VAT3( uC, i, jpl, k)
01387                 + VAT3( uW, ip1, jpl, k)
01388             )
01389             * VAT3( oPN, ii, jj, kk)
01390         ) / (
01391             VAT3( oC, i, jpl, kp1)

```

```

01392             - VAT3( oE, im1, jpl, kpl)
01393             - VAT3( oE, i, jpl, kpl)
01394         );
01395
01396         //fprintf(data, "%19.12E\n", VAT3(uPN, ii, jj, kk));
01397
01398         /* *****
01399         /* *** > uPS;
01400         /* *****
01401
01402         VAT3( uPS, ii, jj, kk) =
01403         (
01404             VAT3( uSE, im1, j, k)
01405             + VAT3( uS, i, j, k)
01406             + VAT3( uSW, ip1, j, k)
01407             + (
01408                 VAT3( oNW, i, jml, kpl)
01409             + VAT3( oN, i, jml, kpl)
01410             + VAT3( oNE, i, jml, kpl)
01411             )
01412             * VAT3( uPC, ii, jj, kk)
01413             + (
01414                 VAT3( uE, im1, jml, k)
01415             + VAT3( uC, i, jml, k)
01416             + VAT3( uW, ip1, jml, k)
01417             )
01418             * VAT3( oPS, ii, jj, kk)
01419         ) / (
01420             VAT3( oC, i, jml, kpl)
01421             - VAT3( oE, im1, jml, kpl)
01422             - VAT3( oE, i, jml, kpl)
01423         );
01424
01425         //fprintf(data, "%19.12E\n", VAT3(uPS, ii, jj, kk));
01426
01427         /* *****
01428         /* *** > uPE;
01429         /* *****
01430
01431         VAT3( uPE, ii, jj, kk) =
01432         (
01433             VAT3( uSE, i, jpl, k)
01434             + VAT3( uS, ip1, jpl, k)
01435             + VAT3( uNE, i, jml, k)
01436             + (
01437                 VAT3( uS, ip1, jpl, k)
01438             + VAT3( uC, ip1, j, k)
01439             + VAT3( uN, ip1, jml, k)
01440             )
01441             * VAT3( oPE, ii, jj, kk)
01442             + (
01443                 VAT3( oNW, ip1, j, kpl)
01444             + VAT3( oE, i, j, kpl)
01445             + VAT3( oNE, i, jml, kpl)
01446             )
01447             * VAT3( uPC, ii, jj, kk)
01448         ) / (
01449             VAT3( oC, ip1, j, kpl)
01450             - VAT3( oN, ip1, j, kpl)
01451             - VAT3( oN, ip1, jml, kpl)
01452         );
01453
01454         //fprintf(data, "%19.12E\n", VAT3(uPE, ii, jj, kk));
01455
01456         /* *****
01457         /* *** > uPW;
01458         /* *****
01459
01460         VAT3( uPW, ii, jj, kk) =
01461         (
01462             VAT3( uSW, i, jpl, k)
01463             + VAT3( uW, i, j, k)
01464             + VAT3( uNW, i, jml, k)
01465             + (
01466                 VAT3( uS, im1, jpl, k)
01467             + VAT3( uC, im1, j, k)
01468             + VAT3( uN, im1, jml, k)
01469             )
01470             * VAT3( oPW, ii, jj, kk)
01471             + (
01472                 VAT3( oNE, im1, j, kpl)

```

```

01473             + VAT3( oE, im1, j, kp1)
01474             + VAT3( oNW, i, jml, kp1)
01475         )
01476     * VAT3( uPC, ii, jj, kk)
01477 ) / (
01478     VAT3( oC, im1, j, kp1)
01479     - VAT3( oN, im1, j, kp1)
01480     - VAT3( oN, im1, jml, kp1)
01481 );
01482
01483 //fprintf(data, "%19.12E\n", VAT3(uPW, ii, jj, kk));
01484
01485 /** *****
01486 /** *** > uPNE;
01487 /** *****
01488
01489 VAT3(uPNE, ii, jj, kk) =
01490 (
01491     VAT3( uNE, i, j, k)
01492     + VAT3( uE, i, jpl, k)
01493     * VAT3( oPN, ii, jj, kk)
01494     + VAT3( uN, ip1, j, k)
01495     * VAT3( oPE, ii, jj, kk)
01496     + VAT3( uC, ip1, jpl, k)
01497     * VAT3( oPNE, ii, jj, kk)
01498     + VAT3( oNE, i, j, kp1)
01499     * VAT3( uPC, ii, jj, kk)
01500     + VAT3( oE, i, jpl, kp1)
01501     * VAT3( uPN, ii, jj, kk)
01502     + VAT3( oN, ip1, j, kp1)
01503     * VAT3( uPE, ii, jj, kk)
01504 )
01505 / VAT3( oC, ip1, jpl, kp1);
01506
01507 //fprintf(data, "%19.12E\n", VAT3(uPNE, ii, jj, kk));
01508
01509 /** *****
01510 /** *** > uPNW;
01511 /** *****
01512
01513 VAT3(uPNW, ii, jj, kk) =
01514 (
01515     VAT3( uNW, i, j, k)
01516     + VAT3( uW, i, jpl, k)
01517     * VAT3( oPN, ii, jj, kk)
01518     + VAT3( uN, im1, j, k)
01519     * VAT3( oPW, ii, jj, kk)
01520     + VAT3( uC, im1, jpl, k)
01521     * VAT3( oPNW, ii, jj, kk)
01522     + VAT3( oNW, i, j, kp1)
01523     * VAT3( uPC, ii, jj, kk)
01524     + VAT3( oE, im1, jpl, kp1)
01525     * VAT3( uPN, ii, jj, kk)
01526     + VAT3( oN, im1, j, kp1)
01527     * VAT3( uPW, ii, jj, kk)
01528 )
01529 / VAT3( oC, im1, jpl, kp1);
01530
01531 //fprintf(data, "%19.12E\n", VAT3(uPNW, ii, jj, kk));
01532
01533 /** *****
01534 /** *** > uPSE;
01535 /** *****
01536
01537 VAT3(uPSE, ii, jj, kk) =
01538 (
01539     VAT3( uSE, i, j, k)
01540     + VAT3( uE, i, jml, k)
01541     * VAT3( oPS, ii, jj, kk)
01542     + VAT3( uS, ip1, j, k)
01543     * VAT3( oPE, ii, jj, kk)
01544     + VAT3( uC, ip1, jml, k)
01545     * VAT3( oPSE, ii, jj, kk)
01546     + VAT3( oNW, ip1, jml, kp1)
01547     * VAT3( uPC, ii, jj, kk)
01548     + VAT3( oE, i, jml, kp1)
01549     * VAT3( uPS, ii, jj, kk)
01550     + VAT3( oN, ip1, jml, kp1)
01551     * VAT3( uPE, ii, jj, kk)
01552 )
01553 / VAT3( oC, ip1, jml, kp1);

```

```

01554
01555 //fprintf(data, "%19.12E\n", VAT3(uPSE, ii, jj, kk));
01556
01557 /* *****
01558 /* *** > uPSW;
01559 /* *****
01560
01561 VAT3(uPSW, ii, jj, kk) =
01562 (
01563     VAT3(uSW, i, j, k)
01564 + VAT3(uW, i, jml, k)
01565 * VAT3(oPS, ii, jj, kk)
01566 + VAT3(uS, iml, j, k)
01567 * VAT3(oPW, ii, jj, kk)
01568 + VAT3(uC, iml, jml, k)
01569 * VAT3(oPSW, ii, jj, kk)
01570 + VAT3(ONE, iml, jml, kp1)
01571 * VAT3(uPC, ii, jj, kk)
01572 + VAT3(oE, iml, jml, kp1)
01573 * VAT3(uPS, ii, jj, kk)
01574 + VAT3(oN, iml, jml, kp1)
01575 * VAT3(uPW, ii, jj, kk)
01576 )
01577 / VAT3(oC, iml, jml, kp1);
01578
01579 //fprintf(data, "%19.12E\n", VAT3(uPSW, ii, jj, kk));
01580
01581 }
01582 }
01583 }
01584 }

```

9.121 buildPd.h

```

00001
00050 #ifndef _BUILDPD_H_
00051 #define _BUILDPD_H_
00052
00053 #include "apbscfg.h"
00054
00055 #include "malloc/malloc.h"
00056
00057 #include "generic/vhal.h"
00058 #include "generic/vmatrix.h"
00059
00060 VEXTERNC void VbuildP(
00061     int *nxf,
00062     int *nyf,
00063     int *nzf,
00064     int *nxc,
00065     int *nyc,
00066     int *nzc,
00067     int *mgprol,
00068     int *ipc,
00069     double *rpc,
00070     double *pc,
00071     double *ac,
00072     double *xf,
00073     double *yf,
00074     double *zf
00075 );
00076
00077 VEXTERNC void VbuildP_trilin(
00078     int *nxf,
00079     int *nyf,
00080     int *nzf,
00081     int *nxc,
00082     int *nyc,
00083     int *nzc,
00084     double *pc,
00085     double *xf,
00086     double *yf,
00087     double *zf
00088 );
00089
00090 VEXTERNC void VbuildPb_trilin(
00091     int *nxf,
00092     int *nyf,

```

```
00093     int     *nzf,
00094     int     *nxc,
00095     int     *nyc,
00096     int     *nzc,
00097     double  *oPC,
00098     double  *oPN,
00099     double  *oPS,
00100     double  *oPE,
00101     double  *oPW,
00102     double  *oPNE,
00103     double  *oPNW,
00104     double  *oPSE,
00105     double  *oPSW,
00106     double  *uPC,
00107     double  *uPN,
00108     double  *uPS,
00109     double  *uPE,
00110     double  *uPW,
00111     double  *uPNE,
00112     double  *uPNW,
00113     double  *uPSE,
00114     double  *uPSW,
00115     double  *dPC,
00116     double  *dPN,
00117     double  *dPS,
00118     double  *dPE,
00119     double  *dPW,
00120     double  *dPNE,
00121     double  *dPNW,
00122     double  *dPSE,
00123     double  *dPSW,
00124     double  *xf,
00125     double  *yf,
00126     double  *zf
00127 );
00128
00129 VEXTERNC void VbuildP_op7(
00130     int     *nxf,
00131     int     *nyf,
00132     int     *nzf,
00133     int     *nxc,
00134     int     *nyc,
00135     int     *nzc,
00136     int     *ipc,
00137     double  *rpc,
00138     double  *ac,
00139     double  *pc
00140 );
00141
00142 VEXTERNC void VbuildPb_op7(
00143     int     *nxf,
00144     int     *nyf,
00145     int     *nzf,
00146     int     *nxc,
00147     int     *nyc,
00148     int     *nzc,
00149     int     *ipc,
00150     double  *rpc,
00151     double  *oC,
00152     double  *oE,
00153     double  *oN,
00154     double  *uC,
00155     double  *oPC,
00156     double  *oPN,
00157     double  *oPS,
00158     double  *oPE,
00159     double  *oPW,
00160     double  *oPNE,
00161     double  *oPNW,
00162     double  *oPSE,
00163     double  *oPSW,
00164     double  *uPC,
00165     double  *uPN,
00166     double  *uPS,
00167     double  *uPE,
00168     double  *uPW,
00169     double  *uPNE,
00170     double  *uPNW,
00171     double  *uPSE,
00172     double  *uPSW,
00173     double  *dPC,
```

```
00174         double *dPN,
00175         double *dPS,
00176         double *dPE,
00177         double *dPW,
00178         double *dPNE,
00179         double *dPNW,
00180         double *dPSE,
00181         double *dPSW
00182 );
00183
00184 VEXTERNC void VbuildP_op27(
00185         int *nxf,
00186         int *nyf,
00187         int *nzf,
00188         int *nxc,
00189         int *nyc,
00190         int *nzc,
00191         int *ipc,
00192         double *rpc,
00193         double *ac,
00194         double *pc
00195 );
00196
00197 VEXTERNC void VbuildPb_op27(
00198         int *nxf,
00199         int *nyf,
00200         int *nzf,
00201         int *nxc,
00202         int *nyc,
00203         int *nzc,
00204         int *ipc,
00205         double *rpc,
00206         double *oC,
00207         double *oE,
00208         double *oN,
00209         double *uC,
00210         double *oNE,
00211         double *oNW,
00212         double *uE,
00213         double *uW,
00214         double *uN,
00215         double *uS,
00216         double *uNE,
00217         double *uNW,
00218         double *uSE,
00219         double *uSW,
00220         double *oPC,
00221         double *oPN,
00222         double *oPS,
00223         double *oPE,
00224         double *oPW,
00225         double *oPNE,
00226         double *oPNW,
00227         double *oPSE,
00228         double *oPSW,
00229         double *uPC,
00230         double *uPN,
00231         double *uPS,
00232         double *uPE,
00233         double *uPW,
00234         double *uPNE,
00235         double *uPNW,
00236         double *uPSE,
00237         double *uPSW,
00238         double *dPC,
00239         double *dPN,
00240         double *dPS,
00241         double *dPE,
00242         double *dPW,
00243         double *dPNE,
00244         double *dPNW,
00245         double *dPSE,
00246         double *dPSW
00247 );
00248
00249 #endif /* _BUILDPD_H_ */
```

9.122 cgd.c

```

00001
00055 #include "cgd.h"
00056
00057 VPUBLIC void Vcghs(int *nx, int *ny, int *nz,
00058                  int *ipc, double *rpc,
00059                  double *ac, double *cc, double *fc,
00060                  double *x, double *p, double *ap, double *r,
00061                  int *itmax, int *iters,
00062                  double *errtol, double *omega,
00063                  int *iresid, int *iadjoint) {
00064
00065     double rsnrm, pAp, denom;
00066     double rhok1, rhok2, alpha, beta;
00067
00068     // Setup for the looping
00069     *iters = 0;
00070
00071     if (*iters >= *itmax && *iresid == 0)
00072         return;
00073
00074     Vmresid(nx, ny, nz, ipc, rpc, ac, cc, fc, x, r);
00075     denom = Vxnorm2(nx, ny, nz, r);
00076
00077     if (denom == 0.0)
00078         return;
00079
00080     if (*iters >= *itmax)
00081         return;
00082
00083     while(1) {
00084
00085         // Compute/check the current stopping test
00086         rhok2 = Vxdot(nx, ny, nz, r, r);
00087         rsnrm = VSQRT(rhok2);
00088
00089         if (rsnrm / denom <= *errtol)
00090             break;
00091
00092         if (*iters >= *itmax)
00093             break;
00094
00095         // Form new direction vector from old one and residual
00096         if (*iters == 0) {
00097             Vxcopy(nx, ny, nz, r, p);
00098         } else {
00099             beta = rhok2 / rhok1;
00100             alpha = 1.0 / beta;
00101             Vxaxpy(nx, ny, nz, &alpha, r, p);
00102             Vxscal(nx, ny, nz, &beta, p);
00103         }
00104
00105         // Linear case: alpha which minimizes energy norm of error
00106         Vmatvec(nx, ny, nz, ipc, rpc, ac, cc, p, ap);
00107         pAp = Vxdot(nx, ny, nz, p, ap);
00108         alpha = rhok2 / pAp;
00109
00110         // Save rhok2 for next iteration
00111         rhok1 = rhok2;
00112
00113         // Update solution in direction p of length alpha
00114         Vxaxpy(nx, ny, nz, &alpha, p, x);
00115
00116         // Update residual
00117         alpha = -alpha;
00118         Vxaxpy(nx, ny, nz, &alpha, ap, r);
00119
00120         // some bookkeeping
00121         (*iters)++;
00122     }
00123 }

```

9.123 cgd.h

```

00001
00050 #ifndef _CGD_H_
00051 #define _CGD_H_

```

```

00052
00053 #include "apbscfg.h"
00054
00055 #include "malloc/malloc.h"
00056
00057 #include "generic/vhal.h"
00058 #include "pmgc/matvecd.h"
00059 #include "pmgc/mikpckd.h"
00060
00061 VEXTERNC void Vcghs(
00062     int *nx,
00063     int *ny,
00064     int *nz,
00065     int *ipc,
00066     double *rpc,
00067     double *ac,
00068     double *cc,
00069     double *fc,
00070     double *x,
00071     double *p,
00072     double *ap,
00073     double *r,
00074     int *itmax,
00075     int *iters,
00076     double *errtol,
00077     double *omega,
00078     int *iresid,
00079     int *iadjoint
00080 );
00081
00082 #endif /* _CGD_H_ */

```

9.124 gsd.c

```

00001
00055 #include "gsd.h"
00056
00057 VPUBLIC void Vgsrb(int *nx, int *ny, int *nz,
00058     int *ipc, double *rpc,
00059     double *ac, double *cc, double *fc,
00060     double *x, double *w1, double *w2, double *r,
00061     int *itmax, int *iters,
00062     double *errtol, double *omega,
00063     int *iresid, int *iadjoint) {
00064
00065     int numdia;
00066
00067     MAT2(ac, *nx * *ny * *nz, 1);
00068
00069     // Do in one step ***
00070     numdia = VAT(ipc, 11);
00071     if (numdia == 7) {
00072         Vgsrb7x(nx, ny, nz,
00073             ipc, rpc,
00074             RAT2(ac, 1,1), cc, fc,
00075             RAT2(ac, 1,2), RAT2(ac, 1,3), RAT2(ac, 1,4),
00076             x, w1, w2, r,
00077             itmax, iters, errtol, omega, iresid, iadjoint);
00078     } else if (numdia == 27) {
00079         Vgsrb27x(nx, ny, nz,
00080             ipc, rpc,
00081             RAT2(ac, 1, 1), cc, fc,
00082             RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
00083             RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00084             RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1,10),
00085             RAT2(ac, 1,11), RAT2(ac, 1,12), RAT2(ac, 1,13), RAT2(ac, 1,14),
00086             x, w1, w2, r,
00087             itmax, iters, errtol, omega, iresid, iadjoint);
00088     } else {
00089         Vnm_print(2, "GSRB: invalid stencil type given...\n");
00090     }
00091 }
00092
00093
00094
00095 VPUBLIC void Vgsrb7x(int *nx,int *ny,int *nz,
00096     int *ipc, double *rpc,
00097     double *oC, double *cc, double *fc,

```



```

00098     double *oE, double *oN, double *uC,
00099     double *x, double *w1, double *w2, double *r,
00100     int *itmax, int *iters,
00101     double *errtol, double *omega,
00102     int *iresid, int *iadjoint) {
00103
00104     int i, j, k, ioff;
00105
00106     MAT3(cc, *nx, *ny, *nz);
00107     MAT3(fc, *nx, *ny, *nz);
00108     MAT3( x, *nx, *ny, *nz);
00109     MAT3(w1, *nx, *ny, *nz);
00110     MAT3(w2, *nx, *ny, *nz);
00111     MAT3( r, *nx, *ny, *nz);
00112
00113     MAT3(oE, *nx, *ny, *nz);
00114     MAT3(oN, *nx, *ny, *nz);
00115     MAT3(uC, *nx, *ny, *nz);
00116     MAT3(oC, *nx, *ny, *nz);
00117
00118     for (*iters=1; *iters<=*itmax; (*iters)++) {
00119
00120         // Do the red points ***
00121         #pragma omp parallel for private(i, j, k, ioff)
00122         for (k=2; k<=*nz-1; k++) {
00123             for (j=2; j<=*ny-1; j++) {
00124                 ioff = (1 - *iadjoint) * ( (j + k + 2) % 2)
00125                     + ( *iadjoint) * (1 - (j + k + 2) % 2);
00126                 for (i=2+ioff; i<=*nx-1; i+=2) {
00127                     VAT3(x, i, j, k) = (
00128                         VAT3(fc, i, j, k)
00129                         + VAT3(oN, i, j, k) * VAT3(x, i, j+1, k)
00130                         + VAT3(oN, i, j-1, k) * VAT3(x, i, j-1, k)
00131                         + VAT3(oE, i, j, k) * VAT3(x, i+1, j, k)
00132                         + VAT3(oE, i-1, j, k) * VAT3(x, i-1, j, k)
00133                         + VAT3( uC, i, j, k-1) * VAT3(x, i, j, k-1)
00134                         + VAT3( uC, i, j, k) * VAT3(x, i, j, k+1)
00135                         ) / (VAT3(oC, i, j, k) + VAT3(cc, i, j, k));
00136                 }
00137             }
00138         }
00139
00140         // Do the black points
00141         #pragma omp parallel for private(i, j, k, ioff)
00142         for (k=2; k<=*nz-1; k++) {
00143             for (j=2; j<=*ny-1; j++) {
00144                 ioff = ( *iadjoint) * ( (j + k + 2) % 2)
00145                     + (1 - *iadjoint) * (1 - (j + k + 2) % 2);
00146                 for (i=2+ioff; i<=*nx-1; i+=2) {
00147                     VAT3(x, i, j, k) = (
00148                         VAT3(fc, i, j, k)
00149                         + VAT3(oN, i, j, k) * VAT3(x, i, j+1, k)
00150                         + VAT3(oN, i, j-1, k) * VAT3(x, i, j-1, k)
00151                         + VAT3(oE, i, j, k) * VAT3(x, i+1, j, k)
00152                         + VAT3(oE, i-1, j, k) * VAT3(x, i-1, j, k)
00153                         + VAT3( uC, i, j, k-1) * VAT3(x, i, j, k-1)
00154                         + VAT3( uC, i, j, k) * VAT3(x, i, j, k+1)
00155                         ) / (VAT3(oC, i, j, k) + VAT3(cc, i, j, k));
00156                 }
00157             }
00158         }
00159     }
00160
00161     if (*iresid == 1)
00162         Vmresid7_ls(nx, ny, nz, ipc, rpc, oC, cc, fc, oE, oN, uC, x, r);
00163 }
00164
00165
00166
00167 VPUBLIC void Vgsrb27x(int *nx,int *ny,int *nz,
00168     int *ipc, double *rpc,
00169     double *oC, double *cc, double *fc,
00170     double *oE, double *oN, double *uC, double *oNE, double *oNW,
00171     double *uE, double *uW, double *uN, double *uS,
00172     double *uNE, double *uNW, double *uSE, double *uSW,
00173     double *x, double *w1, double *w2, double *r,
00174     int *itmax, int *iters,
00175     double *errtol, double *omega,
00176     int *iresid, int *iadjoint) {
00177
00178     int i, j, k;

```

```

00179     int i1, j1, k1;
00180     int i2, j2, k2;
00181     int ioff;
00182     int istep;
00183
00184     double tmpO, tmpU, tmpD;
00185
00186     MAT3( cC, *nx, *ny, *nz);
00187     MAT3( fC, *nx, *ny, *nz);
00188     MAT3( x, *nx, *ny, *nz);
00189     MAT3( w1, *nx, *ny, *nz);
00190     MAT3( w2, *nx, *ny, *nz);
00191     MAT3( r, *nx, *ny, *nz);
00192
00193     MAT3( oE, *nx, *ny, *nz);
00194     MAT3( oN, *nx, *ny, *nz);
00195     MAT3( uC, *nx, *ny, *nz);
00196     MAT3( oC, *nx, *ny, *nz);
00197
00198     MAT3( oNE, *nx, *ny, *nz);
00199     MAT3( oNW, *nx, *ny, *nz);
00200
00201     MAT3( uE, *nx, *ny, *nz);
00202     MAT3( uW, *nx, *ny, *nz);
00203     MAT3( uN, *nx, *ny, *nz);
00204     MAT3( uS, *nx, *ny, *nz);
00205     MAT3( uNE, *nx, *ny, *nz);
00206     MAT3( uNW, *nx, *ny, *nz);
00207     MAT3( uSE, *nx, *ny, *nz);
00208     MAT3( uSW, *nx, *ny, *nz);
00209
00210     // Do the gauss-seidel iteration itmax times
00211
00212     /*
00213     i1 = (1 - *iadjoint) * 2 + ( *iadjoint) * (*nx - 1);
00214     i2 = ( *iadjoint) * 2 + (1 - *iadjoint) * (*nx - 1);
00215     j1 = (1 - *iadjoint) * 2 + ( *iadjoint) * (*ny - 1);
00216     j2 = ( *iadjoint) * 2 + (1 - *iadjoint) * (*ny - 1);
00217     k1 = (1 - *iadjoint) * 2 + ( *iadjoint) * (*nz - 1);
00218     k2 = ( *iadjoint) * 2 + (1 - *iadjoint) * (*nz - 1);
00219     istep = ( *iadjoint) * (-1) + (1 - *iadjoint) * (1);
00220     */
00221
00222     i1 = (1-*iadjoint) * 2 + *iadjoint * (*nx-1);
00223     i2 = *iadjoint * 2 + (1-*iadjoint) * (*nx-1);
00224     j1 = (1-*iadjoint) * 2 + *iadjoint * (*ny-1);
00225     j2 = *iadjoint * 2 + (1-*iadjoint) * (*ny-1);
00226     k1 = (1-*iadjoint) * 2 + *iadjoint * (*nz-1);
00227     k2 = *iadjoint * 2 + (1-*iadjoint) * (*nz-1);
00228     istep = *iadjoint*(-1) + (1-*iadjoint)*(1);
00229
00230     for (*iters=1; *iters<=*itmax; (*iters)++) {
00231
00232         // #pragma omp parallel for private(i, j, k, ioff, tmpO, tmpU, tmpD)
00233         for (k=2; k<=*nz-1; k++) {
00234
00235             for (j=2; j<=*ny-1; j++) {
00236
00237                 ioff = (1 - *iadjoint) * ( (j + k + 2) % 2)
00238                     + ( *iadjoint) * (1 - (j + k + 2) % 2);
00239
00240                 for (i=2+ioff; i<=*nx-1; i+=2) {
00241
00242                     tmpO =
00243                         + VAT3( oN, i, j, k) * VAT3(x, i, j+1, k)
00244                         + VAT3( oN, i, j-1, k) * VAT3(x, i, j-1, k)
00245                         + VAT3( oE, i, j, k) * VAT3(x, i+1, j, k)
00246                         + VAT3( oE, i-1, j, k) * VAT3(x, i-1, j, k)
00247                         + VAT3( oNE, i, j, k) * VAT3(x, i+1, j+1, k)
00248                         + VAT3( oNW, i, j, k) * VAT3(x, i-1, j+1, k)
00249                         + VAT3( oNW, i+1, j-1, k) * VAT3(x, i+1, j-1, k)
00250                         + VAT3( oNE, i-1, j-1, k) * VAT3(x, i-1, j-1, k);
00251
00252                     tmpU =
00253                         + VAT3( uC, i, j, k) * VAT3(x, i, j, k+1)
00254                         + VAT3( uN, i, j, k) * VAT3(x, i, j+1, k+1)
00255                         + VAT3( uS, i, j, k) * VAT3(x, i, j-1, k+1)
00256                         + VAT3( uE, i, j, k) * VAT3(x, i+1, j, k+1)
00257                         + VAT3( uW, i, j, k) * VAT3(x, i-1, j, k+1)
00258                         + VAT3( uNE, i, j, k) * VAT3(x, i+1, j+1, k+1)
00259                         + VAT3( uNW, i, j, k) * VAT3(x, i-1, j+1, k+1)

```

```

00260             + VAT3( uSE,  i,  j,  k) * VAT3(x, i+1, j-1, k+1)
00261             + VAT3( uSW,  i,  j,  k) * VAT3(x, i-1, j-1, k+1);
00262
00263         tmpD =
00264             + VAT3( uC,   i,  j, k-1) * VAT3(x,  i,  j, k-1)
00265             + VAT3( uS,   i, j+1, k-1) * VAT3(x,  i, j+1, k-1)
00266             + VAT3( uN,   i, j-1, k-1) * VAT3(x,  i, j-1, k-1)
00267             + VAT3( uW, i+1,  j, k-1) * VAT3(x, i+1,  j, k-1)
00268             + VAT3( uE, i-1,  j, k-1) * VAT3(x, i-1,  j, k-1)
00269             + VAT3( uSW, i+1, j+1, k-1) * VAT3(x, i+1, j+1, k-1)
00270             + VAT3( uSE, i-1, j+1, k-1) * VAT3(x, i-1, j+1, k-1)
00271             + VAT3( uNW, i+1, j-1, k-1) * VAT3(x, i+1, j-1, k-1)
00272             + VAT3( uNE, i-1, j-1, k-1) * VAT3(x, i-1, j-1, k-1);
00273
00274         VAT3(x, i, j, k) = (VAT3(fc, i, j, k) + (tmpO + tmpU + tmpD))
00275             / (VAT3(oC, i, j, k) + VAT3(cc, i, j, k));
00276
00277     }
00278 }
00279 }
00280
00281 // #pragma omp parallel for private(i, j, k, ioff, tmpO, tmpU, tmpD)
00282 for (k=2; k<=nz-1; k++) {
00283
00284     for (j=2; j<=ny-1; j++) {
00285
00286         ioff = ( *iadjoint) * ( (j + k + 2) % 2)
00287             + (1 - *iadjoint) * (1 - (j + k + 2) % 2);
00288
00289         for (i=2+ioff; i<=nx-1; i+=2) {
00290
00291             tmpO =
00292                 + VAT3( oN,  i,  j,  k) * VAT3(x,  i, j+1,  k)
00293                 + VAT3( oN,  i, j-1,  k) * VAT3(x,  i, j-1,  k)
00294                 + VAT3( oE,  i,  j,  k) * VAT3(x, i+1,  j,  k)
00295                 + VAT3( oE, i-1,  j,  k) * VAT3(x, i-1,  j,  k)
00296                 + VAT3( oNE, i,  j,  k) * VAT3(x, i+1, j+1,  k)
00297                 + VAT3( oNW, i,  j,  k) * VAT3(x, i-1, j+1,  k)
00298                 + VAT3( oNW, i+1, j-1,  k) * VAT3(x, i+1, j-1,  k)
00299                 + VAT3( oNE, i-1, j-1,  k) * VAT3(x, i-1, j-1,  k);
00300
00301             tmpU =
00302                 + VAT3( uC,   i,  j,  k) * VAT3(x,  i,  j, k+1)
00303                 + VAT3( uN,   i,  j,  k) * VAT3(x,  i, j+1, k+1)
00304                 + VAT3( uS,   i,  j,  k) * VAT3(x,  i, j-1, k+1)
00305                 + VAT3( uE,   i,  j,  k) * VAT3(x, i+1,  j, k+1)
00306                 + VAT3( uW,   i,  j,  k) * VAT3(x, i-1,  j, k+1)
00307                 + VAT3( uNE,  i,  j,  k) * VAT3(x, i+1, j+1, k+1)
00308                 + VAT3( uNW,  i,  j,  k) * VAT3(x, i-1, j+1, k+1)
00309                 + VAT3( uSE,  i,  j,  k) * VAT3(x, i+1, j-1, k+1)
00310                 + VAT3( uSW,  i,  j,  k) * VAT3(x, i-1, j-1, k+1);
00311
00312             tmpD =
00313                 + VAT3( uC,   i,  j, k-1) * VAT3(x,  i,  j, k-1)
00314                 + VAT3( uS,   i, j+1, k-1) * VAT3(x,  i, j+1, k-1)
00315                 + VAT3( uN,   i, j-1, k-1) * VAT3(x,  i, j-1, k-1)
00316                 + VAT3( uW, i+1,  j, k-1) * VAT3(x, i+1,  j, k-1)
00317                 + VAT3( uE, i-1,  j, k-1) * VAT3(x, i-1,  j, k-1)
00318                 + VAT3( uSW, i+1, j+1, k-1) * VAT3(x, i+1, j+1, k-1)
00319                 + VAT3( uSE, i-1, j+1, k-1) * VAT3(x, i-1, j+1, k-1)
00320                 + VAT3( uNW, i+1, j-1, k-1) * VAT3(x, i+1, j-1, k-1)
00321                 + VAT3( uNE, i-1, j-1, k-1) * VAT3(x, i-1, j-1, k-1);
00322
00323             VAT3(x, i, j, k) = (VAT3(fc, i, j, k) + (tmpO + tmpU + tmpD))
00324                 / (VAT3(oC, i, j, k) + VAT3(cc, i, j, k));
00325         }
00326     }
00327 }
00328 }
00329
00330 // If specified, return the new residual as well
00331 if (*iresid == 1)
00332     Vmresid27_ls(nx, ny, nz,
00333         ipc, rpc,
00334         oC, cc, fc,
00335         oE, oN, uC,
00336         oNE, oNW,
00337         uE, uW, uN, uS,
00338         uNE, uNW, uSE, uSW,
00339         x, r);
00340 }

```

9.125 gsd.h

```

00001
00049 #ifndef _GSD_H_
00050 #define _GSD_H_
00051
00052 #include "apbscfg.h"
00053
00054 #include "malloc/malloc.h"
00055
00056 #include "generic/vhal.h"
00057 #include "generic/vmatrix.h"
00058 #include "pmgc/matvecd.h"
00059
00066 VEXTERNC void Vgsrb(
00067     int    *nx,
00068     int    *ny,
00069     int    *nz,
00070     int    *ipc,
00071     double *rpc,
00072     double *ac,
00073     double *cc,
00074     double *fc,
00075     double *x,
00076     double *w1,
00077     double *w2,
00078     double *r,
00079     int    *itmax,
00080     int    *iters,
00081     double *errtol,
00082     double *omega,
00083     int    *iresid,
00084     int    *iadjoint
00085 );
00086
00087 VEXTERNC void Vgsrb7x(
00088     int    *nx,
00089     int    *ny,
00090     int    *nz,
00091     int    *ipc,
00092     double *rpc,
00093     double *oC,
00094     double *cc,
00095     double *fc,
00096     double *oE,
00097     double *oN,
00098     double *uC,
00099     double *x,
00100     double *w1,
00101     double *w2,
00102     double *r,
00103     int    *itmax,
00104     int    *iters,
00105     double *errtol,
00106     double *omega,
00107     int    *iresid,
00108     int    *iadjoint
00109 );
00110
00111 VEXTERNC void Vgsrb27x(
00112     int *nx,
00113     int *ny,
00114     int *nz,
00115     int *ipc,
00116     double *rpc,
00117     double *oC,
00118     double *cc,
00119     double *fc,
00120     double *oE,
00121     double *oN,
00122     double *uC,
00123     double *oNE,
00124     double *oNW,
00125     double *uE,
00126     double *uW,
00127     double *uN,
00128     double *uS,
00129     double *uNE,
00130     double *uNW,
00131     double *uSE,

```

```

00132         double *uSW,
00133         double *x,
00134         double *w1,
00135         double *w2,
00136         double *r,
00137         int *itmax,
00138         int *iters,
00139         double *errtol,
00140         double *omega,
00141         int *iresid,
00142         int *iadjoint
00143     );
00144
00145
00146 #endif /* _GSD_H_ */

```

9.126 matvecd.c

```

00001
00055 #include "matvecd.h"
00056
00057 VPUBLIC void Vmatvec(int *nx, int *ny, int *nz,
00058                     int *ipc, double *rpc,
00059                     double *ac, double *cc,
00060                     double *x, double *y) {
00061
00062     int numdia;
00063
00064     // Do in one step
00065     numdia = VAT(ipc, 11);
00066
00067     if (numdia == 7) {
00068         Vmatvec7(nx, ny, nz,
00069                 ipc, rpc,
00070                 ac, cc,
00071                 x, y);
00072     } else if (numdia == 27) {
00073         Vmatvec27(nx, ny, nz,
00074                  ipc, rpc,
00075                  ac, cc,
00076                  x, y);
00077     } else {
00078         Vnm_print(2, "MATVEC: invalid stencil type given...");
00079     }
00080 }
00081
00082 VPUBLIC void Vmatvec7(int *nx, int *ny, int *nz,
00083                      int *ipc, double *rpc,
00084                      double *ac, double *cc,
00085                      double *x, double *y) {
00086
00087     MAT2(ac, *nx * *ny * *nz, 1);
00088
00089     Vmatvec7_ls(nx, ny, nz,
00090                 ipc, rpc,
00091                 RAT2(ac, 1, 1), cc,
00092                 RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
00093                 x, y);
00094 }
00095
00096
00097
00098 VEXTERN void Vmatvec7_ls(int *nx, int *ny, int *nz,
00099                          int *ipc, double *rpc,
00100                          double *oC, double *cc,
00101                          double *oE, double *oN, double *uC,
00102                          double *x, double *y) {
00103
00104     int i, j, k;
00105
00106     MAT3(oE, *nx, *ny, *nz);
00107     MAT3(oN, *nx, *ny, *nz);
00108     MAT3(uC, *nx, *ny, *nz);
00109     MAT3(cc, *nx, *ny, *nz);
00110     MAT3(oC, *nx, *ny, *nz);
00111     MAT3(x, *nx, *ny, *nz);
00112     MAT3(y, *nx, *ny, *nz);
00113

```

```

00114 // Do it
00115 #pragma omp parallel for private(i, j, k)
00116 for (k=2; k<=*nz-1; k++) {
00117     for (j=2; j<=*ny-1; j++) {
00118         for (i=2; i<=*nx-1; i++) {
00119             VAT3(y, i, j, k) =
00120                 - VAT3(oN, i, j, k) * VAT3(x, i, j+1, k)
00121                 - VAT3(oN, i, j-1, k) * VAT3(x, i, j-1, k)
00122                 - VAT3(oE, i, j, k) * VAT3(x, i+1, j, k)
00123                 - VAT3(oE, i-1, j, k) * VAT3(x, i-1, j, k)
00124                 - VAT3(uC, i, j, k-1) * VAT3(x, i, j, k-1)
00125                 - VAT3(uC, i, j, k) * VAT3(x, i, j, k+1)
00126                 + (VAT3(oC, i, j, k) + VAT3(cc, i, j, k)) * VAT3(x, i, j, k);
00127         }
00128     }
00129 }
00130 }
00131
00132
00133
00134 VPUBLIC void Vmatvec27(int *nx, int *ny, int *nz,
00135     int *ipc, double *rpc,
00136     double *ac, double *cc,
00137     double *x, double *y) {
00138
00139     MAT2(ac, *nx * *ny * *nz, 1);
00140
00141     Vmatvec27_ls(nx, ny, nz,
00142         ipc, rpc,
00143         RAT2(ac, 1, 1), cc,
00144         RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
00145         RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00146         RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1, 10),
00147         RAT2(ac, 1, 11), RAT2(ac, 1, 12), RAT2(ac, 1, 13), RAT2(ac, 1, 14),
00148         x, y);
00149 }
00150
00151
00152
00153 VPUBLIC void Vmatvec27_ls(int *nx, int *ny, int *nz,
00154     int *ipc, double *rpc,
00155     double *oC, double *cc,
00156     double *oE, double *oN, double *uC,
00157     double *oNE, double *oNW,
00158     double *uE, double *uW, double *uN, double *uS,
00159     double *uNE, double *uNW, double *uSE, double *uSW,
00160     double *x, double *y) {
00161
00162     int i, j, k;
00163
00164     double tmpO, tmpU, tmpD;
00165
00166     MAT3(cc, *nx, *ny, *nz);
00167     MAT3(x, *nx, *ny, *nz);
00168     MAT3(y, *nx, *ny, *nz);
00169
00170     MAT3(oC, *nx, *ny, *nz);
00171     MAT3(oE, *nx, *ny, *nz);
00172     MAT3(oN, *nx, *ny, *nz);
00173     MAT3(oNE, *nx, *ny, *nz);
00174     MAT3(oNW, *nx, *ny, *nz);
00175
00176     MAT3(uC, *nx, *ny, *nz);
00177     MAT3(uE, *nx, *ny, *nz);
00178     MAT3(uW, *nx, *ny, *nz);
00179     MAT3(uN, *nx, *ny, *nz);
00180     MAT3(uS, *nx, *ny, *nz);
00181     MAT3(uNE, *nx, *ny, *nz);
00182     MAT3(uNW, *nx, *ny, *nz);
00183     MAT3(uSE, *nx, *ny, *nz);
00184     MAT3(uSW, *nx, *ny, *nz);
00185
00186 // Do it
00187 #pragma omp parallel for private(i, j, k, tmpO, tmpU, tmpD)
00188 for (k=2; k<=*nz-1; k++) {
00189     for (j=2; j<=*ny-1; j++) {
00190         for (i=2; i<=*nx-1; i++) {
00191             tmpO =
00192                 - VAT3(oN, i, j, k) * VAT3(x, i, j+1, k)
00193                 - VAT3(oN, i, j-1, k) * VAT3(x, i, j-1, k)
00194                 - VAT3(oE, i, j, k) * VAT3(x, i+1, j, k)

```

```

00195         - VAT3( oE, i-1, j, k) * VAT3(x, i-1, j, k)
00196         - VAT3( oNE, i, j, k) * VAT3(x, i+1, j+1, k)
00197         - VAT3( oNW, i, j, k) * VAT3(x, i-1, j+1, k)
00198         - VAT3( oNW, i+1, j-1, k) * VAT3(x, i+1, j-1, k)
00199         - VAT3( oNE, i-1, j-1, k) * VAT3(x, i-1, j-1, k);
00200
00201     tmpU =
00202         - VAT3( uC, i, j, k) * VAT3(x, i, j, k+1)
00203         - VAT3( uN, i, j, k) * VAT3(x, i, j+1, k+1)
00204         - VAT3( uS, i, j, k) * VAT3(x, i, j-1, k+1)
00205         - VAT3( uE, i, j, k) * VAT3(x, i+1, j, k+1)
00206         - VAT3( uW, i, j, k) * VAT3(x, i-1, j, k+1)
00207         - VAT3( uNE, i, j, k) * VAT3(x, i+1, j+1, k+1)
00208         - VAT3( uNW, i, j, k) * VAT3(x, i-1, j+1, k+1)
00209         - VAT3( uSE, i, j, k) * VAT3(x, i+1, j-1, k+1)
00210         - VAT3( uSW, i, j, k) * VAT3(x, i-1, j-1, k+1);
00211
00212     tmpD =
00213         - VAT3( uC, i, j, k-1) * VAT3(x, i, j, k-1)
00214         - VAT3( uS, i, j+1, k-1) * VAT3(x, i, j+1, k-1)
00215         - VAT3( uN, i, j-1, k-1) * VAT3(x, i, j-1, k-1)
00216         - VAT3( uW, i+1, j, k-1) * VAT3(x, i+1, j, k-1)
00217         - VAT3( uE, i-1, j, k-1) * VAT3(x, i-1, j, k-1)
00218         - VAT3( uSW, i+1, j+1, k-1) * VAT3(x, i+1, j+1, k-1)
00219         - VAT3( uSE, i-1, j+1, k-1) * VAT3(x, i-1, j+1, k-1)
00220         - VAT3( uNW, i+1, j-1, k-1) * VAT3(x, i+1, j-1, k-1)
00221         - VAT3( uNE, i-1, j-1, k-1) * VAT3(x, i-1, j-1, k-1);
00222
00223     VAT3(y, i, j, k) = tmpO + tmpU + tmpD
00224         + (VAT3(oC, i, j, k) + VAT3(cc, i, j, k)) * VAT3(x, i, j, k);
00225     }
00226 }
00227 }
00228 }
00229
00230
00231
00232 VEXTERNC void Vnmatvec(int *nx, int *ny, int *nz,
00233     int *ipc, double *rpc,
00234     double *ac, double *cc, double *x, double *y, double *w1) {
00235
00236     int numdia;
00237
00238     // Do in one step
00239     numdia = VAT(ipc, 11);
00240
00241     if (numdia == 7) {
00242         Vnmatvec7(nx, ny, nz,
00243             ipc, rpc,
00244             ac, cc,
00245             x, y, w1);
00246     } else if (numdia == 27) {
00247         Vnmatvec27(nx, ny, nz,
00248             ipc, rpc,
00249             ac, cc,
00250             x, y, w1);
00251     } else {
00252         Vnm_print(2, "MATVEC: invalid stencil type given...");
00253     }
00254 }
00255
00256
00257
00258 VPUBLIC void Vnmatvec7(int *nx, int *ny, int *nz,
00259     int *ipc, double *rpc,
00260     double *ac, double *cc,
00261     double *x, double *y, double *w1) {
00262
00263     MAT2(ac, *nx * *ny * *nz, 1);
00264
00265     WARN_UNTESTED;
00266
00267     Vnmatvecd7_ls(nx, ny, nz,
00268         ipc, rpc,
00269         RAT2(ac, 1, 1), cc,
00270         RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
00271         x, y, w1);
00272 }
00273
00274
00275

```

```

00276 VPUBLIC void Vnmatvecd7_ls(int *nx, int *ny, int *nz,
00277     int *ipc, double *rpc,
00278     double *oC, double *cc,
00279     double *oE, double *oN, double *uC,
00280     double *x, double *y, double *w1) {
00281
00282     int i, j, k;
00283     int ipkey;
00284
00285     MAT3(oE, *nx, *ny, *nz);
00286     MAT3(oN, *nx, *ny, *nz);
00287     MAT3(uC, *nx, *ny, *nz);
00288     MAT3(cc, *nx, *ny, *nz);
00289     MAT3(oC, *nx, *ny, *nz);
00290     MAT3( x, *nx, *ny, *nz);
00291     MAT3( y, *nx, *ny, *nz);
00292     MAT3(w1, *nx, *ny, *nz);
00293
00294     WARN_UNTESTED;
00295
00296     // first get vector nonlinear term to avoid subroutine calls
00297     ipkey = VAT(ipc, 10);
00298     Vc_vec(cc, x, w1, nx, ny, nz, &ipkey);
00299
00300     // The operator
00301     #pragma omp parallel for private(i, j, k)
00302     for (k=2; k<=*nz-1; k++)
00303         for (j=2; j<=*ny-1; j++)
00304             for (i=2; i<=*nx-1; i++)
00305                 VAT3(y, i, j, k) =
00306                     - VAT3(oN, i, j, k) * VAT3(x, i, j+1, k)
00307                     - VAT3(oN, i, j-1, k) * VAT3(x, i, j-1, k)
00308                     - VAT3(oE, i, j, k) * VAT3(x, i+1, j, k)
00309                     - VAT3(oE, i-1, j, k) * VAT3(x, i-1, j, k)
00310                     - VAT3(uC, i, j, k-1) * VAT3(x, i, j, k-1)
00311                     - VAT3(uC, i, j, k) * VAT3(x, i, j, k+1)
00312                     + VAT3(oC, i, j, k) * VAT3(x, i, j, k)
00313                     + VAT3(w1, i, j, k);
00314 }
00315
00316
00317 VPUBLIC void Vnmatvec27(int *nx, int *ny, int *nz,
00318     int *ipc, double *rpc,
00319     double *ac, double *cc,
00320     double *x, double *y, double *w1) {
00321
00322     MAT2(ac, *nx * *ny * *nz, 1);
00323
00324     WARN_UNTESTED;
00325
00326     // Do in one step
00327     Vnmatvecd27_ls(nx, ny, nz,
00328         ipc, rpc,
00329         RAT2(ac, 1, 1), cc,
00330         RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
00331         RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00332         RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1,10),
00333         RAT2(ac, 1,11), RAT2(ac, 1,12), RAT2(ac, 1,13), RAT2(ac, 1,14),
00334         x, y, w1);
00335 }
00336
00337
00338
00339 VPUBLIC void Vnmatvecd27_ls(int *nx, int *ny, int *nz,
00340     int *ipc, double *rpc,
00341     double *oC, double *cc,
00342     double *oE, double *oN, double *uC,
00343     double *oNE, double *oNW,
00344     double *uE, double *uW, double *uN, double *uS,
00345     double *uNE, double *uNW, double *uSE, double *uSW,
00346     double *x, double *y, double *w1) {
00347
00348     int i, j, k;
00349     int ipkey;
00350
00351     double tmpO, tmpU, tmpD;
00352
00353     MAT3( oE, *nx, *ny, *nz);
00354     MAT3( oN, *nx, *ny, *nz);
00355     MAT3( uC, *nx, *ny, *nz);
00356     MAT3(oNE, *nx, *ny, *nz);

```



```

00357     MAT3(oNW, *nx, *ny, *nz);
00358     MAT3( uE, *nx, *ny, *nz);
00359     MAT3( uW, *nx, *ny, *nz);
00360     MAT3( uN, *nx, *ny, *nz);
00361     MAT3( uS, *nx, *ny, *nz);
00362     MAT3(uNE, *nx, *ny, *nz);
00363     MAT3(uNW, *nx, *ny, *nz);
00364     MAT3(uSE, *nx, *ny, *nz);
00365     MAT3(uSW, *nx, *ny, *nz);
00366     MAT3( cc, *nx, *ny, *nz);
00367     MAT3( oC, *nx, *ny, *nz);
00368     MAT3( x, *nx, *ny, *nz);
00369     MAT3( y, *nx, *ny, *nz);
00370     MAT3( w1, *nx, *ny, *nz);
00371
00372     WARN_UNTESTED;
00373
00374     // First get vector noNlinear term to avoid subroutine calls
00375     ipkey = VAT(ipc, 10);
00376     Vc_vec(cc, x, w1, nx, ny, nz, &ipkey);
00377
00378     // The operator
00379     #pragma omp parallel for private(i, j, k, tmpO, tmpU, tmpD)
00380     for (k=2; k<=*nz-1; k++) {
00381         for (j=2; j<=*ny-1; j++) {
00382             for(i=2; i<=*nx-1; i++) {
00383
00384                 tmpO =
00385                 - VAT3( oN, i, j, k) * VAT3(x, i, j+1, k)
00386                 - VAT3( oN, i, j-1, k) * VAT3(x, i, j-1, k)
00387                 - VAT3( oE, i, j, k) * VAT3(x, i+1, j, k)
00388                 - VAT3( oE, i-1, j, k) * VAT3(x, i-1, j, k)
00389                 - VAT3( oNE, i, j, k) * VAT3(x, i+1, j+1, k)
00390                 - VAT3( oNW, i, j, k) * VAT3(x, i-1, j+1, k)
00391                 - VAT3( oNW, i+1, j-1, k) * VAT3(x, i+1, j-1, k)
00392                 - VAT3( oNE, i-1, j-1, k) * VAT3(x, i-1, j-1, k);
00393
00394                 tmpU =
00395                 - VAT3( uC, i, j, k) * VAT3(x, i, j, k+1)
00396                 - VAT3( uN, i, j, k) * VAT3(x, i, j+1, k+1)
00397                 - VAT3( uS, i, j, k) * VAT3(x, i, j-1, k+1)
00398                 - VAT3( uE, i, j, k) * VAT3(x, i+1, j, k+1)
00399                 - VAT3( uW, i, j, k) * VAT3(x, i-1, j, k+1)
00400                 - VAT3( uNE, i, j, k) * VAT3(x, i+1, j+1, k+1)
00401                 - VAT3( uNW, i, j, k) * VAT3(x, i-1, j+1, k+1)
00402                 - VAT3( uSE, i, j, k) * VAT3(x, i+1, j-1, k+1)
00403                 - VAT3( uSW, i, j, k) * VAT3(x, i-1, j-1, k+1);
00404
00405                 tmpD =
00406                 - VAT3( uC, i, j, k-1) * VAT3(x, i, j, k-1)
00407                 - VAT3( uS, i, j+1, k-1) * VAT3(x, i, j+1, k-1)
00408                 - VAT3( uN, i, j-1, k-1) * VAT3(x, i, j-1, k-1)
00409                 - VAT3( uW, i+1, j, k-1) * VAT3(x, i+1, j, k-1)
00410                 - VAT3( uE, i-1, j, k-1) * VAT3(x, i-1, j, k-1)
00411                 - VAT3( uSW, i+1, j+1, k-1) * VAT3(x, i+1, j+1, k-1)
00412                 - VAT3( uSE, i-1, j+1, k-1) * VAT3(x, i-1, j+1, k-1)
00413                 - VAT3( uNW, i+1, j-1, k-1) * VAT3(x, i+1, j-1, k-1)
00414                 - VAT3( uNE, i-1, j-1, k-1) * VAT3(x, i-1, j-1, k-1);
00415
00416                 VAT3(y, i, j, k) = tmpO + tmpU + tmpD
00417                 + VAT3(oC, i, j, k) * VAT3(x, i, j, k)
00418                 + VAT3(w1, i, j, k);
00419             }
00420         }
00421     }
00422 }
00423
00424
00425
00426 VPUBLIC void Vmresid(int *nx, int *ny, int *nz,
00427     int *ipc, double *rpc,
00428     double *ac, double *cc, double *fc,
00429     double *x, double *r) {
00430
00431     int numdia;
00432
00433     // Do in one step
00434     numdia = VAT(ipc, 11);
00435     if (numdia == 7) {
00436         Vmresid7(nx, ny, nz, ipc, rpc, ac, cc, fc, x, r);
00437     } else if (numdia == 27) {

```

```

00438     Vmresid27(nx, ny, nz, ipc, rpc, ac, cc, fc, x, r);
00439 } else {
00440     Vnm_print(2, "Vmresid: invalid stencil type given...\n");
00441 }
00442 }
00443
00444
00445
00446 VPUBLIC void Vmresid7(int *nx, int *ny, int *nz,
00447     int *ipc, double *rpc,
00448     double *ac, double *cc, double *fc,
00449     double *x, double *r) {
00450
00451     MAT2(ac, *nx * *ny * *nz, 1);
00452
00453     // Do in one step
00454     Vmresid7_ls(nx, ny, nz,
00455         ipc, rpc,
00456         RAT2(ac, 1,1), cc, fc,
00457         RAT2(ac, 1,2), RAT2(ac, 1,3), RAT2(ac, 1,4),
00458         x,r);
00459 }
00460
00461 VPUBLIC void Vmresid7_ls(int *nx, int *ny, int *nz,
00462     int *ipc, double *rpc,
00463     double *oC, double *cc, double *fc,
00464     double *oE, double *oN, double *uC,
00465     double *x, double *r) {
00466
00467     int i, j, k;
00468
00469     MAT3(oE, *nx, *ny, *nz);
00470     MAT3(oN, *nx, *ny, *nz);
00471     MAT3(uC, *nx, *ny, *nz);
00472     MAT3(cc, *nx, *ny, *nz);
00473     MAT3(fc, *nx, *ny, *nz);
00474     MAT3(oC, *nx, *ny, *nz);
00475     MAT3(x, *nx, *ny, *nz);
00476     MAT3(r, *nx, *ny, *nz);
00477
00478     // Do it
00479     #pragma omp parallel for private(i, j, k)
00480     for (k=2; k<=*nz-1; k++) {
00481         for (j=2; j<=*ny-1; j++) {
00482             for (i=2; i<=*nx-1; i++) {
00483                 VAT3(r, i, j, k) = VAT3(fc, i, j, k)
00484                     + VAT3(oN, i, j, k) * VAT3(x, i, j+1, k)
00485                     + VAT3(oN, i, j-1, k) * VAT3(x, i, j-1, k)
00486                     + VAT3(oE, i, j, k) * VAT3(x, i+1, j, k)
00487                     + VAT3(oE, i-1, j, k) * VAT3(x, i-1, j, k)
00488                     + VAT3(uC, i, j, k-1) * VAT3(x, i, j, k-1)
00489                     + VAT3(uC, i, j, k) * VAT3(x, i, j, k+1)
00490                     - (VAT3(oC, i, j, k) + VAT3(cc, i, j, k)) * VAT3(x, i, j, k);
00491             }
00492         }
00493     }
00494 }
00495
00496
00497
00498 VPUBLIC void Vmresid27(int *nx, int *ny, int *nz,
00499     int *ipc, double *rpc,
00500     double *ac, double *cc, double *fc,
00501     double *x, double *r) {
00502
00503     MAT2(ac, *nx * *ny * *nz, 1);
00504
00505     // Do in one step
00506     Vmresid27_ls(nx, ny, nz,
00507         ipc, rpc,
00508         RAT2(ac, 1, 1), cc, fc,
00509         RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
00510         RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00511         RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1,10),
00512         RAT2(ac, 1,11), RAT2(ac, 1,12), RAT2(ac, 1,13), RAT2(ac, 1,14),
00513         x,r);
00514 }
00515
00516
00517
00518 VPUBLIC void Vmresid27_ls(int *nx, int *ny, int *nz,

```

```

00519     int *ipc, double *rpc,
00520     double *oC, double *cc, double *fc,
00521     double *oE, double *oN, double *uC,
00522     double *oNE, double *oNW,
00523     double *uE, double *uW, double *uN, double *uS,
00524     double *uNE, double *uNW, double *uSE, double *uSW,
00525     double *x, double *r) {
00526
00527     int i, j, k;
00528
00529     double tmpO, tmpU, tmpD;
00530
00531     MAT3(cc, *nx, *ny, *nz);
00532     MAT3(fc, *nx, *ny, *nz);
00533     MAT3(x, *nx, *ny, *nz);
00534     MAT3(r, *nx, *ny, *nz);
00535
00536     MAT3(oC, *nx, *ny, *nz);
00537     MAT3(oE, *nx, *ny, *nz);
00538     MAT3(oN, *nx, *ny, *nz);
00539     MAT3(oNE, *nx, *ny, *nz);
00540     MAT3(oNW, *nx, *ny, *nz);
00541
00542     MAT3(uC, *nx, *ny, *nz);
00543     MAT3(uE, *nx, *ny, *nz);
00544     MAT3(uW, *nx, *ny, *nz);
00545     MAT3(uN, *nx, *ny, *nz);
00546     MAT3(uS, *nx, *ny, *nz);
00547     MAT3(uNE, *nx, *ny, *nz);
00548     MAT3(uNW, *nx, *ny, *nz);
00549     MAT3(uSE, *nx, *ny, *nz);
00550     MAT3(uSW, *nx, *ny, *nz);
00551
00552     #pragma omp parallel for private(i, j, k, tmpO, tmpU, tmpD)
00553     for (k=2; k<=*nz-1; k++) {
00554         for (j=2; j<=*ny-1; j++) {
00555             for (i=2; i<=*nx-1; i++) {
00556
00557                 tmpO =
00558                     + VAT3( oN, i, j, k) * VAT3(x, i, j+1, k)
00559                     + VAT3( oN, i, j-1, k) * VAT3(x, i, j-1, k)
00560                     + VAT3( oE, i, j, k) * VAT3(x, i+1, j, k)
00561                     + VAT3( oE, i-1, j, k) * VAT3(x, i-1, j, k)
00562                     + VAT3( oNE, i, j, k) * VAT3(x, i+1, j+1, k)
00563                     + VAT3( oNW, i, j, k) * VAT3(x, i-1, j+1, k)
00564                     + VAT3( oNW, i+1, j-1, k) * VAT3(x, i+1, j-1, k)
00565                     + VAT3( oNE, i-1, j-1, k) * VAT3(x, i-1, j-1, k);
00566
00567                 tmpU =
00568                     + VAT3( uC, i, j, k) * VAT3(x, i, j, k+1)
00569                     + VAT3( uN, i, j, k) * VAT3(x, i, j+1, k+1)
00570                     + VAT3( uS, i, j, k) * VAT3(x, i, j-1, k+1)
00571                     + VAT3( uE, i, j, k) * VAT3(x, i+1, j, k+1)
00572                     + VAT3( uW, i, j, k) * VAT3(x, i-1, j, k+1)
00573                     + VAT3( uNE, i, j, k) * VAT3(x, i+1, j+1, k+1)
00574                     + VAT3( uNW, i, j, k) * VAT3(x, i-1, j+1, k+1)
00575                     + VAT3( uSE, i, j, k) * VAT3(x, i+1, j-1, k+1)
00576                     + VAT3( uSW, i, j, k) * VAT3(x, i-1, j-1, k+1);
00577
00578                 tmpD =
00579                     + VAT3( uC, i, j, k-1) * VAT3(x, i, j, k-1)
00580                     + VAT3( uS, i, j+1, k-1) * VAT3(x, i, j+1, k-1)
00581                     + VAT3( uN, i, j-1, k-1) * VAT3(x, i, j-1, k-1)
00582                     + VAT3( uW, i+1, j, k-1) * VAT3(x, i+1, j, k-1)
00583                     + VAT3( uE, i-1, j, k-1) * VAT3(x, i-1, j, k-1)
00584                     + VAT3( uSW, i+1, j+1, k-1) * VAT3(x, i+1, j+1, k-1)
00585                     + VAT3( uSE, i-1, j+1, k-1) * VAT3(x, i-1, j+1, k-1)
00586                     + VAT3( uNW, i+1, j-1, k-1) * VAT3(x, i+1, j-1, k-1)
00587                     + VAT3( uNE, i-1, j-1, k-1) * VAT3(x, i-1, j-1, k-1);
00588
00589                 VAT3(r, i, j, k) = VAT3(fc, i, j, k) + tmpO + tmpU + tmpD
00590                     - (VAT3(oC, i, j, k) + VAT3(cc, i, j, k)) * VAT3(x, i, j, k);
00591             }
00592         }
00593     }
00594 }
00595
00596
00597
00598 VPUBLIC void Vnmresid(int *nx, int *ny, int *nz,
00599     int *ipc, double *rpc,

```

```

00600         double *ac, double *cc, double *fc,
00601         double *x, double *r, double *w1) {
00602
00603     int numdia;
00604
00605     // Do in oNe step ***
00606     numdia = VAT(ipc, 11);
00607     if (numdia == 7) {
00608         Vnmresid7(nx, ny, nz, ipc, rpc, ac, cc, fc, x, r, w1);
00609     } else if (numdia == 27) {
00610         Vnmresid27(nx, ny, nz, ipc, rpc, ac, cc, fc, x, r, w1);
00611     } else {
00612         Vnm_print(2, "Vnmresid: invalid stencil type given...\n");
00613     }
00614 }
00615
00616
00617
00618 VPUBLIC void Vnmresid7(int *nx, int *ny, int *nz,
00619 int *ipc, double *rpc,
00620 double *ac, double *cc, double *fc,
00621 double *x, double *r, double *w1) {
00622
00623     MAT2(ac, *nx * *ny * *nz, 1);
00624
00625     // Do in oNe step
00626     Vnmresid7_ls(nx, ny, nz,
00627         ipc, rpc,
00628         RAT2(ac, 1, 1), cc, fc,
00629         RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
00630         x, r, w1);
00631 }
00632
00633 VPUBLIC void Vnmresid7_ls(int *nx, int *ny, int *nz,
00634 int *ipc, double *rpc,
00635 double *oC, double *cc, double *fc,
00636 double *oE, double *oN, double *uC,
00637 double *x, double *r, double *w1) {
00638
00639     int i, j, k;
00640     int ipkey;
00641
00642     MAT3(oE, *nx, *ny, *nz);
00643     MAT3(oN, *nx, *ny, *nz);
00644     MAT3(uC, *nx, *ny, *nz);
00645     MAT3(cc, *nx, *ny, *nz);
00646     MAT3(fc, *nx, *ny, *nz);
00647     MAT3(oC, *nx, *ny, *nz);
00648     MAT3(x, *nx, *ny, *nz);
00649     MAT3(r, *nx, *ny, *nz);
00650     MAT3(w1, *nx, *ny, *nz);
00651
00652     // First get vector nonlinear term to avoid subroutine calls
00653     ipkey = VAT(ipc, 10);
00654     Vc_vec(cc, x, w1, nx, ny, nz, &ipkey);
00655
00656     // The residual
00657     for (k=2; k<=*nz-1; k++) {
00658         for (j=2; j<=*ny-1; j++) {
00659             for (i=2; i<=*nx-1; i++) {
00660                 VAT3(r, i, j, k) = VAT3(fc, i, j, k)
00661                     + VAT3(oN, i, j, k) * VAT3(x, i, j+1, k)
00662                     + VAT3(oN, i, j-1, k) * VAT3(x, i, j-1, k)
00663                     + VAT3(oE, i, j, k) * VAT3(x, i+1, j, k)
00664                     + VAT3(oE, i-1, j, k) * VAT3(x, i-1, j, k)
00665                     + VAT3(uC, i, j, k-1) * VAT3(x, i, j, k-1)
00666                     + VAT3(uC, i, j, k) * VAT3(x, i, j, k+1)
00667                     - VAT3(oC, i, j, k) * VAT3(x, i, j, k)
00668                     - VAT3(w1, i, j, k);
00669             }
00670         }
00671     }
00672 }
00673
00674
00675
00676 VPUBLIC void Vnmresid27(int *nx, int *ny, int *nz,
00677 int *ipc, double *rpc,
00678 double *ac, double *cc, double *fc,
00679 double *x, double *r, double *w1) {
00680

```

```

00681     MAT2(ac, *nx * *ny * *nz, 1);
00682
00683     // Do in oNe step
00684     Vnmresid27_ls(nx, ny, nz,
00685         ipc, rpc,
00686         RAT2(ac, 1, 1), cc, fc,
00687         RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
00688         RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00689         RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1, 10),
00690         RAT2(ac, 1, 11), RAT2(ac, 1, 12), RAT2(ac, 1, 13), RAT2(ac, 1, 14),
00691         x, r, wl);
00692 }
00693
00694
00695
00696 VPUBLIC void Vnmresid27_ls(int *nx, int *ny, int *nz,
00697     int *ipc, double *rpc,
00698     double *oC, double *cc, double *fc,
00699     double *oE, double *oN, double *uC,
00700     double *oNE, double *oNW,
00701     double *uE, double *uW, double *uN, double *uS,
00702     double *uNE, double *uNW, double *uSE, double *uSW,
00703     double *x, double *r, double *wl) {
00704
00705     int i, j, k;
00706     int ipkey;
00707     double tmpO, tmpU, tmpD;
00708
00709     MAT3( oC, *nx, *ny, *nz);
00710     MAT3( cc, *nx, *ny, *nz);
00711     MAT3( fc, *nx, *ny, *nz);
00712     MAT3( oE, *nx, *ny, *nz);
00713     MAT3( oN, *nx, *ny, *nz);
00714     MAT3( uC, *nx, *ny, *nz);
00715     MAT3( oNE, *nx, *ny, *nz);
00716     MAT3( oNW, *nx, *ny, *nz);
00717     MAT3( uE, *nx, *ny, *nz);
00718     MAT3( uW, *nx, *ny, *nz);
00719     MAT3( uN, *nx, *ny, *nz);
00720     MAT3( uS, *nx, *ny, *nz);
00721     MAT3( uNE, *nx, *ny, *nz);
00722     MAT3( uNW, *nx, *ny, *nz);
00723     MAT3( uSE, *nx, *ny, *nz);
00724     MAT3( uSW, *nx, *ny, *nz);
00725     MAT3( x, *nx, *ny, *nz);
00726     MAT3( r, *nx, *ny, *nz);
00727     MAT3( wl, *nx, *ny, *nz);
00728
00729     // First get vector noNlinear term to avoid subroutine calls
00730     ipkey = VAT(ipc, 10);
00731     Vc_vec(cc, x, wl, nx, ny, nz, &ipkey);
00732
00733     // The residual
00734     for (k=2; k<=*nz-1; k++) {
00735         for (j=2; j<=*ny-1; j++) {
00736             for (i=2; i<=*nx-1; i++) {
00737
00738                 tmpO =
00739                     + VAT3( oN, i, j, k) * VAT3(x, i, j+1, k)
00740                     + VAT3( oN, i, j-1, k) * VAT3(x, i, j-1, k)
00741                     + VAT3( oE, i, j, k) * VAT3(x, i+1, j, k)
00742                     + VAT3( oE, i-1, j, k) * VAT3(x, i-1, j, k)
00743                     + VAT3( oNE, i, j, k) * VAT3(x, i+1, j+1, k)
00744                     + VAT3( oNW, i, j, k) * VAT3(x, i-1, j+1, k)
00745                     + VAT3( oNW, i+1, j-1, k) * VAT3(x, i+1, j-1, k)
00746                     + VAT3( oNE, i-1, j-1, k) * VAT3(x, i-1, j-1, k);
00747
00748                 tmpU =
00749                     + VAT3( uC, i, j, k) * VAT3(x, i, j, k+1)
00750                     + VAT3( uN, i, j, k) * VAT3(x, i, j+1, k+1)
00751                     + VAT3( uS, i, j, k) * VAT3(x, i, j-1, k+1)
00752                     + VAT3( uE, i, j, k) * VAT3(x, i+1, j, k+1)
00753                     + VAT3( uW, i, j, k) * VAT3(x, i-1, j, k+1)
00754                     + VAT3( uNE, i, j, k) * VAT3(x, i+1, j+1, k+1)
00755                     + VAT3( uNW, i, j, k) * VAT3(x, i-1, j+1, k+1)
00756                     + VAT3( uSE, i, j, k) * VAT3(x, i+1, j-1, k+1)
00757                     + VAT3( uSW, i, j, k) * VAT3(x, i-1, j-1, k+1);
00758
00759                 tmpD =
00760                     + VAT3( uC, i, j, k-1) * VAT3(x, i, j, k-1)
00761                     + VAT3( uS, i, j+1, k-1) * VAT3(x, i, j+1, k-1)

```

```

00762         + VAT3( uN, i, j-1, k-1) * VAT3(x, i, j-1, k-1)
00763         + VAT3( uW, i+1, j, k-1) * VAT3(x, i+1, j, k-1)
00764         + VAT3( uE, i-1, j, k-1) * VAT3(x, i-1, j, k-1)
00765         + VAT3( uSW, i+1, j+1, k-1) * VAT3(x, i+1, j+1, k-1)
00766         + VAT3( uSE, i-1, j+1, k-1) * VAT3(x, i-1, j+1, k-1)
00767         + VAT3( uNW, i+1, j-1, k-1) * VAT3(x, i+1, j-1, k-1)
00768         + VAT3( uNE, i-1, j-1, k-1) * VAT3(x, i-1, j-1, k-1);
00769
00770     VAT3(r, i, j, k) =
00771         + tmpO + tmpU + tmpD
00772         + VAT3(fc, i, j, k)
00773         - VAT3(oC, i, j, k) * VAT3(x, i, j, k)
00774         - VAT3(w1, i, j, k);
00775     }
00776 }
00777 }
00778 }
00779
00780
00781
00782 VPUBLIC void Vrestrc(int *nxf, int *nyf, int *nzf,
00783     int *nxc, int *nyc, int *nzc,
00784     double *xin, double *xout, double *pc) {
00785
00786     MAT2(pc, *nxc * *nyc * *nzc, 1 );
00787
00788     Vrestrc2(nxf, nyf, nzf,
00789         nxc, nyc, nzc,
00790         xin, xout,
00791         RAT2(pc, 1, 1), RAT2(pc, 1, 2), RAT2(pc, 1, 3), RAT2(pc, 1, 4), RAT2(pc, 1, 5),
00792         RAT2(pc, 1, 6), RAT2(pc, 1, 7), RAT2(pc, 1, 8), RAT2(pc, 1, 9),
00793         RAT2(pc, 1,10), RAT2(pc, 1,11), RAT2(pc, 1,12), RAT2(pc, 1,13), RAT2(pc, 1,14),
00794         RAT2(pc, 1,15), RAT2(pc, 1,16), RAT2(pc, 1,17), RAT2(pc, 1,18),
00795         RAT2(pc, 1,19), RAT2(pc, 1,20), RAT2(pc, 1,21), RAT2(pc, 1,22), RAT2(pc, 1,23),
00796         RAT2(pc, 1,24), RAT2(pc, 1,25), RAT2(pc, 1,26), RAT2(pc, 1,27));
00797 }
00798
00799
00800
00801 VEXTERNC void Vrestrc2(int *nxf, int *nyf, int *nzf,
00802     int *nxc, int *nyc, int *nzc,
00803     double *xin, double *xout,
00804     double *oPC, double *oPN, double *oPS, double *oPE, double *oPW,
00805     double *oPNE, double *oPNW, double *oPSE, double *oPSW,
00806     double *uPC, double *uPN, double *uPS, double *uPE, double *uPW,
00807     double *uPNE, double *uPNW, double *uPSE, double *uPSW,
00808     double *dPC, double *dPN, double *dPS, double *dPE, double *dPW,
00809     double *dPNE, double *dPNW, double *dPSE, double *dPSW) {
00810
00811     int i, j, k;
00812     int ii, jj, kk;
00813     int idimenshun = 3;
00814
00815     double tmpO, tmpU, tmpD;
00816     double dimfac;
00817
00818     MAT3(xin, *nxf, *nyf, *nzf);
00819     MAT3(xout, *nxc, *nyc, *nzc);
00820
00821     MAT3(oPC, *nxc, *nyc, *nzc);
00822     MAT3(oPN, *nxc, *nyc, *nzc);
00823     MAT3(oPS, *nxc, *nyc, *nzc);
00824     MAT3(oPE, *nxc, *nyc, *nzc);
00825     MAT3(oPW, *nxc, *nyc, *nzc);
00826
00827     MAT3(oPNE, *nxc, *nyc, *nzc);
00828     MAT3(oPNW, *nxc, *nyc, *nzc);
00829     MAT3(oPSE, *nxc, *nyc, *nzc);
00830     MAT3(oPSW, *nxc, *nyc, *nzc);
00831
00832     MAT3(uPC, *nxc, *nyc, *nzc);
00833     MAT3(uPN, *nxc, *nyc, *nzc);
00834     MAT3(uPS, *nxc, *nyc, *nzc);
00835     MAT3(uPE, *nxc, *nyc, *nzc);
00836     MAT3(uPW, *nxc, *nyc, *nzc);
00837
00838     MAT3(uPNE, *nxc, *nyc, *nzc);
00839     MAT3(uPNW, *nxc, *nyc, *nzc);
00840     MAT3(uPSE, *nxc, *nyc, *nzc);
00841     MAT3(uPSW, *nxc, *nyc, *nzc);
00842

```

```

00843     MAT3(dPC, *nxc, *nyc, *nzc);
00844     MAT3(dPN, *nxc, *nyc, *nzc);
00845     MAT3(dPS, *nxc, *nyc, *nzc);
00846     MAT3(dPE, *nxc, *nyc, *nzc);
00847     MAT3(dPW, *nxc, *nyc, *nzc);
00848
00849     MAT3(dPNE, *nxc, *nyc, *nzc);
00850     MAT3(dPNW, *nxc, *nyc, *nzc);
00851     MAT3(dPSE, *nxc, *nyc, *nzc);
00852     MAT3(dPSW, *nxc, *nyc, *nzc);
00853
00854     // Verify correctness of the input boundary points
00855     VfboundPMG00(nxf, nyf, nzf, xin);
00856
00857     dimfac = VPOW(2.0, idimenshun);
00858
00859     // Handle the interior points as average of 5 finer grid pts ***
00860     #pragma omp parallel for private(k, kk, j, jj, i, ii, tmpO, tmpU, tmpD)
00861     for (k=2; k<=*nzc-1; k++) {
00862         kk = (k - 1) * 2 + 1;
00863
00864         for (j=2; j<=*nyc-1; j++) {
00865             jj = (j - 1) * 2 + 1;
00866
00867             for (i=2; i<=*nxc-1; i++) {
00868                 ii = (i - 1) * 2 + 1;
00869
00870                 // Compute the restriction
00871                 tmpO =
00872                     + VAT3( oPC, i, j, k) * VAT3(xin, ii, jj, kk)
00873                     + VAT3( oPN, i, j, k) * VAT3(xin, ii, jj+1, kk)
00874                     + VAT3( oPS, i, j, k) * VAT3(xin, ii, jj-1, kk)
00875                     + VAT3( oPE, i, j, k) * VAT3(xin, ii+1, jj, kk)
00876                     + VAT3( oPW, i, j, k) * VAT3(xin, ii-1, jj, kk)
00877                     + VAT3( oPNE, i, j, k) * VAT3(xin, ii+1, jj+1, kk)
00878                     + VAT3( oPNW, i, j, k) * VAT3(xin, ii-1, jj+1, kk)
00879                     + VAT3( oPSE, i, j, k) * VAT3(xin, ii+1, jj-1, kk)
00880                     + VAT3( oPSW, i, j, k) * VAT3(xin, ii-1, jj-1, kk);
00881
00882                 tmpU =
00883                     + VAT3( uPC, i, j, k) * VAT3(xin, ii, jj, kk+1)
00884                     + VAT3( uPN, i, j, k) * VAT3(xin, ii, jj+1, kk+1)
00885                     + VAT3( uPS, i, j, k) * VAT3(xin, ii, jj-1, kk+1)
00886                     + VAT3( uPE, i, j, k) * VAT3(xin, ii+1, jj, kk+1)
00887                     + VAT3( uPW, i, j, k) * VAT3(xin, ii-1, jj, kk+1)
00888                     + VAT3( uPNE, i, j, k) * VAT3(xin, ii+1, jj+1, kk+1)
00889                     + VAT3( uPNW, i, j, k) * VAT3(xin, ii-1, jj+1, kk+1)
00890                     + VAT3( uPSE, i, j, k) * VAT3(xin, ii+1, jj-1, kk+1)
00891                     + VAT3( uPSW, i, j, k) * VAT3(xin, ii-1, jj-1, kk+1);
00892
00893                 tmpD =
00894                     + VAT3( dPC, i, j, k) * VAT3(xin, ii, jj, kk-1)
00895                     + VAT3( dPN, i, j, k) * VAT3(xin, ii, jj+1, kk-1)
00896                     + VAT3( dPS, i, j, k) * VAT3(xin, ii, jj-1, kk-1)
00897                     + VAT3( dPE, i, j, k) * VAT3(xin, ii+1, jj, kk-1)
00898                     + VAT3( dPW, i, j, k) * VAT3(xin, ii-1, jj, kk-1)
00899                     + VAT3( dPNE, i, j, k) * VAT3(xin, ii+1, jj+1, kk-1)
00900                     + VAT3( dPNW, i, j, k) * VAT3(xin, ii-1, jj+1, kk-1)
00901                     + VAT3( dPSE, i, j, k) * VAT3(xin, ii+1, jj-1, kk-1)
00902                     + VAT3( dPSW, i, j, k) * VAT3(xin, ii-1, jj-1, kk-1);
00903
00904                 VAT3(xout, i, j, k) = tmpO + tmpU + tmpD;
00905             }
00906         }
00907     }
00908
00909     // Verify correctness of the output boundary points
00910     VfboundPMG00(nxc, nyc, nzc, xout);
00911 }
00912
00913
00914
00915 VPUBLIC void VinterpPMG(int *nxc, int *nyc, int *nzc,
00916     int *nxf, int *nyf, int *nzf,
00917     double *xin, double *xout,
00918     double *pc) {
00919
00920     MAT2(pc, *nxc * *nyc * *nzc, 1);
00921
00922     VinterpPMG2(nxc, nyc, nzc,
00923         nxf, nyf, nzf,

```

```

00924         xin, xout,
00925         RAT2(pc, 1, 1), RAT2(pc, 1, 2), RAT2(pc, 1, 3), RAT2(pc, 1, 4), RAT2(pc, 1, 5),
00926         RAT2(pc, 1, 6), RAT2(pc, 1, 7), RAT2(pc, 1, 8), RAT2(pc, 1, 9),
00927         RAT2(pc, 1,10), RAT2(pc, 1,11), RAT2(pc, 1,12), RAT2(pc, 1,13), RAT2(pc, 1,14),
00928         RAT2(pc, 1,15), RAT2(pc, 1,16), RAT2(pc, 1,17), RAT2(pc, 1,18),
00929         RAT2(pc, 1,19), RAT2(pc, 1,20), RAT2(pc, 1,21), RAT2(pc, 1,22), RAT2(pc, 1,23),
00930         RAT2(pc, 1,24), RAT2(pc, 1,25), RAT2(pc, 1,26), RAT2(pc, 1,27));
00931 }
00932
00933
00934
00935 VPUBLIC void VinterpPMG2(int *nxc, int *nyc, int *nzc,
00936 int *nxf, int *nyf, int *nzf,
00937 double *xin, double *xout,
00938 double *oPC, double *oPN, double *oPS, double *oPE, double *oPW,
00939 double *oPNE, double *oPNW, double *oPSE, double *oPSW,
00940 double *uPC, double *uPN, double *uPS, double *uPE, double *uPW,
00941 double *uPNE, double *uPNW, double *uPSE, double *uPSW,
00942 double *dPC, double *dPN, double *dPS, double *dPE, double *dPW,
00943 double *dPNE, double *dPNW, double *dPSE, double *dPSW) {
00944
00945     int i, j, k;
00946     int ii, jj, kk;
00947
00948     MAT3( xin, *nxc, *nyc, *nzc);
00949     MAT3(xout, *nxf, *nyf, *nzf);
00950
00951     MAT3( oPC, *nxc, *nyc, *nzc);
00952     MAT3( oPN, *nxc, *nyc, *nzc);
00953     MAT3( oPS, *nxc, *nyc, *nzc);
00954     MAT3( oPE, *nxc, *nyc, *nzc);
00955     MAT3( oPW, *nxc, *nyc, *nzc);
00956
00957     MAT3(oPNE, *nxc, *nyc, *nzc);
00958     MAT3(oPNW, *nxc, *nyc, *nzc);
00959     MAT3(oPSE, *nxc, *nyc, *nzc);
00960     MAT3(oPSW, *nxc, *nyc, *nzc);
00961
00962     MAT3( uPC, *nxc, *nyc, *nzc);
00963     MAT3( uPN, *nxc, *nyc, *nzc);
00964     MAT3( uPS, *nxc, *nyc, *nzc);
00965     MAT3( uPE, *nxc, *nyc, *nzc);
00966     MAT3( uPW, *nxc, *nyc, *nzc);
00967
00968     MAT3(uPNE, *nxc, *nyc, *nzc);
00969     MAT3(uPNW, *nxc, *nyc, *nzc);
00970     MAT3(uPSE, *nxc, *nyc, *nzc);
00971     MAT3(uPSW, *nxc, *nyc, *nzc);
00972
00973     MAT3( dPC, *nxc, *nyc, *nzc);
00974     MAT3( dPN, *nxc, *nyc, *nzc);
00975     MAT3( dPS, *nxc, *nyc, *nzc);
00976     MAT3( dPE, *nxc, *nyc, *nzc);
00977     MAT3( dPW, *nxc, *nyc, *nzc);
00978
00979     MAT3(dPNE, *nxc, *nyc, *nzc);
00980     MAT3(dPNW, *nxc, *nyc, *nzc);
00981     MAT3(dPSE, *nxc, *nyc, *nzc);
00982     MAT3(dPSW, *nxc, *nyc, *nzc);
00983
00984     /* *****
00985     * Setup
00986     * *****
00987
00988     // Verify correctness of the input boundary points ***
00989     VfboundPMG00(nxc, nyc, nzc, xin);
00990
00991     // Do it
00992     for (k=1; k<=*nzf-2; k+=2) {
00993         kk = (k - 1) / 2 + 1;
00994
00995         for (j=1; j<=*nyf-2; j+=2) {
00996             jj = (j - 1) / 2 + 1;
00997
00998             for (i=1; i<=*nxf-2; i+=2) {
00999                 ii = (i - 1) / 2 + 1;
01000
01001                 /* *****
01002                 * Type 1 -- Fine grid points common to a coarse grid point *
01003                 * ***** */
01004

```



```

01005         // Copy coinciding points from coarse grid to fine grid
01006         VAT3(xout, i, j, k) = VAT3(xin, ii, jj, kk);
01007
01008         /* *****
01009          * type 2 -- fine grid points common to a coarse grid plane *
01010          * ***** */
01011
01012         // Fine grid pts common only to y-z planes on coarse grid
01013         // (intermediate pts between 2 grid points on x-row)
01014         VAT3(xout, i+1, j, k) = VAT3(oPE, ii, jj, kk) * VAT3(xin, ii, jj, kk)
01015             + VAT3(oPW, ii+1, jj, kk) * VAT3(xin, ii+1, jj, kk);
01016
01017         // Fine grid pts common only to x-z planes on coarse grid
01018         // (intermediate pts between 2 grid points on a y-row)
01019         VAT3(xout, i, j+1, k) = VAT3(oPN, ii, jj, kk) * VAT3(xin, ii, jj, kk)
01020             + VAT3(oPS, ii, jj+1, kk) * VAT3(xin, ii, jj+1, kk);
01021
01022         // Fine grid pts common only to x-y planes on coarse grid
01023         // (intermediate pts between 2 grid points on a z-row)
01024         VAT3(xout, i, j, k+1) = VAT3(uPC, ii, jj, kk) * VAT3(xin, ii, jj, kk)
01025             + VAT3(dPC, ii, jj, kk+1) * VAT3(xin, ii, jj, kk+1);
01026
01027         /* *****
01028          * type 3 -- fine grid points common to a coarse grid line *
01029          * ***** */
01030
01031         // Fine grid pts common only to z planes on coarse grid
01032         // (intermediate pts between 4 grid pts on the xy-plane)
01033
01034         VAT3(xout, i+1, j+1, k) = VAT3(oPNE, ii, jj, kk) * VAT3(xin, ii, jj, kk)
01035             + VAT3(oPNW, ii+1, jj, kk) * VAT3(xin, ii+1, jj, kk)
01036             + VAT3(oPSE, ii, jj+1, kk) * VAT3(xin, ii, jj+1, kk)
01037             + VAT3(oPSW, ii+1, jj+1, kk) * VAT3(xin, ii+1, jj+1, kk);
01038
01039         // Fine grid pts common only to y planes on coarse grid
01040         // (intermediate pts between 4 grid pts on the xz-plane)
01041         VAT3(xout, i+1, j, k+1) = VAT3(uPE, ii, jj, kk) * VAT3(xin, ii, jj, kk)
01042             + VAT3(uPW, ii+1, jj, kk) * VAT3(xin, ii+1, jj, kk)
01043             + VAT3(dPE, ii, jj, kk+1) * VAT3(xin, ii, jj, kk+1)
01044             + VAT3(dPW, ii+1, jj, kk+1) * VAT3(xin, ii+1, jj, kk+1);
01045
01046         // Fine grid pts common only to x planes on coarse grid
01047         // (intermediate pts between 4 grid pts on the yz-plane)
01048         VAT3(xout, i, j+1, k+1) = VAT3(uPN, ii, jj, kk) * VAT3(xin, ii, jj, kk)
01049             + VAT3(uPS, ii, jj+1, kk) * VAT3(xin, ii, jj+1, kk)
01050             + VAT3(dPN, ii, jj, kk+1) * VAT3(xin, ii, jj, kk+1)
01051             + VAT3(dPS, ii, jj+1, kk+1) * VAT3(xin, ii, jj+1, kk+1);
01052
01053         /* *****
01054          * type 4 -- fine grid points not common to *
01055          * coarse grid pts/lines/planes *
01056          * ***** */
01057
01058         // Completely interior points
01059         VAT3(xout, i+1, j+1, k+1) =
01060             + VAT3(uPNE, ii, jj, kk) * VAT3(xin, ii, jj, kk)
01061             + VAT3(uPNW, ii+1, jj, kk) * VAT3(xin, ii+1, jj, kk)
01062             + VAT3(uPSE, ii, jj+1, kk) * VAT3(xin, ii, jj+1, kk)
01063             + VAT3(uPSW, ii+1, jj+1, kk) * VAT3(xin, ii+1, jj+1, kk)
01064             + VAT3(dPNE, ii, jj, kk+1) * VAT3(xin, ii, jj, kk+1)
01065             + VAT3(dPNW, ii+1, jj, kk+1) * VAT3(xin, ii+1, jj, kk+1)
01066             + VAT3(dPSE, ii, jj+1, kk+1) * VAT3(xin, ii, jj+1, kk+1)
01067             + VAT3(dPSW, ii+1, jj+1, kk+1) * VAT3(xin, ii+1, jj+1, kk+1);
01068     }
01069 }
01070
01071 // Verify correctness of the output boundary points ***
01072 VfboundPMG00(nxf, nyf, nzf, xout);
01073 }
01074
01075
01076
01077
01078 VPUBLIC void Vextrac(int *nxf, int *nyf, int *nzf,
01079     int *nxc, int *nyc, int *nzc,
01080     double *xin, double *xout) {
01081
01082     int i, j, k;
01083     int ii, jj, kk;
01084
01085     MAT3( xin, *nxf, *nyf, *nzf);

```

```

01086     MAT3(xout, *nxc, *nyc, *nzc);
01087
01088     // Verify correctness of the input boundary points
01089     VfboundPMG00(nxf, nyf, nzf, xin);
01090
01091     // Do it
01092     for (k=2; k<=*nzc-1; k++) {
01093         kk = (k - 1) * 2 + 1;
01094
01095         for (j=2; j<=*nyc-1; j++) {
01096             jj = (j - 1) * 2 + 1;
01097
01098             for (i=2; i<=*nxc-1; i++) {
01099                 ii = (i - 1) * 2 + 1;
01100
01101                 // Compute the restriction
01102                 VAT3(xout, i, j, k) = VAT3(xin, ii, jj, kk);
01103             }
01104         }
01105     }
01106
01107     // Verify correctness of the output boundary points
01108     VfboundPMG00(nxc, nyc, nzc, xout);
01109 }

```

9.127 matvecd.h

```

00001
00049 #ifndef _MATVECD_H_
00050 #define _MATVECD_H_
00051
00052 #include "apbscfg.h"
00053
00054 #include "generic/vhal.h"
00055 #include "generic/vmatrix.h"
00056 #include "pmgc/mikpckd.h"
00057 #include "pmgc/myppdec.h"
00058
00066 VEXTERNC void Vmatvec(
00067     int    *nx,
00068     int    *ny,
00069     int    *nz,
00070     int    *ipc,
00071     double *rpc,
00072     double *ac,
00073     double *cc,
00074     double *x,
00075     double *y
00076 );
00077
00078 VEXTERNC void Vmatvec7(
00079     int    *nx,
00080     int    *ny,
00081     int    *nz,
00082     int    *ipc,
00083     double *rpc,
00084     double *ac,
00085     double *cc,
00086     double *x,
00087     double *y
00088 );
00089
00090 VEXTERNC void Vmatvec7_ls(
00091     int    *nx,
00092     int    *ny,
00093     int    *nz,
00094     int    *ipc,
00095     double *rpc,
00096     double *oC,
00097     double *cc,
00098     double *oE,
00099     double *oN,
00100     double *uC,
00101     double *x,
00102     double *y
00103 );
00104
00105

```

```
00106
00107 VEXTERNC void Vmatvec27(
00108     int    *nx,
00109     int    *ny,
00110     int    *nz,
00111     int    *ipc,
00112     double *rpc,
00113     double *ac,
00114     double *cc,
00115     double *x,
00116     double *y
00117 );
00118
00119 VEXTERNC void Vmatvec27_ls(
00120     int    *nx,
00121     int    *ny,
00122     int    *nz,
00123     int    *ipc,
00124     double *rpc,
00125     double *oC,
00126     double *cc,
00127     double *oE,
00128     double *oN,
00129     double *uC,
00130     double *oNE,
00131     double *oNW,
00132     double *uE,
00133     double *uW,
00134     double *uN,
00135     double *uS,
00136     double *uNE,
00137     double *uNW,
00138     double *uSE,
00139     double *uSW,
00140     double *x,
00141     double *y
00142 );
00143
00144
00152 VEXTERNC void Vnmatvec(
00153     int *nx,
00154     int *ny,
00155     int *nz,
00156     int *ipc,
00157     double *rpc,
00158     double *ac,
00159     double *cc,
00160     double *x,
00161     double *y,
00162     double *wl
00163 );
00164
00165 VEXTERNC void Vnmatvec7(
00166     int *nx,
00167     int *ny,
00168     int *nz,
00169     int *ipc,
00170     double *rpc,
00171     double *ac,
00172     double *cc,
00173     double *x,
00174     double *y,
00175     double *wl
00176 );
00177
00178 VEXTERNC void Vnmatvecd7_ls(
00179     int *nx,
00180     int *ny,
00181     int *nz,
00182     int *ipc,
00183     double *rpc,
00184     double *oC,
00185     double *cc,
00186     double *oE,
00187     double *oN,
00188     double *uC,
00189     double *x,
00190     double *y,
00191     double *wl
00192 );
00193
```

```
00194 VEXTERNC void Vnmatvec27(  
00195     int    *nx,  
00196     int    *ny,  
00197     int    *nz,  
00198     int    *ipc,  
00199     double *rpc,  
00200     double *ac,  
00201     double *cc,  
00202     double *x,  
00203     double *y,  
00204     double *wl  
00205 );  
00206  
00207 VEXTERNC void Vnmatvecd27_1s(  
00208     int    *nx,  
00209     int    *ny,  
00210     int    *nz,  
00211     int    *ipc,  
00212     double *rpc,  
00213     double *oC,  
00214     double *cc,  
00215     double *oE,  
00216     double *oN,  
00217     double *uC,  
00218     double *oNE,  
00219     double *oNW,  
00220     double *uE,  
00221     double *uW,  
00222     double *uN,  
00223     double *uS,  
00224     double *uNE,  
00225     double *uNW,  
00226     double *uSE,  
00227     double *uSW,  
00228     double *x,  
00229     double *y,  
00230     double *wl  
00231 );  
00232  
00233  
00241 VEXTERNC void Vmresid(  
00242     int    *nx,  
00243     int    *ny,  
00244     int    *nz,  
00245     int    *ipc,  
00246     double *rpc,  
00247     double *ac,  
00248     double *cc,  
00249     double *fc,  
00250     double *x,  
00251     double *r  
00252 );  
00253  
00254 VEXTERNC void Vmresid7(  
00255     int    *nx,  
00256     int    *ny,  
00257     int    *nz,  
00258     int    *ipc,  
00259     double *rpc,  
00260     double *ac,  
00261     double *cc,  
00262     double *fc,  
00263     double *x,  
00264     double *r  
00265 );  
00266  
00267 VEXTERNC void Vmresid7_1s(  
00268     int *nx,  
00269     int *ny,  
00270     int *nz,  
00271     int *ipc,  
00272     double *rpc,  
00273     double *oC,  
00274     double *cc,  
00275     double *fc,  
00276     double *oE,  
00277     double *oN,  
00278     double *uC,  
00279     double *x,  
00280     double *r  
00281 );
```

```
00282
00283 VEXTERNC void Vmresid27(
00284     int    *nx,
00285     int    *ny,
00286     int    *nz,
00287     int    *ipc,
00288     double *rpc,
00289     double *ac,
00290     double *cc,
00291     double *fc,
00292     double *x,
00293     double *r
00294 );
00295
00296 VEXTERNC void Vmresid27_ls(
00297     int *nx,
00298     int *ny,
00299     int *nz,
00300     int *ipc,
00301     double *rpc,
00302     double *oC,
00303     double *cc,
00304     double *fc,
00305     double *oE,
00306     double *oN,
00307     double *uC,
00308     double *oNE,
00309     double *oNW,
00310     double *uE,
00311     double *uW,
00312     double *uN,
00313     double *uS,
00314     double *uNE,
00315     double *uNW,
00316     double *uSE,
00317     double *uSW,
00318     double *x,
00319     double *r
00320 );
00321
00322
00323
00331 VEXTERNC void Vnmresid(
00332     int    *nx,
00333     int    *ny,
00334     int    *nz,
00335     int    *ipc,
00336     double *rpc,
00337     double *ac,
00338     double *cc,
00339     double *fc,
00340     double *x,
00341     double *r,
00342     double *wl
00343 );
00344
00345 VEXTERNC void Vnmresid7(
00346     int *nx,
00347     int *ny,
00348     int *nz,
00349     int *ipc,
00350     double *rpc,
00351     double *ac,
00352     double *cc,
00353     double *fc,
00354     double *x,
00355     double *r,
00356     double *wl
00357 );
00358
00359 VEXTERNC void Vnmresid7_ls(
00360     int *nx,
00361     int *ny,
00362     int *nz,
00363     int *ipc,
00364     double *rpc,
00365     double *oC,
00366     double *cc,
00367     double *fc,
00368     double *oE,
00369     double *oN,
```

```
00370         double *uC,
00371         double *x,
00372         double *r,
00373         double *wl
00374     );
00375
00376 VEXTERNC void Vnmresid27(
00377     int *nx,
00378     int *ny,
00379     int *nz,
00380     int *ipc,
00381     double *rpc,
00382     double *ac,
00383     double *cc,
00384     double *fc,
00385     double *x,
00386     double *r,
00387     double *wl
00388 );
00389
00390 VEXTERNC void Vnmresid27_1s(
00391     int *nx,
00392     int *ny,
00393     int *nz,
00394     int *ipc,
00395     double *rpc,
00396     double *oC,
00397     double *cc,
00398     double *fc,
00399     double *oE,
00400     double *oN,
00401     double *uC,
00402     double *oNE,
00403     double *oNW,
00404     double *uE,
00405     double *uW,
00406     double *uN,
00407     double *uS,
00408     double *uNE,
00409     double *uNW,
00410     double *uSE,
00411     double *uSW,
00412     double *x,
00413     double *r,
00414     double *wl
00415 );
00416
00417
00418
00425 VEXTERNC void Vrestrc(
00426     int *nxf,
00427     int *nyf,
00428     int *nzf,
00429     int *nxc,
00430     int *nyc,
00431     int *nzc,
00432     double *xin,
00433     double *xout,
00434     double *pc
00435 );
00436
00437 VEXTERNC void Vrestrc2(
00438     int *nxf,
00439     int *nyf,
00440     int *nzf,
00441     int *nxc,
00442     int *nyc,
00443     int *nzc,
00444     double *xin,
00445     double *xout,
00446     double *oPC,
00447     double *oPN,
00448     double *oPS,
00449     double *oPE,
00450     double *oPW,
00451     double *oPNE,
00452     double *oPNW,
00453     double *oPSE,
00454     double *oPSW,
00455     double *uPC,
00456     double *uPN,
```

```
00457         double *uPS,
00458         double *uPE,
00459         double *uPW,
00460         double *uPNE,
00461         double *uPNW,
00462         double *uPSE,
00463         double *uPSW,
00464         double *dPC,
00465         double *dPN,
00466         double *dPS,
00467         double *dPE,
00468         double *dPW,
00469         double *dPNE,
00470         double *dPNW,
00471         double *dPSE,
00472         double *dPSW
00473     );
00474
00481 VEXTERNC void VinterpPMG(
00482     int     *nxc,
00483     int     *nyc,
00484     int     *nzc,
00485     int     *nxf,
00486     int     *nyf,
00487     int     *nzf,
00488     double *xin,
00489     double *xout,
00490     double *pc
00491 );
00492
00493 VEXTERNC void VinterpPMG2(
00494     int     *nxc,
00495     int     *nyc,
00496     int     *nzc,
00497     int     *nxf,
00498     int     *nyf,
00499     int     *nzf,
00500     double *xin,
00501     double *xout,
00502     double *oPC,
00503     double *oPN,
00504     double *oPS,
00505     double *oPE,
00506     double *oPW,
00507     double *oPNE,
00508     double *oPNW,
00509     double *oPSE,
00510     double *oPSW,
00511     double *uPC,
00512     double *uPN,
00513     double *uPS,
00514     double *uPE,
00515     double *uPW,
00516     double *uPNE,
00517     double *uPNW,
00518     double *uPSE,
00519     double *uPSW,
00520     double *dPC,
00521     double *dPN,
00522     double *dPS,
00523     double *dPE,
00524     double *dPW,
00525     double *dPNE,
00526     double *dPNW,
00527     double *dPSE,
00528     double *dPSW
00529 );
00530
00537 VEXTERNC void Vextrac(
00538     int *nxf,
00539     int *nyf,
00540     int *nzf,
00541     int *nxc,
00542     int *ny,
00543     int *nzc,
00544     double *xin,
00545     double *xout
00546 );
00547
00548 #endif /* _MATVECD_H_ */
```

9.128 mgcsd.c

```

00001
00055 #include "mgcsd.h"
00056
00057 VEXTERNC void Vmvecs(int *nx, int *ny, int *nz,
00058     double *x,
00059     int *iz,
00060     double *w0, double *w1, double *w2, double *w3,
00061     int *istop, int *itmax, int *iters, int *ierror,
00062     int *nlev, int *ilev, int *nlev_real,
00063     int *mgsolv, int *iok, int *iinfo,
00064     double *epsiln, double *errtol, double *omega,
00065     int *nul, int *nu2,
00066     int *mgsmoo,
00067     int *ipc, double *rpc,
00068     double *pc, double *ac, double *cc, double *fc, double *tru) {
00069
00070     int level;          // @todo: doc
00071     int lev;            // @todo: doc
00072     int itmax_s;        // @todo: doc
00073     int iters_s;        // @todo: doc
00074     int nuu;           // @todo: doc
00075     int mgsmoo_s;      // @todo: doc
00076     int iresid;        // @todo: doc
00077     int nxf;           // @todo: doc
00078     int nyf;           // @todo: doc
00079     int nzf;           // @todo: doc
00080     int nxc;           // @todo: doc
00081     int nyc;           // @todo: doc
00082     int nzc;           // @todo: doc
00083     int lpv;           // @todo: doc
00084     int n;              // @todo: doc
00085     int m;              // @todo: doc
00086     int iadjoin;       // @todo: doc
00087     double errtol_s;    // @todo: doc
00088     double rsden;       // @todo: doc
00089     double rsnrm;       // @todo: doc
00090     double orsnrm;      // @todo: doc
00091     double xnum;        // @todo: doc
00092     double xden;        // @todo: doc
00093     double xdamp;       // @todo: doc
00094     int lda;            // @todo: doc
00095
00096     double alpha;        // A utility variable used to pass a parameter to xaxpy
00097     int numlev;          // A utility variable used to pass a parameter to mkcors
00098
00099     MAT2(iz, 50, 1);
00100
00101     // Recover level information
00102     level = 1;
00103     lev = (*ilev - 1) + level;
00104
00105     // Recover grid sizes
00106     nxf = *nx;
00107     nyf = *ny;
00108     nzf = *nz;
00109     numlev = *nlev - 1;
00110     Vmkcors(&numlev, &nxf, &nyf, &nzf, &nxc, &nyc, &nzc);
00111
00112     // Do some i/o if requested
00113     if (*iinfo > 1) {
00114         VMESSEGE0("Starting mvcs operation");
00115         VMESSEGE3("Fine Grid Size: (%d, %d, %d)", nxf, nyf, nzf);
00116         VMESSEGE3("Coarse Grid Size: (%d, %d, %d)", nxc, nyc, nzc);
00117     }
00118
00119     if (*iok != 0) {
00120         Vprtstp(*iok, -1, 0.0, 0.0, 0.0);
00121     }
00122 }
00123
00124 /* *****
00125  * *** Note: if (iok != 0) then: use a stopping test. ***
00126  * *** else: use just the itmax to stop iteration. ***
00127  * *****
00128  * *** istop=0 most efficient (whatever it is) ***
00129  * *** istop=1 relative residual ***
00130  * *** istop=2 rms difference of successive iterates ***
00131  * *** istop=3 relative true error (provided for testing) ***

```



```

00132      *      *****/
00133
00134      // Compute denominator for stopping criterion
00135      if (*iok != 0) {
00136          if (*istop == 0) {
00137              rsden = 1.0;
00138          }
00139          else if (*istop == 1) {
00140              rsden = Vxnrml(&nxf, &nyf, &nzf, RAT(fc, VAT2(iz, 1,lev)));
00141          }
00142          else if (*istop == 2) {
00143              rsden = VSQRT(nxf * nyf * nzf);
00144          }
00145          else if (*istop == 3) {
00146              rsden = Vxnrml2(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1,lev)));
00147          }
00148          else if (*istop == 4) {
00149              rsden = Vxnrml2(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1,lev)));
00150          }
00151          else if (*istop == 5) {
00152              Vmatvec(&nxf, &nyf, &nzf,
00153                  RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00154                  RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)),
00155                  RAT(tru, VAT2(iz, 1,lev)), w1);
00156              rsden = VSQRT(Vxdot(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1,lev)), w1));
00157          }
00158          else {
00159              VABORT_MSG1("Bad istop value: %d", *istop);
00160          }
00161
00162          if (rsden == 0.0) {
00163              rsden = 1.0;
00164              VERRMSG0("rhs is zero on finest level");
00165          }
00166          rsnm = rsden;
00167          orsnm = rsnm;
00168          iters_s = 0;
00169
00170          Vprtstp(*iok, 0, rsnm, rsden, orsnm);
00171      }
00172
00173
00174
00175      /* *****/
00176      * *** solve directly if nlev = 1
00177      * *****/
00178
00179      // Solve directly if on the coarse grid
00180      if (*nlev == 1) {
00181
00182          // Use iterative method?
00183          if (*mgsolv == 0) {
00184
00185              // solve on coarsest grid with cgls, mgsmoo_s=4 (no residual)
00186              iresid = 0;
00187              iadjoin = 0;
00188              itmax_s = 100;
00189              iters_s = 0;
00190              errtol_s = *epsiln;
00191              mgsmoo_s = 4;
00192
00193              Vazeros(&nxf, &nyf, &nzf, RAT(x, VAT2(iz, 1,lev)));
00194
00195              Vsmooth(&nxf, &nyf, &nzf,
00196                  RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00197                  RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)), RAT(fc, VAT2(iz, 1,lev)),
00198                  RAT(x, VAT2(iz, 1,lev)), w1, w2, w3,
00199                  &itmax_s, &iters_s, &errtol_s, omega,
00200                  &iresid, &iadjoin, &mgsmoo_s);
00201
00202              // Check for trouble on the coarse grid
00203              VWARN_MSG2(iters_s <= itmax_s,
00204                  "Exceeded maximum iterations: iters_s=%d, itmax_s=%d",
00205                  iters_s, itmax_s);
00206
00207          } else if (*mgsolv == 1) {
00208
00209              // Use direct method?
00210
00211              // Setup lpv to access the factored/banded operator
00212              lpv = lev + 1;

```

```

00213
00214 // setup for banded format
00215 n = *RAT(ipc, (VAT2(iz, 5,lpv) - 1) + 1);
00216 m = *RAT(ipc, (VAT2(iz, 5,lpv) - 1) + 2);
00217 lda = *RAT(ipc, (VAT2(iz, 5,lpv) - 1) + 3);
00218
00219 // Call dpbsl to solve
00220 Vxcopy_small(&nxf, &nyf, &nzf, RAT(fc, VAT2(iz, 1,lev)), w1);
00221 Vdpbsl(RAT(ac, VAT2(iz, 7,lpv)), &lda, &n, &m, w1);
00222 Vxcopy_large(&nxf, &nyf, &nzf, w1, RAT(x, VAT2(iz, 1,lev)));
00223 VfboundPMG00(&nxf, &nyf, &nzf, RAT(x, VAT2(iz, 1,lev)));
00224
00225 } else {
00226     VABORT_MSG1("Invalid coarse solver requested: %d", *mgsolv);
00227 }
00228
00229
00230 // Compute the stopping test
00231 *iters = 1;
00232 if (*iok != 0) {
00233
00234     orsnrm = rsnm;
00235
00236     if (*istop == 0) {
00237
00238         Vmresid(&nxf, &nyf, &nzf,
00239             RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00240             RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00241             RAT(fc, VAT2(iz, 1,lev)),
00242             RAT(x, VAT2(iz, 1, lev)), w1);
00243
00244         rsnm = Vxnrm1(&nxf, &nyf, &nzf, w1);
00245     }
00246
00247     else if (*istop == 1) {
00248
00249         Vmresid(&nxf, &nyf, &nzf,
00250             RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00251             RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00252             RAT(fc, VAT2(iz, 1, lev)), RAT(x, VAT2(iz, 1, lev)),
00253             w1);
00254         rsnm = Vxnrm1(&nxf, &nyf, &nzf, w1);
00255     }
00256
00257     else if (*istop == 2) {
00258
00259         alpha = -1.0;
00260
00261         Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1,lev)), w1);
00262         Vxaxpy(&nxf, &nyf, &nzf, &alpha,
00263             RAT(x, VAT2(iz, 1,lev)), w1);
00264         rsnm = Vxnrm1(&nxf, &nyf, &nzf, w1);
00265         Vxcopy(&nxf, &nyf, &nzf, RAT(x, VAT2(iz, 1,lev)), RAT(tru, VAT2(iz, 1,lev)));
00266     }
00267
00268     else if (*istop == 3) {
00269
00270         alpha = -1.0;
00271
00272         Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1,lev)), w1);
00273         Vxaxpy(&nxf, &nyf, &nzf, &alpha, RAT(x, VAT2(iz, 1,lev)), w1);
00274         rsnm = Vxnrm2(&nxf, &nyf, &nzf, w1);
00275     }
00276
00277     else if (*istop == 4) {
00278
00279         alpha = -1.0;
00280
00281         Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1,lev)), w1);
00282         Vxaxpy(&nxf, &nyf, &nzf, &alpha, RAT(x, VAT2(iz, 1,lev)), w1);
00283         rsnm = Vxnrm2(&nxf, &nyf, &nzf, w1);
00284     }
00285
00286     else if (*istop == 5) {
00287
00288         alpha = -1.0;
00289
00290         Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1,lev)), w1);
00291         Vxaxpy(&nxf, &nyf, &nzf, &alpha, RAT(x, VAT2(iz, 1,lev)), w1);
00292
00293         Vmatvec(&nxf, &nyf, &nzf,

```

```

00294         RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00295         RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)),
00296         w1, w2);
00297     rsnrm = VSQRT(Vxdot(&nxf, &nyf, &nzf, w1, w2));
00298 }
00299
00300     else {
00301         VABORT_MSG1("Bad istop value: %d\n", *istop);
00302     }
00303     Vprtstp(*iok, *iters, rsnrm, rsden, orsnrm);
00304 }
00305 return;
00306 }
00307
00308
00309 /* *****
00310  * *** begin mg iteration (note nxf,nyf,nzf changes during loop)
00311  * *****/
00312
00313 // Setup for the v-cycle looping
00314 *iters = 0;
00315 do {
00316
00317     // Finest level initialization
00318     level = 1;
00319     lev = (*ilev - 1) + level;
00320
00321     // nul pre-smoothings on fine grid (with residual)
00322     iresid = 1;
00323     iadjoint = 0;
00324     iters_s = 0;
00325     errtol_s = 0.0;
00326     nuuu = Vivariv(nul, &lev);
00327
00328     Vsmooth(&nxf, &nyf, &nzf,
00329         RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00330         RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)), RAT(fc, VAT2(iz, 1,lev)),
00331         RAT(x, VAT2(iz, 1,lev)), w2, w3, w1,
00332         &nuuu, &iters_s,
00333         &errtol_s, omega,
00334         &iresid, &iadjoint, mgsmoo);
00335
00336     Vxcopy(&nxf, &nyf, &nzf, w1, RAT(w0, VAT2(iz, 1,lev)));
00337
00338
00339
00340 /* *****
00341  * begin cycling down to coarse grid
00342  * *****/
00343
00344 // Go down grids: restrict resid to coarser and smooth
00345 for (level=2; level<=*nlev; level++) {
00346
00347     lev = (*ilev - 1) + level;
00348
00349     // Find new grid size
00350     numlev = 1;
00351     Vmkcors(&numlev, &nxf, &nyf, &nzf, &nxc, &nyc, &nzc);
00352
00353     // Restrict residual to coarser grid ***
00354     Vrestrc(&nxf, &nyf, &nzf,
00355         &nxc, &nyc, &nzc,
00356         w1, RAT(w0, VAT2(iz, 1,lev)), RAT(pc, VAT2(iz, 11,lev-1)));
00357
00358     nxf = nxc;
00359     nyf = nyc;
00360     nzf = nzc;
00361
00362
00363     // if not on coarsest level yet...
00364     if (level != *nlev) {
00365
00366         // nul pre-smoothings on this level (with residual)
00367         // (w1 has residual...)
00368         Vazeros(&nxf, &nyf, &nzf, RAT(x, VAT2(iz, 1,lev)));
00369         iresid = 1;
00370         iadjoint = 0;
00371         iters_s = 0;
00372         errtol_s = 0.0;
00373         nuuu = Vivariv(nul, &lev);
00374         Vsmooth(&nxf, &nyf, &nzf,
00375             RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),

```

```

00376         RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)), RAT(w0, VAT2(iz, 1,lev)),
00377         RAT(x, VAT2(iz, 1,lev)), w2, w3, w1,
00378         &nuuu, &iters_s,
00379         &errtol_s, omega ,
00380         &iresid, &iadjoin, mgsmoo);
00381     }
00382     // End of cycling down to coarse grid loop
00383 }
00384
00385
00386
00387 /* *****
00388  * begin coarse grid
00389  * *****/
00390
00391 // Coarsest level
00392 level = *nlev;
00393 lev = (*ilev - 1) + level;
00394
00395 // Use iterative method?
00396 if (*mgsolv == 0) {
00397
00398     // solve on coarsest grid with cghs, mgsmoo_s=4 (no residual)
00399     iresid = 0;
00400     iadjoin = 0;
00401     itmax_s = 100;
00402     iters_s = 0;
00403     errtol_s = *epsiln;
00404     mgsmoo_s = 4;
00405     Vazeros(&nxf, &nyf, &nzf, RAT(x, VAT2(iz, 1,lev)));
00406     Vsmooth(&nxf, &nyf, &nzf,
00407             RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00408             RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)), RAT(w0, VAT2(iz, 1,lev)),
00409             RAT(x, VAT2(iz, 1,lev)), w1, w2, w3,
00410             &itmax_s, &iters_s,
00411             &errtol_s, omega,
00412             &iresid, &iadjoin, &mgsmoo_s);
00413
00414     // Check for trouble on the coarse grid
00415     VWARN_MSG2(iters_s <= itmax_s,
00416               "Exceeded maximum iterations: iters_s=%d, itmax_s=%d",
00417               iters_s, itmax_s);
00418 } else if (*mgsolv == 1) {
00419
00420     // use direct method?
00421
00422     // Setup lpv to access the factored/banded operator
00423     lpv = lev + 1;
00424
00425     // Setup for banded format
00426     n = VAT(ipc, (VAT2(iz, 5, lpv) - 1) + 1);
00427     m = VAT(ipc, (VAT2(iz, 5, lpv) - 1) + 2);
00428     lda = VAT(ipc, (VAT2(iz, 5, lpv) - 1) + 3);
00429
00430     // Call dpbsl to solve
00431     Vxcopy_small(&nxf, &nyf, &nzf, RAT(w0, VAT2(iz, 1,lev)), w1);
00432     Vdpbsl(RAT(ac, VAT2(iz, 7,lpv)), &lda, &n, &m, w1);
00433     Vxcopy_large(&nxf, &nyf, &nzf, w1, RAT(x, VAT2(iz, 1,lev)));
00434     VfboundPMG00(&nxf, &nyf, &nzf, RAT(x, VAT2(iz, 1,lev)));
00435
00436 } else {
00437     VABORT_MSG1("Invalid coarse solver requested: %d", *mgsolv);
00438 }
00439
00440
00441 /* *****
00442  * begin cycling back to fine grid
00443  * *****/
00444
00445
00446 // Move up grids: interpolate resid to finer and smooth
00447 for (level=*nlev-1; level>=1; level--) {
00448
00449     lev = (*ilev - 1) + level;
00450
00451     // Find new grid size
00452     numlev = 1;
00453     Vmkfine(&numlev,
00454             &nxf, &nyf, &nzf,
00455             &nxc, &nyc, &nzc);
00456

```

```

00457         // Interpolate to next finer grid
00458         VinterpPMG(&nxf, &nyf, &nzf,
00459                 &nxc, &nyc, &nzc,
00460                 RAT(x, VAT2(iz, 1,lev+1)), w1, RAT(pc, VAT2(iz, 1,lev)));
00461
00462         /* Compute the hackbusch/reusken damping parameter
00463         * which is equivalent to the standard linear cg steplength
00464         */
00465         Vmatvec(&nxf, &nyf, &nzf,
00466                 RAT(ipc, VAT2(iz, 5,lev+1)), RAT(rpc, VAT2(iz, 6,lev+1)),
00467                 RAT(ac, VAT2(iz, 7,lev+1)), RAT(cc, VAT2(iz, 1,lev+1)),
00468                 RAT(x, VAT2(iz, 1,lev+1)), w2);
00469
00470         xnum = Vxdot(&nxf, &nyf, &nzf,
00471                 RAT(x, VAT2(iz, 1,lev+1)), RAT(w0, VAT2(iz, 1,lev+1)));
00472
00473         xden = Vxdot(&nxf, &nyf, &nzf,
00474                 RAT(x, VAT2(iz, 1,lev+1)), w2);
00475         xdamp = xnum / xden;
00476
00477         // New grid size
00478         nxf = nxc;
00479         nyf = nyc;
00480         nzf = nzc;
00481
00482         // perform the coarse grid correction
00483         // xdamp = 1.0d0
00484         Vxaxpy(&nxf, &nyf, &nzf,
00485                 &xdamp, w1, RAT(x, VAT2(iz, 1,lev)));
00486
00487         // nu2 post-smoothings for correction (no residual)
00488         iresid = 0;
00489         iadjoint = 1;
00490         iters_s = 0;
00491         errtol_s = 0.0;
00492         nuuu = Vivariv(nu2, &lev);
00493         if (level == 1) {
00494             Vsmooth(&nxf, &nyf, &nzf,
00495                     RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00496                     RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)), RAT(fc, VAT2(iz, 1,lev)),
00497                     RAT(x, VAT2(iz, 1,lev)), w1, w2, w3,
00498                     &nuuu, &iters_s, &errtol_s, omega,
00499                     &iresid, &iadjoint, mgsmoo);
00500         } else {
00501             Vsmooth(&nxf, &nyf, &nzf,
00502                     RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00503                     RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)), RAT(w0, VAT2(iz, 1,lev)),
00504                     RAT(x, VAT2(iz, 1,lev)), w1, w2, w3,
00505                     &nuuu, &iters_s, &errtol_s, omega,
00506                     &iresid, &iadjoint, mgsmoo);
00507         }
00508     }
00509
00510     /* *****
00511     * iteration complete: do some i/o
00512     * *****
00513
00514     // Increment the iteration counter
00515     (*iters)++;
00516
00517     // Compute/check the current stopping test
00518     if (iok != 0) {
00519         orsnrm = rsnm;
00520         if (*istop == 0) {
00521             Vmresid(&nxf, &nyf, &nzf,
00522                     RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00523                     RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)), RAT(fc, VAT2(iz, 1,lev)),
00524                     RAT(x, VAT2(iz, 1,lev)), w1);
00525             rsnm = Vxnrm1(&nxf, &nyf, &nzf, w1);
00526         } else if (*istop == 1) {
00527             Vmresid(&nxf, &nyf, &nzf,
00528                     RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00529                     RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)), RAT(fc, VAT2(iz, 1,lev)),
00530                     RAT(x, VAT2(iz, 1,lev)), w1);
00531             rsnm = Vxnrm1(&nxf, &nyf, &nzf, w1);
00532         } else if (*istop == 2) {
00533             Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1,lev)), w1);
00534             alpha = -1.0;
00535             Vxaxpy(&nxf, &nyf, &nzf, &alpha, RAT(x, VAT2(iz, 1,lev)), w1);
00536             rsnm = Vxnrm1(&nxf, &nyf, &nzf, w1);
00537             Vxcopy(&nxf, &nyf, &nzf, RAT(x, VAT2(iz, 1,lev)), RAT(tru, VAT2(iz, 1,lev)));

```

```

00538     } else if (*istop == 3) {
00539         Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1,lev)), w1);
00540         alpha = -1.0;
00541         Vxaxpy(&nxf, &nyf, &nzf, &alpha, RAT(x, VAT2(iz, 1,lev)), w1);
00542         rsnmr = Vxnmr2(&nxf, &nyf, &nzf, w1);
00543     } else if (*istop == 4) {
00544         Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1,lev)), w1);
00545         alpha = -1.0;
00546         Vxaxpy(&nxf, &nyf, &nzf, &alpha, RAT(x, VAT2(iz, 1,lev)), w1);
00547         rsnmr = Vxnmr2(&nxf, &nyf, &nzf, w1);
00548     } else if (*istop == 5) {
00549         Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1,lev)), w1);
00550         alpha = -1.0;
00551         Vxaxpy(&nxf, &nyf, &nzf, &alpha, RAT(x, VAT2(iz, 1,lev)), w1);
00552         Vmatvec(&nxf, &nyf, &nzf,
00553             RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00554             RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)),
00555             w1, w2);
00556         rsnmr = VSQRT(Vxdot(&nxf, &nyf, &nzf, w1, w2));
00557     } else {
00558         VABORT_MSG1("Bad istop value: %d", *istop);
00559     }
00560     Vprtstp(*iok, *iters, rsnmr, rsden, orsnmr);
00561 }
00562 } while (*iters<*itmax && (rsnmr/rsden) > *errtol);
00563
00564 *ierror = *iters < *itmax ? 0 : 1;
00565 }

```

9.129 mgcsd.h

```

00001
00050 #ifndef _MGCSH_H_
00051 #define _MGCSH_H_
00052
00053 #include "apbscfg.h"
00054
00055 #include "malloc/malloc.h"
00056
00057 #include "generic/vhal.h"
00058 #include "generic/vmatrix.h"
00059 #include "pmgc/mgsd.h"
00060 #include "pmgc/mikpckd.h"
00061 #include "pmgc/smoothd.h"
00062 #include "pmgc/gsd.h"
00063 #include "pmgc/matvecd.h"
00064 #include "pmgc/mlinpcd.h"
00065
00106 VEXTERN void Vmvs(
00107     int    *nx,
00108     int    *ny,
00109     int    *nz,
00110     double *x,
00111     int    *iz,
00112     double *w0,
00113     double *w1,
00114     double *w2,
00115     double *w3,
00116     int    *istop,
00117     int    *itmax,
00118     int    *iters,
00119     int    *ierror,
00120     int    *nlev,
00121     int    *ilev,
00122     int    *nlev_real,
00123     int    *mgsolv,
00124     int    *iok,
00125     int    *iinfo,
00126     double *epsiln,
00127     double *errtol,
00128     double *omega,
00129     int    *nul,
00130     int    *nu2,
00131     int    *mgsmoo,
00132     int    *ipc,
00133     double *rpc,
00134     double *pc,
00135     double *ac,

```

```

00136         double *cc,
00137         double *fc,
00138         double *tru
00139     );
00140
00141 #endif /* _MGCSH_H_ */

```

9.130 mgdrvd.c

```

00001
00055 #include "mgdrvd.h"
00056
00057 VPUBLIC void Vmgdriv(int* iparm, double* rparm,
00058                     int* iwork, double* rwork, double* u,
00059                     double* xf, double* yf, double* zf,
00060                     double* gxcf, double* gycf, double* gzcf,
00061                     double* alcf, double* a2cf, double* a3cf,
00062                     double* ccf, double* fcf, double* tcf) {
00063
00064     // The following variables will be returned from mgsz
00065     int nxc = 0;
00066     int nyc = 0;
00067     int nzc = 0;
00068     int nf = 0;
00069     int nc = 0;
00070     int narr = 0;
00071     int narrc = 0;
00072     int n_rpc = 0;
00073     int n_iz = 0;
00074     int n_ipc = 0;
00075     int iretot = 0;
00076     int iintot = 0;
00077
00078     // Miscellaneous variables
00079     int nrwk = 0;
00080     int niwk = 0;
00081     int nx = 0;
00082     int ny = 0;
00083     int nz = 0;
00084     int nlev = 0;
00085     int ierror = 0;
00086     int mxlv = 0;
00087     int mgcoar = 0;
00088     int mgdisc = 0;
00089     int mgsolv = 0;
00090     int k_iz = 0;
00091     int k_ipc = 0;
00092     int k_rpc = 0;
00093     int k_ac = 0;
00094     int k_cc = 0;
00095     int k_fc = 0;
00096     int k_pc = 0;
00097
00098     // Utility pointers to help in passing values
00099     int *iz = VNULL;
00100     int *ipc = VNULL;
00101     double *rpc = VNULL;
00102     double *pc = VNULL;
00103     double *ac = VNULL;
00104     double *cc = VNULL;
00105     double *fc = VNULL;
00106
00107     // Decode some parameters
00108     nrwk = VAT(iparm, 1);
00109     niwk = VAT(iparm, 2);
00110     nx = VAT(iparm, 3);
00111     ny = VAT(iparm, 4);
00112     nz = VAT(iparm, 5);
00113     nlev = VAT(iparm, 6);
00114
00115     // Perform some checks on input
00116     VASSERT_MSG1(nlev > 0, "nlev must be positive: %d", nlev);
00117     VASSERT_MSG1(nx > 0, "nx must be positive: %d", nx);
00118     VASSERT_MSG1(ny > 0, "ny must be positive: %d", ny);
00119     VASSERT_MSG1(nz > 0, "nz must be positive: %d", nz);
00120
00121     mxlv = Vmaxlev(nx, ny, nz);
00122     VASSERT_MSG2(

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00123         nlev <= mxlv,
00124         "number of levels exceeds maximum: %d > %d",
00125         nlev, mxlv
00126     );
00127
00128
00129     // Extract basic grid sizes, etc.
00130     mgcoar = VAT(iparm, 18);
00131     mgdisc = VAT(iparm, 19);
00132     mgsolv = VAT(iparm, 21);
00133
00134     Vmgksz(&mgcoar, &mgdisc, &mgsolv,
00135           &nx, &ny, &nz,
00136           &nlev,
00137           &nxc, &nyc, &nzc,
00138           &nf, &nc,
00139           &narr, &narrc,
00140           &n_rpc, &n_iz, &n_ipc,
00141           &iRETOT, &iINTOT);
00142
00143     // Perform some more checks on input
00144     VASSERT_MSG2(
00145         iRETOT >= nrwk,
00146         "real workspace exceeds maximum size: %d > %d",
00147         nrwk, iRETOT
00148     );
00149     VASSERT_MSG2(
00150         iINTOT >= niwk,
00151         "integer workspace exceeds maximum size: %d > %d",
00152         niwk, iINTOT
00153     );
00154
00155     // Split up the integer work array
00156     k_iz = 1;
00157     k_ipc = k_iz + n_iz;
00158
00159     // Split up the real work array ***
00160     k_rpc = 1;
00161     k_cc = k_rpc + n_rpc;
00162     k_fc = k_cc + narr;
00163     k_pc = k_fc + narr;
00164     k_ac = k_pc + 27 * narrc;
00165     // k_ac_after = 4 * nf + 4 * narrc;
00166     // k_ac_after = 4 * nf + 14 * narrc;
00167     // k_ac_after = 14 * nf + 14 * narrc;
00168
00169     iz = RAT(iwork, k_iz);
00170     ipc = RAT(iwork, k_ipc);
00171
00172     rpc = RAT(rwork, k_rpc);
00173     pc = RAT(rwork, k_pc);
00174     ac = RAT(rwork, k_ac);
00175     cc = RAT(rwork, k_cc);
00176     fc = RAT(rwork, k_fc);
00177
00178     // Call the multigrid driver
00179     Vmgdriv2(iparm, rparm,
00180             &nx, &ny, &nz,
00181             u,
00182             iz, ipc, rpc,
00183             pc, ac, cc, fc,
00184             xf, yf, zf,
00185             gxcf, gycf, gzcf,
00186             alcf, a2cf, a3cf,
00187             ccf, fcf, tcf);
00188 }
00189
00190 VPUBLIC void Vmgdriv2(int *iparm, double *rparm,
00191                     int *nx, int *ny, int *nz,
00192                     double *u,
00193                     int *iz, int *ipc, double *rpc,
00194                     double *pc, double *ac, double *cc, double *fc,
00195                     double *xf, double *yf, double *zf,
00196                     double *gxcf, double *gycf, double *gzcf,
00197                     double *alcf, double *a2cf, double *a3cf,
00198                     double *ccf, double *fcf, double *tcf) {
00199
00200     // @todo Document this function
00201
00202     // Miscellaneous Variables
00203     int mgkey = 0;

```



```
00204     int itmax      = 0;
00205     int iok        = 0;
00206     int iinfo       = 0;
00207     int istop       = 0;
00208     int ipkey       = 0;
00209     int nul         = 0;
00210     int nu2         = 0;
00211     int ilev        = 0;
00212     int ido         = 0;
00213     int iters       = 0;
00214     int ierror      = 0;
00215     int nlev_real   = 0;
00216     int ibound      = 0;
00217     int mgprol      = 0;
00218     int mgcoar      = 0;
00219     int mgsolv      = 0;
00220     int mgdisc      = 0;
00221     int mgsmoo      = 0;
00222     int iperf       = 0;
00223     int mode        = 0;
00224
00225     double epsiln   = 0.0;
00226     double epsmac   = 0.0;
00227     double errtol   = 0.0;
00228     double omegal   = 0.0;
00229     double omegan   = 0.0;
00230     double bf       = 0.0;
00231     double oh       = 0.0;
00232     double tsetupf  = 0.0;
00233     double tsetupc  = 0.0;
00234     double tsolve   = 0.0;
00235
00236
00237
00238     // More miscellaneous variables
00239     int itmax_p = 0;
00240     int iters_p = 0;
00241     int iok_p  = 0;
00242     int iinfo_p = 0;
00243
00244     double errtol_p = 0.0;
00245     double rho_p    = 0.0;
00246     double rho_min  = 0.0;
00247     double rho_max  = 0.0;
00248     double rho_min_mod = 0.0;
00249     double rho_max_mod = 0.0;
00250
00251     int nxf = 0;
00252     int nyf = 0;
00253     int nzf = 0;
00254     int nxc = 0;
00255     int nyc = 0;
00256     int nzc = 0;
00257     int level = 0;
00258     int nlevd = 0;
00259
00260
00261
00262     // Utility variables
00263     int numlev = 0;
00264
00265     // Get the value of nlev here because it is needed for the iz matrix
00266     int nlev = VAT(iparm, 6);
00267     MAT2(iz, 50, nlev);
00268
00269     // Decode integer parameters from the iparm array
00270     nul = VAT(iparm, 7);
00271     nu2 = VAT(iparm, 8);
00272     mgkey = VAT(iparm, 9);
00273     itmax = VAT(iparm, 10);
00274     istop = VAT(iparm, 11);
00275     iinfo = VAT(iparm, 12);
00276     ipkey = VAT(iparm, 14);
00277     mode = VAT(iparm, 16);
00278     mgprol = VAT(iparm, 17);
00279     mgcoar = VAT(iparm, 18);
00280     mgdisc = VAT(iparm, 19);
00281     mgsmoo = VAT(iparm, 20);
00282     mgsolv = VAT(iparm, 21);
00283     iperf = VAT(iparm, 22);
00284
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00285 // Decode real parameters from the rparm array
00286 errtol = VAT(rparm, 1);
00287 omegal = VAT(rparm, 9);
00288 omegan = VAT(rparm, 10);
00289
00291 Vprtstp(0, -99, 0.0, 0.0, 0.0);
00292
00293 // Build the multigrid data structure in iz
00294 Vbuildstr(nx, ny, nz, &nlev, iz);
00295
00296 // Start the timer
00297 Vnm_tstart(30, "Vmgsdrv2: fine problem setup");
00298
00299 // Build operator and rhs on fine grid
00300 ido = 0;
00301 Vbuildops(nx, ny, nz,
00302           &nlev, &ipkey, &iinfo, &ido, iz,
00303           &mgsprol, &mgscoar, &mgsolv, &mgsdisc,
00304           ipc, rpc, pc, ac, cc, fc,
00305           xf, yf, zf,
00306           gxcf, gycf, gzcfc,
00307           alcfc, a2cfc, a3cfc,
00308           ccfc, fcfc, tcfc);
00309
00310 // Stop the timer
00311 Vnm_tstop(30, "Vmgsdrv2: fine problem setup");
00312
00313 // Start the timer
00314 Vnm_tstart(30, "Vmgsdrv2: coarse problem setup");
00315
00316 // Build operator and rhs on all coarse grids
00317 ido = 1;
00318 Vbuildops(nx, ny, nz,
00319           &nlev, &ipkey, &iinfo, &ido, iz,
00320           &mgsprol, &mgscoar, &mgsolv, &mgsdisc,
00321           ipc, rpc, pc, ac, cc, fc,
00322           xf, yf, zf,
00323           gxcf, gycf, gzcfc,
00324           alcfc, a2cfc, a3cfc,
00325           ccfc, fcfc, tcfc);
00326
00327 // Stop the timer
00328 Vnm_tstop(30, "Vmgsdrv2: coarse problem setup");
00329
00330 // Determine Machine Epsilon
00331 epsiln = Vnm_epsmac();
00332
00333 /*****
00334 *** analysis ***
00335 *** note: we destroy the rhs function "fc" here in "mpower" ***
00336 *****/
00337
00338 // errtol and itmax
00339 itmax_p = 1000;
00340 iok_p = 0;
00341 nlev_real = nlev;
00342 nlevd = nlev_real;
00343
00344 // Finest level initialization
00345 nxf = *nx;
00346 nyf = *ny;
00347 nzf = *nz;
00348
00349 // Go down grids: compute max/min eigenvalues of all operators
00350 for (level=1; level <= nlev_real; level++) {
00351     nlevd = nlev_real - level + 1;
00352
00353     // Move down the grids
00354     if (level != 1) {
00355
00356         // Find new grid size
00357         numlev = 1;
00358         Vmkcoars(&numlev, &nxf, &nyf, &nzf, &nxc, &nyc, &nzc);
00359
00360         // New grid size ***
00361         nxf = nxc;
00362         nyf = nyc;
00363         nzf = nzc;
00364     }
00365
00366     if (iinfo > 1) {

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00367         VMESAGE3("Analysis ==> (%3d, %3d, %3d)", nxf, nyf, nzf);
00368     }
00369
00370
00371     // Largest eigenvalue of the system matrix A
00372     if (iperf == 1 || iperf == 3) {
00373
00374         if (iinfo > 1) {
00375             VMESAGE0("Power calculating rho(A)");
00376         }
00377
00378         iters_p = 0;
00379         iinfo_p = iinfo;
00380         errtol_p = 1.0e-4;
00381
00382         Vpower(&nxf, &nyf, &nzf,
00383             iz, &level,
00384             ipc, rpc, ac, cc,
00385             alcf, a2cf, a3cf, ccf,
00386             &rho_max, &rho_max_mod, &errtol_p,
00387             &itmax_p, &iters_p, &iinfo_p);
00388
00389         if (iinfo > 1) {
00390             VMESAGE1("Power iters = %d", iters_p);
00391             VMESAGE1("Power eigmax = %f", rho_max);
00392             VMESAGE1("Power (MODEL) = %f", rho_max_mod);
00393         }
00394
00395         // Smallest eigenvalue of the system matrix A
00396         if (iinfo > 1) {
00397             VMESAGE0("Ipower calculating lambda_min(A)...");
00398         }
00399
00400         iters_p = 0;
00401         iinfo_p = iinfo;
00402         errtol_p = 1.0e-4;
00403
00404         Vazeros(&nxf, &nyf, &nzf, u);
00405
00406         Vipower(&nxf, &nyf, &nzf, u, iz,
00407             alcf, a2cf, a3cf, ccf, fcf,
00408             &rho_min, &rho_min_mod, &errtol_p, &itmax_p, &iters_p,
00409             &nlevd, &level, &nlev_real, &mgsolv,
00410             &iok_p, &iinfo_p, &epsiln, &errtol, &omegal,
00411             &nul, &nu2, &mgs moo,
00412             ipc, rpc, pc, ac, cc, tcf);
00413
00414         if (iinfo > 1) {
00415             VMESAGE1("Ipower iters = %d", iters_p);
00416             VMESAGE1("Ipower eigmin = %f", rho_min);
00417             VMESAGE1("Ipower (MODEL) = %f", rho_min_mod);
00418
00419             // Condition number estimate
00420             VMESAGE1("Condition number = %f", rho_max / rho_min);
00421             VMESAGE1("Condition (MODEL) = %f", rho_max_mod / rho_min_mod);
00422         }
00423     }
00424
00425     // Spectral radius of the multigrid operator M
00426     // NOTE: due to lack of vectors, we destroy "fc" in mpower...
00427     if (iperf == 2 || iperf == 3) {
00428
00429         if (iinfo > 1) {
00430             VMESAGE0("Mpower calculating rho(M)");
00431         }
00432
00433         iters_p = 0;
00434         iinfo_p = iinfo;
00435         errtol_p = epsiln;
00436
00437         Vazeros(&nxf, &nyf, &nzf, RAT(u, VAT2(iz, 1, level)));
00438
00439         WARN_UNTESTED;
00440         Vmpower(&nxf, &nyf, &nzf, u, iz,
00441             alcf, a2cf, a3cf, ccf, fcf,
00442             &rho_p, &errtol_p, &itmax_p, &iters_p,
00443             &nlevd, &level, &nlev_real, &mgsolv,
00444             &iok_p, &iinfo_p, &epsiln,
00445             &errtol, &omegal, &nul, &nu2, &mgs moo,
00446             ipc, rpc, pc, ac, cc, fc, tcf);
00447

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00448         if (iinfo > 1) {
00449             VMESAGE1("Mpower iters = %d", iters_p);
00450             VMESAGE1("Mpower rho(M) = %f", rho_p);
00451         }
00452     }
00453
00454     // Reinitialize the solution function
00455
00456     Vazeros(&nxf, &nyf, &nzf, RAT(u, VAT2(iz, 1, level)));
00457
00458     // Next grid
00459 }
00460
00461 // Reinitialize the solution function
00462     Vazeros(nx, ny, nz, u);
00463
00464 /*****
00465 *** this overwrites the rhs array provided by pde specification ***
00466 **** compute an algebraically produced rhs for the given tcf *****/
00467
00468 if (istop == 4 || istop == 5 || iperf != 0 ) {
00469
00470     if (iinfo > 1) {
00471         VMESAGE0("Generating algebraic RHS from your soln...");
00472     }
00473
00474
00475     WARN_UNTESTED;
00476     Vbuildalg(nx, ny, nz, &mode, &nlev, iz,
00477             ipc, rpc, ac, cc, ccf, tcf, fc, fcf);
00478 }
00479
00480 /*****/
00481
00482 // Impose zero dirichlet boundary conditions (now in source fcn)
00483     VfboundPMG00(nx, ny, nz, u);
00484
00485 // Start the timer
00486     Vnm_tstart(30, "Vmgsdrv2: solve");
00487
00488 // Call specified multigrid method
00489 if (mode == 0 || mode == 2) {
00490     nlev_real = nlev;
00491     iok = 1;
00492     ilev = 1;
00493
00494     if (mgkey == 0) {
00495
00496         Vmvcs(nx, ny, nz,
00497             u, iz, alcf, a2cf, a3cf, ccf,
00498             &istop, &itmax, &iters, &ierror, &nlev,
00499             &ilev, &nlev_real, &mgsolv,
00500             &iok, &iinfo, &epsiln, &errtol, &omegal,
00501             &nul, &nu2, &mgs moo,
00502             ipc, rpc, pc, ac, cc, fc, tcf);
00503
00504     } else if (mgkey == 1) {
00505
00506         Vmvcs(nx, ny, nz,
00507             u, iz, alcf, a2cf, a3cf, ccf,
00508             &istop, &itmax, &iters, &ierror, &nlev,
00509             &ilev, &nlev_real, &mgsolv,
00510             &iok, &iinfo, &epsiln, &errtol, &omegal,
00511             &nul, &nu2, &mgs moo,
00512             ipc, rpc, pc, ac, cc, fc, tcf);
00513
00514     } else {
00515         VABORT_MSG1("Bad mgkey given: %d", mgkey);
00516     }
00517 }
00518
00519 if (mode == 1 || mode == 2) {
00520
00521     nlev_real = nlev;
00522     iok = 1;
00523     ilev = 1;
00524
00525     if (mgkey == 0) {
00526
00527         Vmvfas(nx, ny, nz,
00528             u, iz, alcf, a2cf, a3cf, ccf, fcf,

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```

00529             &istop, &itmax, &iters, &ierror, &nlev,
00530             &ilev, &nlev_real, &mgsolv,
00531             &iok, &iinfo, &epsiln, &errtol, &omegan,
00532             &nul, &nu2, &mgsmoo,
00533             ipc, rpc, pc, ac, cc, fc, tcf);
00534
00535     } else if (mgkey == 1) {
00536
00537         Vfmvfas(nx, ny, nz,
00538             u, iz,
00539             alcf, a2cf, a3cf, ccf, fcf,
00540             &istop, &itmax, &iters, &ierror, &nlev,
00541             &ilev, &nlev_real, &mgsolv,
00542             &iok, &iinfo, &epsiln, &errtol, &omegan,
00543             &nul, &nu2, &mgsmoo,
00544             ipc, rpc, pc, ac, cc, fc, tcf);
00545
00546     } else {
00547         VABORT_MSG1("Bad mgkey given: %d", mgkey);
00548     }
00549 }
00550
00551 // Stop the timer
00552 Vnm_tstop(30, "Vmgsdrv2: solve");
00553
00554 // Restore boundary conditions
00555 ibound = 1;
00556
00557 VfboundPMG(&ibound, nx, ny, nz, u, gxcf, gycf, gzcf);
00558 }
00559
00560
00561
00562 VPUBLIC void Vmgsz(int *mgcoar, int *mgdisc, int *mgsolv,
00563     int *nx, int *ny, int *nz,
00564     int *nlev,
00565     int *nxc, int *nyc, int *nzc,
00566     int *nf, int *nc,
00567     int *narr, int *narrc,
00568     int *n_rpc, int *n_iz, int *n_ipc,
00569     int *iretot, int *iintot) {
00570
00571     // Constants: num of different types of arrays in mg code
00572     int num_nf = 0;
00573     int num_narr = 2;
00574     int num_narrc = 27;
00575
00576     // Misc variables
00577     int nc_band, num_band, n_band;
00578     int nxf, nyf, nzf;
00579     int level;
00580     int num_nf_oper, num_narrc_oper;
00581
00582     // Utility variables
00583     int numlev;
00584
00585     // Go down grids: compute max/min eigenvalues of all operators
00586     *nf = *nx * *ny * *nz;
00587
00588     *narr = *nf;
00589
00590     nxf = *nx;
00591     nyf = *ny;
00592     nzf = *nz;
00593
00594     *nxc = *nx;
00595     *nyc = *ny;
00596     *nzc = *nz;
00597
00598     for (level=2; level<=*nlev; level++) {
00599
00600         //find new grid size ***
00601
00602         numlev = 1;
00603         Vmkcors(&numlev, &nxf, &nyf, &nzf, nxc, nyc, nzc);
00604
00605         // New grid size
00606         nxf = *nxc;
00607         nyf = *nyc;
00608         nzf = *nzc;
00609

```

```

00610         // Add the unknowns on this level to the total
00611         *narr += nxf * nyf * nzf;
00612     }
00613     *nc = *nxc * *nyc * *nzc;
00614     *narrc = *narr - *nf;
00615
00616     // Box or fem on fine grid?
00617     if (*mgdisc == 0) {
00618         num_nf_oper = 4;
00619     } else if (*mgdisc == 1) {
00620         num_nf_oper = 14;
00621     } else {
00622         Vnm_print(2, "Vmgsz: invalid mgdisc parameter: %d\n", *mgdisc);
00623     }
00624
00625     // Galerkin or standard coarsening?
00626     if ((*mgcoar == 0 || *mgcoar == 1) && *mgdisc == 0) {
00627         num_narrc_oper = 4;
00628     } else if (*mgcoar == 2) {
00629         num_narrc_oper = 14;
00630     } else {
00631         Vnm_print(2, "Vmgsz: invalid mgcoar parameter: %d\n", *mgcoar);
00632     }
00633
00634     // Symmetric banded linpack storage on coarse grid
00635     if (*mgsolv == 0) {
00636         n_band = 0;
00637     } else if (*mgsolv == 1) {
00638         if ((*mgcoar == 0 || *mgcoar == 1) && *mgdisc == 0) {
00639             num_band = 1 + (*nxc - 2) * (*nyc - 2);
00640         } else {
00641             num_band = 1 + (*nxc - 2) * (*nyc - 2) + (*nxc - 2) + 1;
00642         }
00643         nc_band = (*nxc - 2) * (*nyc - 2) * (*nzc - 2);
00644         n_band = nc_band * num_band;
00645     } else {
00646         Vnm_print(2, "Vmgsz: invalid mgsolv parameter: %d\n", *mgsolv);
00647     }
00648
00649     // Info work array required storage
00650     *n_rpc = 100 * (*nlev + 1);
00651
00652     // Resulting total required real storage for method
00653     *iretot = num_narr * *narr
00654         + (num_nf + num_nf_oper) * *nf
00655         + (num_narrc + num_narrc_oper) * *narrc
00656         + n_band
00657         + *n_rpc;
00658
00659     // The integer storage parameters ***
00660     *n_iz = 50 * (*nlev + 1);
00661     *n_ipc = 100 * (*nlev + 1);
00662
00663     // Resulting total required integer storage for method
00664     *iintot = *n_iz + *n_ipc;
00665 }

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9.131 mgdrvd.h

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00001
00054 #ifndef _MGDRVD_H_
00055 #define _MGDRVD_H_
00056
00057 #include "apbscfg.h"
00058
00059 #include "malloc/malloc.h"
00060
00061 #include "generic/vhal.h"
00062 #include "generic/vmatrix.h"
00063 #include "pmgc/mgsabd.h"
00064 #include "pmgc/mgcsd.h"
00065 #include "pmgc/powerd.h"
00066 #include "pmgc/mgfasd.h"
00067
00074 VEXTERN void Vmgdriv(
00075     int* iparm,
00076     double* rparm,
00077     int* iwork,

```

```

00078         double* rwork,
00079         double* u,
00080         double* xf,
00081         double* yf,
00082         double* zf,
00083         double* gxcf,
00084         double* gycf,
00085         double* gzcf,
00086         double* alcf,
00087         double* a2cf,
00088         double* a3cf,
00089         double* ccf,
00090         double* fcf,
00091         double* tcf
00092     );
00093
00130 VEXTERNC void Vmgdriv2(
00131     int *iparm,
00132     double *rparm,
00133     int *nx,
00134     int *ny,
00135     int *nz,
00136     double *u,
00137     int *iz,
00138     int *ipc,
00139     double *rpc,
00140     double *pc,
00141     double *ac,
00142     double *cc,
00143     double *fc,
00144     double *xf,
00145     double *yf,
00146     double *zf,
00147     double *gxcf,
00148     double *gycf,
00149     double *gzcf,
00150     double *alcf,
00151     double *a2cf,
00152     double *a3cf,
00153     double *ccf,
00154     double *fcf,
00155     double *tcf
00156 );
00157
00158
00159
00229 VEXTERNC void Vmgisz(
00230     int *mgcoar,
00231     int *mgdisc,
00232     int *mgsolv,
00233     int *nx,
00234     int *ny,
00235     int *nz,
00236     int *nlev,
00237     int *nxc,
00238     int *nyc,
00239     int *nzc,
00240     int *nf,
00241     int *nc,
00242     int *narr,
00243     int *narre,
00244     int *n_rpc,
00245     int *n_iz,
00246     int *n_ipc,
00247     int *iretot,
00248     int *iintot
00249 );
00250
00251
00252
00253 #endif /* _MGDRVD_H_ */

```

9.132 mgfasd.c

```

00001
00055 #include "mgfasd.h"
00056
00057 VPUBLIC void Vfmvfas(int *nx, int *ny, int *nz,

```

```

00058     double *x,
00059     int *iz,
00060     double *w0, double *w1, double *w2, double *w3, double *w4,
00061     int *istop, int *itmx, int *iters, int *ierror,
00062     int *nlev, int *ilev, int *nlev_real,
00063     int *mgsolv, int *iok, int *iinfo,
00064     double *epsiln, double *errtol, double *omega,
00065     int *nu1, int *nu2, int *mgsmoo,
00066     int *ipc, double *rpc,
00067     double *pc, double *ac, double *cc, double *fc, double *tru) {
00068
00069     // Other Declarations
00070     int level, itmx, nlev, iter, iok;
00071     int nxf, nyf, nzf;
00072     int nxc, nyc, nzc;
00073     int istp, iinfod;
00074     double errd;
00075
00076     // Utility variables
00077     int numlev;
00078
00079     MAT2(iz, 50, *nlev);
00080
00081     // Recover gridsizes
00082     nxf = *nx;
00083     nyf = *ny;
00084     nzf = *nz;
00085
00086     numlev = *nlev - 1;
00087     Vmkcors(&numlev, &nxf, &nyf, &nzf, &nxc, &nyc, &nzc);
00088
00089     // Move up grids: interpolate solution to finer, do v cycle
00090     if (*iinfo != 0) {
00091         Vnm_print(2, "Vfmvfas: starting: (%d,%d,%d) (%d,%d,%d)\n",
00092                 nxf, nyf, nzf, nxc, nyc, nzc);
00093     }
00094
00095     for (level = *nlev_real; level >= *ilev + 1; level--) {
00096
00097         // Call mv cycle
00098         errd = 1.0e-5;
00099         itmx = 1;
00100         nlev = *nlev_real - level + 1;
00101         iter = 0;
00102         iok = 2;
00103         iinfod = *iinfo;
00104         istp = *istop;
00105         if (*iinfo >= 2)
00106             iok = 2;
00107
00108         Vmvfas(&nxc, &nyc, &nzc,
00109              x,
00110              iz,
00111              w0, w1, w2, w3, w4,
00112              &istp, &itmx, &iter, ierror,
00113              &nlev, &level, nlev_real,
00114              mgsolv, &iok, &iinfod,
00115              epsiln, errtol, omega,
00116              nu1, nu2, mgsmoo,
00117              ipc, rpc,
00118              pc, ac, cc, fc, tru);
00119
00120
00121         // Find new grid size
00122         numlev = 1;
00123         Vmkfine(&numlev, &nxc, &nyc, &nzc, &nxf, &nyf, &nzf);
00124
00125         // Interpolate to next finer grid
00126         VinterpPMG(&nxc, &nyc, &nzc,
00127                  &nxf, &nyf, &nzf,
00128                  RAT(x, VAT2(iz, 1, level)),
00129                  RAT(x, VAT2(iz, 1, level-1)),
00130                  RAT(pc, VAT2(iz, 11, level-1)));
00131
00132         // New grid size
00133         nxc = nxf;
00134         nyc = nyf;
00135         nzc = nzf;
00136     }
00137
00138

```



```

00139
00140 // Call mv cycle
00141 level = *ilev;
00142
00143 Vmvmfas(&nxf, &nyf, &nzf,
00144         x, iz,
00145         w0, w1, w2, w3, w4,
00146         istop, itmax, iters,
00147         ierror, nlev, &level, nlev_real,
00148         mgsolv, iok, iinfo,
00149         epsiln, ertol, omega,
00150         nul, nu2, mgsmoo,
00151         ipc, rpc,
00152         pc, ac, cc, fc, tru);
00153 }
00154
00155
00156
00157 VPUBLIC void Vmvmfas(int *nx, int *ny, int *nz,
00158                     double *x,
00159                     int *iz,
00160                     double *w0, double *w1, double *w2, double *w3, double *w4,
00161                     int *istop, int *itmax, int *iters, int *ierror,
00162                     int *nlev, int *ilev, int *nlev_real,
00163                     int *mgsolv, int *iok, int *iinfo,
00164                     double *epsiln, double *ertol, double *omega,
00165                     int *nul, int *nu2, int *mgsmoo,
00166                     int *ipc, double *rpc,
00167                     double *pc, double *ac, double *cc, double *fc, double *tru) {
00168
00169 // Other declarations
00170 int level, lev;
00171 int itmax_s, iters_s, nuuu, ivariv, mgsmoo_s, iresid;
00172 int nxf, nyf, nzf;
00173 int nxc, nyc, nzc;
00174 int iadjoint;
00175 double ertol_s;
00176 double rsden, rsnm, orsnrm;
00177 double xdamp;
00178
00179 int numlev;
00180 double alpha;
00181
00182 MAT2(iz, 50, *nlev);
00183
00184 WARN_UNTESTED;
00185
00186 // Recover level information
00187 level = 1;
00188 lev = (*ilev - 1) + level;
00189
00190 // Recover gridsizes
00191 nxf = *nx;
00192 nyf = *ny;
00193 nzf = *nz;
00194
00195 numlev = *nlev - 1;
00196 Vmkcors(&numlev, &nxf, &nyf, &nzf, &nxc, &nyc, &nzc);
00197
00198 // Do some i/o if requested
00199 if (*iinfo != 0) {
00200     Vnm_print(2, "Vmvmfas: starting: (%d, %d, %d) (%d, %d, %d)\n",
00201              nxf, nyf, nzf, nxc, nyc, nzc);
00202 }
00203
00204 // Initial wall clock
00205 if (*iok != 0) {
00206     Vprtstp(*iok, -1, 0.0, 0.0, 0.0);
00207 }
00208
00209 /*****
00210 *** note: if (iok != 0) then: use a stopping test. ***
00211 *** else: use just the itmax to stop iteration. ***
00212 *****/
00213 *** istop=0 most efficient (whatever it is) ***
00214 *** istop=1 relative residual ***
00215 *** istop=2 rms difference of successive iterates ***
00216 *** istop=3 relative true error (provided for testing) ***
00217 *****/
00218
00219 // Compute denominator for stopping criterion

```

```

00220     if (*iok != 0) {
00221         if (*istop == 0) {
00222             rsden = 1.0;
00223         } else if (*istop == 1) {
00224
00225             // Compute initial residual with zero initial guess
00226             // this is analogous to the linear case where one can
00227             // simply take norm of rhs for a zero initial guess
00228             Vazeros(&nxf, &nyf, &nzf, w1);
00229
00230             Vnmresid(&nxf, &nyf, &nzf,
00231                     RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00232                     RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00233                     RAT(fc, VAT2(iz, 1, lev)),
00234                     w1, w2, w3);
00235
00236             rsden = Vxnrm1(&nxf, &nyf, &nzf, w2);
00237
00238         } else if (*istop == 2) {
00239             rsden = VSQRT(nxf * nyf * nzf);
00240         } else if (*istop == 3) {
00241             rsden = Vxnrm2(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1, lev)));
00242         } else if (*istop == 4) {
00243             rsden = Vxnrm2(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1, lev)));
00244         } else if (*istop == 5) {
00245             Vnmvec(&nxf, &nyf, &nzf,
00246                  RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00247                  RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00248                  RAT(tru, VAT2(iz, 1, lev)),
00249                  w1, w2);
00250             rsden = VSQRT(Vxdot(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1, lev)), w1));
00251         } else {
00252             Vnm_print(2, "Vmvfas: bad istop value: %d\n", *istop);
00253         }
00254         if (rsden == 0.0) {
00255             rsden = 1.0;
00256             Vnm_print(2, "Vmfas: rhs is zero on finest level\n");
00257         }
00258         rsnm = rsden;
00259         orsnm = rsnm;
00260
00261         Vprtstp(*iok, 0, rsnm, rsden, orsnm);
00262     }
00263
00264
00265
00266     /*****
00267     *** solve directly if nlev = 1
00268     *****/
00269
00270     // Solve directly if on the coarse grid
00271     if (*nlev == 1) {
00272
00273         //solve with ncghs, mgsmoo_s=4 (no residual)
00274         iresid = 0;
00275         iadjoint = 0;
00276         itmax_s = 100;
00277         iters_s = 0;
00278         errtol_s = *epsiln;
00279         mgsmoo_s = *mgsmoo;
00280         Vazeros(&nxf, &nyf, &nzf, RAT(x, VAT2(iz, 1, lev)));
00281         Vnsmooth(&nxf, &nyf, &nzf,
00282                RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00283                RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00284                RAT(fc, VAT2(iz, 1, lev)),
00285                RAT(x, VAT2(iz, 1, lev)),
00286                w1, w2, w3,
00287                &itmax_s, &iters_s, &errtol_s, omega,
00288                &iresid, &iadjoint, &mgsmoo_s);
00289
00290         // Compute the stopping test
00291         *iters = 1;
00292         if (*iok != 0) {
00293             orsnm = rsnm;
00294             if (*istop == 0) {
00295                 Vnmresid(&nxf, &nyf, &nzf,
00296                        RAT(ipc, VAT2(iz, 5, lev)),
00297                        RAT(rpc, VAT2(iz, 6, lev)),
00298                        RAT(ac, VAT2(iz, 7, lev)),
00299                        RAT(cc, VAT2(iz, 1, lev)),
00300                        RAT(fc, VAT2(iz, 1, lev)),

```

```

00301         RAT( x, VAT2(iz, 1, lev)),
00302         w1, w2);
00303         rsnrn = Vxnrm1(&nxf, &nyf, &nzf, w1);
00304     } else if (*istop == 1) {
00305         Vnmresid(&nxf, &nyf, &nzf,
00306                 RAT(ipc, VAT2(iz, 5, lev)),
00307                 RAT(rpc, VAT2(iz, 6, lev)),
00308                 RAT( ac, VAT2(iz, 7, lev)),
00309                 RAT( cc, VAT2(iz, 1, lev)),
00310                 RAT( fc, VAT2(iz, 1, lev)),
00311                 RAT( x, VAT2(iz, 1, lev)),
00312                 w1, w2);
00313         rsnrn = Vxnrm1(&nxf, &nyf, &nzf, w1);
00314     } else if (*istop == 2) {
00315         Vxcopy(&nxf, &nyf, &nzf,
00316               RAT(tru, VAT2(iz, 1, lev)),
00317               w1);
00318         alpha = -1.0;
00319         Vxaxpy(&nxf, &nyf, &nzf,
00320               &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00321         rsnrn = Vxnrm1(&nxf, &nyf, &nzf, w1);
00322         Vxcopy(&nxf, &nyf, &nzf,
00323               RAT(x, VAT2(iz, 1, lev)),
00324               RAT(tru, VAT2(iz, 1, lev)));
00325     } else if (*istop == 3) {
00326         Vxcopy(&nxf, &nyf, &nzf,
00327               RAT(tru, VAT2(iz, 1, lev)),
00328               w1);
00329         alpha = -1.0;
00330         Vxaxpy(&nxf, &nyf, &nzf,
00331               &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00332         rsnrn = Vxnrm2(&nxf, &nyf, &nzf, w1);
00333     } else if (*istop == 4) {
00334         Vxcopy(&nxf, &nyf, &nzf,
00335               RAT(tru, VAT2(iz, 1, lev)),
00336               w1);
00337         alpha = -1.0;
00338         Vxaxpy(&nxf, &nyf, &nzf,
00339               &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00340         rsnrn = Vxnrm2(&nxf, &nyf, &nzf, w1);
00341     } else if (*istop == 5) {
00342         Vxcopy(&nxf, &nyf, &nzf,
00343               RAT(tru, VAT2(iz, 1, lev)),
00344               w1);
00345         alpha = -1.0;
00346         Vxaxpy(&nxf, &nyf, &nzf,
00347               &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00348         Vnmatvec(&nxf, &nyf, &nzf,
00349                 RAT(ipc, VAT2(iz, 5, lev)),
00350                 RAT(rpc, VAT2(iz, 6, lev)),
00351                 RAT( ac, VAT2(iz, 7, lev)),
00352                 RAT( cc, VAT2(iz, 1, lev)),
00353                 w1, w2, w3);
00354         rsnrn = VSQRT(Vxdot(&nxf, &nyf, &nzf, w1, w2));
00355     } else {
00356         Vnm_print(2, "Vmcs: bad istop value: %d\n", *istop);
00357     }
00358
00359     Vprtstp(*iok, *iters, rsnrn, rsden, orsnrm);
00360 }
00361 return;
00362 }
00363
00364 /*****
00365 *** begin mg iteration (note nxf,nyf,nzf changes during loop)
00366 *****/
00367
00368 // setup for the v-cycle looping ***
00369 *iters = 0;
00370 while(1) {
00371
00372     // Finest level initialization
00373     level = 1;
00374     lev  = (*ilev - 1) + level;
00375
00376     // Nul pre-smoothings on fine grid (with residual)
00377     iresid = 1;
00378     iadjoin = 0;
00379     iters_s = 0;
00380     errtol_s = 0.0;
00381     nuu = Vivariv(nul, &lev);

```

```

00382     Vnsmooth(&nxf, &nyf, &nzf,
00383             RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00384             RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00385             RAT(fc, VAT2(iz, 1, lev)), RAT(x, VAT2(iz, 1, lev)),
00386             w2, w3, w1,
00387             &nuuu, &iters_s, &errtol_s, omega,
00388             &iresid, &iadjoint, mgsmoo);
00389     Vxcopy(&nxf, &nyf, &nzf, w1, RAT(w0, VAT2(iz, 1, lev)));
00390
00391     /* *****
00392     * begin cycling down to coarse grid
00393     * *****
00394
00395     // Go down grids: restrict resid to coarser and smooth
00396     for (level = 2; level <= *nlev; level++) {
00397         lev = (*ilev - 1) + level;
00398
00399         // Find new grid size
00400         numlev = 1;
00401         Vmkcors(&numlev, &nxf, &nyf, &nzf, &nxc, &nyc, &nzc);
00402
00403         // Restrict residual to coarser grid
00404         Vrestrc(&nxf, &nyf, &nzf, &nxc, &nyc, &nzc,
00405             w1, RAT(w0, VAT2(iz, 1, lev)),
00406             RAT(pc, VAT2(iz, 11, lev-1)));
00407
00408         // Restrict (extract) solution to coarser grid
00409         Vextrac(&nxf, &nyf, &nzf, &nxc, &nyc, &nzc,
00410             RAT(x, VAT2(iz, 1, lev-1)), RAT(w4, VAT2(iz, 1, lev)));
00411
00412         // New grid size
00413         nxf = nxc;
00414         nyf = nyc;
00415         nzf = nzc;
00416
00417         // Apply coarse grid operator to coarse grid soln
00418         Vnmatvec(&nxf, &nyf, &nzf,
00419             RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00420             RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00421             RAT(w4, VAT2(iz, 1, lev)), RAT(fc, VAT2(iz, 1, lev)),
00422             w3);
00423
00424         // Build coarse grid right hand side
00425         alpha = 1.0;
00426         Vxaxpy(&nxf, &nyf, &nzf, &alpha,
00427             RAT(w0, VAT2(iz, 1, lev)), RAT(fc, VAT2(iz, 1, lev)));
00428
00429         // If not on coarsest level yet...
00430         if (level != *nlev) {
00431
00432             // nul pre-smoothings on this level (with residual)
00433             Vxcopy(&nxf, &nyf, &nzf,
00434                 RAT(w4, VAT2(iz, 1, lev)), RAT(x, VAT2(iz, 1, lev)));
00435             iresid = 1;
00436             iadjoint = 0;
00437             iters_s = 0;
00438             errtol_s = 0.0;
00439             nuuu = Vivariv(nul, &lev);
00440             Vnsmooth(&nxf, &nyf, &nzf,
00441                 RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00442                 RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00443                 RAT(fc, VAT2(iz, 1, lev)),
00444                 RAT(x, VAT2(iz, 1, lev)),
00445                 w2, w3, w1,
00446                 &nuuu, &iters_s, &errtol_s, omega,
00447                 &iresid, &iadjoint, mgsmoo);
00448         }
00449
00450         // End of cycling down to coarse grid loop
00451     }
00452
00453     /* *****
00454     * begin coarse grid
00455     * *****
00456
00457     // Coarsest level
00458     level = *nlev;
00459     lev = (*ilev - 1) + level;
00460
00461
00462

```

```

00463      // Solve on coarsest grid with ncghs, mgsmoo_s=4 (no residual)
00464      iresid = 0;
00465      iadjoint = 0;
00466      itmax_s = 100;
00467      iters_s = 0;
00468      errtol_s = *epsiln;
00469      mgsmoo_s = *mgsmoo;
00470      Vazeros(&nxf, &nyf, &nzf, RAT(x, VAT2(iz, 1, lev)));
00471      Vnsmooth(&nxf, &nyf, &nzf,
00472              RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00473              RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00474              RAT(fc, VAT2(iz, 1, lev)),
00475              RAT(x, VAT2(iz, 1, lev)),
00476              w1, w2, w3,
00477              &itmax_s, &iters_s, &errtol_s, omega,
00478              &iresid, &iadjoint, &mgsmoo_s);
00479
00480      /* *****
00481      * begin cycling back to fine grid
00482      * *****/
00483
00484      // Move up grids: interpolate resid to finer and smooth
00485      for (level = *nlev - 1; level >= 1; level--) {
00486          lev = (*ilev - 1) + level;
00487
00488          // Find new grid size
00489          numlev = 1;
00490          Vmkfine(&numlev, &nxf, &nyf, &nzf, &nxc, &nyc, &nzc);
00491
00492          // Form difference of new approx at the coarse grid
00493          alpha = -1.0;
00494          Vxaxpy(&nxf, &nyf, &nzf, &alpha,
00495              RAT(w4, VAT2(iz, 1, lev + 1)), RAT(x, VAT2(iz, 1, lev + 1)));
00496
00497          // Call the line search (on the coarser level)
00498          Vlinesearch(&nxf, &nyf, &nzf, &xdamp,
00499              RAT(ipc, VAT2(iz, 5, lev + 1)),
00500              RAT(rpc, VAT2(iz, 6, lev + 1)),
00501              RAT(ac, VAT2(iz, 7, lev + 1)),
00502              RAT(cc, VAT2(iz, 1, lev + 1)),
00503              RAT(fc, VAT2(iz, 1, lev + 1)),
00504              RAT(x, VAT2(iz, 1, lev + 1)),
00505              RAT(w4, VAT2(iz, 1, lev + 1)),
00506              RAT(w0, VAT2(iz, 1, lev + 1)),
00507              w1, w2, w3);
00508
00509          // Interpolate to next finer grid
00510          VinterpMG(&nxf, &nyf, &nzf, &nxc, &nyc, &nzc,
00511              RAT(x, VAT2(iz, 1, lev + 1)),
00512              w1,
00513              RAT(pc, VAT2(iz, 11, lev)));
00514
00515          // New grid size
00516          nxf = nxc;
00517          nyf = nyc;
00518          nzf = nzc;
00519
00520          // Perform the coarse grid correction
00521          Vxaxpy(&nxf, &nyf, &nzf, &xdamp, w1, RAT(x, VAT2(iz, 1, lev)));
00522
00523          // nu2 post-smoothings for correction (no residual) ***
00524          iresid = 0;
00525          iadjoint = 1;
00526          iters_s = 0;
00527          errtol_s = 0.0;
00528          nuuu = Vivariv(nu2, &lev);
00529          Vnsmooth(&nxf, &nyf, &nzf,
00530              RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00531              RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00532              RAT(fc, VAT2(iz, 1, lev)),
00533              RAT(x, VAT2(iz, 1, lev)),
00534              w1, w2, w3,
00535              &nuuu, &iters_s, &errtol_s, omega,
00536              &iresid, &iadjoint, mgsmoo);
00537      }
00538
00539
00540      /* *****
00541      * iteration complete: do some i/o
00542      * *****/
00543

```

```

00544      // Increment the iteration counter
00545      iters = iters + 1;
00546
00547      // Compute/check the current stopping test
00548      if (*iok != 0) {
00549          orsnrm = rsnm;
00550          if (*istop == 0) {
00551              Vnmresid(&nxf, &nyf, &nzf,
00552                      RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00553                      RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00554                      RAT(fc, VAT2(iz, 1, lev)), RAT(x, VAT2(iz, 1, lev)),
00555                      w1, w2);
00556              rsnm = Vxnrm1(&nxf, &nyf, &nzf, w1);
00557          } else if (*istop == 1) {
00558              Vnmresid(&nxf, &nyf, &nzf,
00559                      RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00560                      RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00561                      RAT(fc, VAT2(iz, 1, lev)), RAT(x, VAT2(iz, 1, lev)),
00562                      w1, w2);
00563              rsnm = Vxnrm1(&nxf, &nyf, &nzf, w1);
00564          } else if (*istop == 2) {
00565              Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1, lev)), w1);
00566              alpha = -1.0;
00567              Vxaxpy(&nxf, &nyf, &nzf, &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00568              rsnm = Vxnrm1(&nxf, &nyf, &nzf, w1);
00569              Vxcopy(&nxf, &nyf, &nzf,
00570                      RAT(x, VAT2(iz, 1, lev)),
00571                      RAT(tru, VAT2(iz, 1, lev)));
00572          } else if (*istop == 3) {
00573              Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1, lev)), w1);
00574              alpha = -1.0;
00575              Vxaxpy(&nxf, &nyf, &nzf, &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00576              rsnm = Vxnrm2(&nxf, &nyf, &nzf, w1);
00577          } else if (*istop == 4) {
00578              Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1, lev)), w1);
00579              alpha = -1.0;
00580              Vxaxpy(&nxf, &nyf, &nzf, &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00581              rsnm = Vxnrm2(&nxf, &nyf, &nzf, w1);
00582          } else if (*istop == 5) {
00583              Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1, lev)), w1);
00584              alpha = -1.0;
00585              Vxaxpy(&nxf, &nyf, &nzf, &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00586              Vnmatvec(&nxf, &nyf, &nzf,
00587                      RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00588                      RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00589                      w1, w2, w3);
00590              rsnm = VSQRT(Vxdot(&nxf, &nyf, &nzf, w1, w2));
00591          } else {
00592              VABORT_MSG1("Bad istop value: %d", *istop);
00593          }
00594
00595          Vprtstp(*iok, *iters, rsnm, rsden, orsnrm);
00596
00597          if ((rsnm / rsden) <= *errtol)
00598              break;
00599      }
00600
00601      if (*iters >= *itmax) {
00602          *ierror = 1;
00603          break;
00604      }
00605  }
00606 }

```

9.133 mgfasd.h

```

00001
00049 #ifndef _MGFASD_H_
00050 #define _MGFASD_H_
00051
00052 #include "apbsefg.h"
00053
00054 #include "maloc/maloc.h"
00055
00056 #include "generic/vhal.h"
00057 #include "pmgc/smoothd.h"
00058 #include "pmgc/mgsbd.h"
00059

```

```
00072 VEXTERNC void Vfmvfas(
00073     int      *nx,
00074     int      *ny,
00075     int      *nz,
00076     double   *x,
00077     int      *iz,
00078     double   *w0,
00079     double   *w1,
00080     double   *w2,
00081     double   *w3,
00082     double   *w4,
00083     int      *istop,
00084     int      *itmax,
00085     int      *iters,
00086     int      *ierror,
00087     int      *nlev,
00088     int      *ilev,
00089     int      *nlev_real,
00090     int      *mgsolv,
00091     int      *iok,
00092     int      *iinfo,
00093     double   *epsiln,
00094     double   *errtol,
00095     double   *omega,
00096     int      *nul,
00097     int      *nu2,
00098     int      *mgsmoo,
00099     int      *ipc,
00100     double   *rpc,
00101     double   *pc,
00102     double   *ac,
00103     double   *cc,
00104     double   *fc,
00105     double   *tru
00106 );
00107
00108
00109
00151 VEXTERNC void Vmvfas(
00152     int      *nx,
00153     int      *ny,
00154     int      *nz,
00155     double   *x,
00156     int      *iz,
00157     double   *w0,
00158     double   *w1,
00159     double   *w2,
00160     double   *w3,
00161     double   *w4,
00162     int      *istop,
00163     int      *itmax,
00164     int      *iters,
00165     int      *ierror,
00166     int      *nlev,
00167     int      *ilev,
00168     int      *nlev_real,
00169     int      *mgsolv,
00170     int      *iok,
00171     int      *iinfo,
00172     double   *epsiln,
00173     double   *errtol,
00174     double   *omega,
00175     int      *nul,
00176     int      *nu2,
00177     int      *mgsmoo,
00178     int      *ipc,
00179     double   *rpc,
00180     double   *pc,
00181     double   *ac,
00182     double   *cc,
00183     double   *fc,
00184     double   *tru
00185 );
00186
00187 #endif /* _MGFASD_H_ */
00188
```

9.134 mgsbnd.c

```

00001
00055 #include "mgsbnd.h"
00056
00057 VPUBLIC void Vbuildops(
00058     int *nx, int *ny, int *nz,
00059     int *nlev, int *ipkey, int *iinfo,
00060     int *ido, int *iz,
00061     int *mgprol, int *mgcoar, int *mgsolv, int *mgdisc, int *ipc,
00062     double *rpc, double *pc, double *ac, double *cc, double *fc,
00063     double *xf, double *yf, double *zf,
00064     double *gxcf, double *gycf, double *gzcf,
00065     double *alcf, double *a2cf, double *a3cf,
00066     double *ccf, double *fcf, double *tcf
00067 ) {
00068
00069     // @todo Document this function
00070     int lev = 0;
00071     int nxx = 0;
00072     int nyy = 0;
00073     int nzz = 0;
00074     int nxold = 0;
00075     int nyold = 0;
00076     int nzold = 0;
00077     int numdia = 0;
00078     int key = 0;
00079
00080     // Utility variables
00081     int i;
00082
00083     MAT2(iz, 50, *nlev);
00084
00085     // Setup
00086     nxx = *nx;
00087     nyy = *ny;
00088     nzz = *nz;
00089
00090     // Build the operator a on the finest level
00091     if (*ido == 0 || *ido == 2) {
00092
00093         lev = 1;
00094
00095         // Some i/o
00096         if (*iinfo > 0)
00097             VMESAGE3("Fine: (%03d, %03d, %03d)", nxx, nyy, nzz);
00098
00099         // Finest level discretization
00100         VbuildA(&nxx, &nyy, &nzz,
00101             ipkey, mgdisc, &numdia,
00102             RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00103             RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)), RAT(fc, VAT2(iz, 1,lev)),
00104             RAT(xf, VAT2(iz, 8,lev)), RAT(yf, VAT2(iz, 9,lev)), RAT(zf, VAT2(iz, 10,lev)),
00105             RAT(gxcf, VAT2(iz, 2,lev)), RAT(gycf, VAT2(iz, 3,lev)), RAT(gzcf, VAT2(iz, 4,lev)),
00106             RAT(alcf, VAT2(iz, 1,lev)), RAT(a2cf, VAT2(iz, 1,lev)), RAT(a3cf, VAT2(iz, 1,lev)),
00107             RAT(ccf, VAT2(iz, 1,lev)), RAT(fcf, VAT2(iz, 1,lev)));
00108
00109         VMESAGE2("Operator stencil (lev, numdia) = (%d, %d)", lev, numdia);
00110
00111         // Now initialize the differential operator offset
00112         VAT2(iz, 7, lev+1) = VAT2(iz, 7, lev) + numdia * nxx * nyy * nzz;
00113
00114         // Debug
00115         if (*iinfo > 7) {
00116             Vprtmtd(&nxx, &nyy, &nzz,
00117                 RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)), RAT(ac, VAT2(iz, 7,lev)));
00118         }
00119     }
00120
00121     // Build the (nlev-1) level operators
00122     if (*ido == 1 || *ido == 2 || *ido == 3) {
00123
00124         for (lev=2; lev<=*nlev; lev++) {
00125             nxold = nxx;
00126             nyold = nyy;
00127             nzold = nzz;
00128             i = 1;
00129
00130             Vmkcors(&i, &nxold, &nyold, &nzold, &nxx, &nyy, &nzz);
00131

```



```

00132         if (*ido != 3) {
00133
00134             // Build the interpolation operator on this level
00135             VbuildP(&nxold, &nyold, &nzold,
00136                 &nxx, &nyy, &nzz,
00137                 mgprol,
00138                 RAT(ipc, VAT2(iz, 5, lev-1)), RAT(rpc, VAT2(iz, 6, lev-1)),
00139                 RAT(pc, VAT2(iz, 11, lev-1)), RAT(ac, VAT2(iz, 7, lev-1)),
00140                 RAT(xf, VAT2(iz, 8, lev-1)), RAT(yf, VAT2(iz, 9, lev-1)), RAT(zf, VAT2(iz,
10, lev-1)));
00141
00142             // Differential operator this level with standard disc.
00143             if (*mgcoar == 0) {
00144
00145                 // Some i/o
00146                 if (*iinfo > 0)
00147                     VMESAGE3("Stand: (%03d, %03d, %03d)", nxx, nyy, nzz);
00148
00149
00150
00151                 Vbuildcopy0(&nxx, &nyy, &nzz,
00152                     &nxold, &nyold, &nzold,
00153                     RAT(xf, VAT2(iz, 8, lev )), RAT(yf, VAT2(iz, 9, lev )), RAT(zf, VAT2(iz,
10, lev )),
00154                     RAT(gxcf, VAT2(iz, 2, lev )), RAT(gycf, VAT2(iz, 3, lev )), RAT(gzcf, VAT2(iz,
4, lev )),
00155                     RAT(alcf, VAT2(iz, 1, lev )), RAT(a2cf, VAT2(iz, 1, lev )), RAT(a3cf, VAT2(iz,
1, lev )),
00156                     RAT(ccf, VAT2(iz, 1, lev )), RAT(fcf, VAT2(iz, 1, lev )), RAT(tcf, VAT2(iz,
1, lev )),
00157                     RAT(xf, VAT2(iz, 8, lev-1)), RAT(yf, VAT2(iz, 9, lev-1)), RAT(zf, VAT2(iz,
10, lev-1)),
00158                     RAT(gxcf, VAT2(iz, 2, lev-1)), RAT(gycf, VAT2(iz, 3, lev-1)), RAT(gzcf, VAT2(iz,
4, lev-1)),
00159                     RAT(alcf, VAT2(iz, 1, lev-1)), RAT(a2cf, VAT2(iz, 1, lev-1)), RAT(a3cf, VAT2(iz,
1, lev-1)),
00160                     RAT(ccf, VAT2(iz, 1, lev-1)), RAT(fcf, VAT2(iz, 1, lev-1)), RAT(tcf, VAT2(iz,
1, lev-1)));
00161
00162                 VbuildA(&nxx, &nyy, &nzz,
00163                     ipkey, mgdisc, &numdia,
00164                     RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00165                     RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)), RAT(fc, VAT2(iz,
1, lev)),
00166                     RAT(xf, VAT2(iz, 8, lev)), RAT(yf, VAT2(iz, 9, lev)), RAT(zf, VAT2(iz,
10, lev)),
00167                     RAT(gxcf, VAT2(iz, 2, lev)), RAT(gycf, VAT2(iz, 3, lev)), RAT(gzcf, VAT2(iz,
4, lev)),
00168                     RAT(alcf, VAT2(iz, 1, lev)), RAT(a2cf, VAT2(iz, 1, lev)), RAT(a3cf, VAT2(iz,
1, lev)),
00169                     RAT(ccf, VAT2(iz, 1, lev)), RAT(fcf, VAT2(iz, 1, lev)));
00170             }
00171
00172             // Differential operator this level with harmonic disc.
00173             else if (*mgcoar == 1) {
00174
00175                 // Some i/o
00176                 if (*iinfo > 0)
00177                     VMESAGE3("Harm0: (%03d, %03d, %03d)", nxx, nyy, nzz);
00178
00179
00180                 Vbuildharm0(&nxx, &nyy, &nzz, &nxold, &nyold, &nzold,
00181                     RAT(xf, VAT2(iz, 8, lev )), RAT(yf, VAT2(iz, 9, lev )), RAT(zf,
VAT2(iz, 10, lev )),
00182                     RAT(gxcf, VAT2(iz, 2, lev )), RAT(gycf, VAT2(iz, 3, lev )), RAT(gzcf,
VAT2(iz, 4, lev )),
00183                     RAT(alcf, VAT2(iz, 1, lev )), RAT(a2cf, VAT2(iz, 1, lev )), RAT(a3cf,
VAT2(iz, 1, lev )),
00184                     RAT(ccf, VAT2(iz, 1, lev )), RAT(fcf, VAT2(iz, 1, lev )), RAT(tcf,
VAT2(iz, 1, lev )),
00185                     RAT(xf, VAT2(iz, 8, lev-1)), RAT(yf, VAT2(iz, 9, lev-1)), RAT(zf,
VAT2(iz, 10, lev-1)),
00186                     RAT(gxcf, VAT2(iz, 2, lev-1)), RAT(gycf, VAT2(iz, 3, lev-1)), RAT(gzcf,
VAT2(iz, 4, lev-1)),
00187                     RAT(alcf, VAT2(iz, 1, lev-1)), RAT(a2cf, VAT2(iz, 1, lev-1)), RAT(a3cf,
VAT2(iz, 1, lev-1)),
00188                     RAT(ccf, VAT2(iz, 1, lev-1)), RAT(fcf, VAT2(iz, 1, lev-1)), RAT(tcf,
VAT2(iz, 1, lev-1)));
00189
00190                 VbuildA(&nxx, &nyy, &nzz,
00191                     ipkey, mgdisc, &numdia,
00192                     RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),

```

```

00192         RAT(ac, VAT2(iz, 7,lev)),    RAT(cc, VAT2(iz, 1,lev)),    RAT(fc, VAT2(iz,
00193         1,lev)),
00193         RAT(xf, VAT2(iz, 8,lev)),    RAT(yf, VAT2(iz, 9,lev)),    RAT(zf, VAT2(iz,
00194         10,lev)),
00194         RAT(gxcf, VAT2(iz, 2,lev)), RAT(gycf, VAT2(iz, 3,lev)), RAT(gzcf, VAT2(iz,
00195         4,lev)),
00195         RAT(alcf, VAT2(iz, 1,lev)), RAT(a2cf, VAT2(iz, 1,lev)), RAT(a3cf, VAT2(iz,
00196         1,lev)),
00196         RAT(ccf, VAT2(iz, 1,lev)),    RAT(fcf, VAT2(iz, 1,lev));
00197     }
00198
00199     // Differential operator with galerkin formulation ***
00200     else if (*mgcoar == 2) {
00201
00202         // Some i/o
00203         if (*iinfo > 0)
00204             VMESAGE3("Galer: (%03d, %03d, %03d)", nxx, nyy, nzz);
00205
00206         Vbuidgaler0(&nxold, &nyold, &nzold,
00207             &nxx, &nyy, &nzz,
00208             ipkey, &numdia,
00209             RAT(pc, VAT2(iz, 11,lev-1)),
00210             RAT(ipc, VAT2(iz, 5,lev-1)), RAT(rpc, VAT2(iz, 6,lev-1)),
00211             RAT(ac, VAT2(iz, 7,lev-1)),    RAT(cc, VAT2(iz, 1,lev-1)), RAT(fc, VAT2(iz,
00212         1,lev-1)),
00212             RAT(ipc, VAT2(iz, 5,lev )), RAT(rpc, VAT2(iz, 6,lev )),
00213             RAT(ac, VAT2(iz, 7,lev )),    RAT(cc, VAT2(iz, 1,lev )), RAT(fc, VAT2(iz,
00214         1,lev  )));
00214
00215
00216
00217         Vextrac(&nxold, &nyold, &nzold,
00218             &nxx, &nyy, &nzz,
00219             RAT(tcf, VAT2(iz, 1,lev-1)), RAT(tcf, VAT2(iz, 1,lev)));
00220     }
00221     else {
00222         VABORT_MSG1("Bad mgcoar value given: %d", *mgcoar);
00223     }
00224
00225     // Now initialize the differential operator offset
00226     // Vnm_print(0, "BUILDOPS: operator stencil (lev,numdia) = (%d, %d)\n",
00227     //     lev,numdia);
00228     VAT2(iz, 7, lev+1) = VAT2(iz, 7,lev) + numdia * nxx * nyy * nzz;
00229
00230     // Debug
00231     if (*iinfo > 8) {
00232
00233         Vprtmatd(&nxx, &nyy, &nzz,
00234             RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)), RAT(ac, VAT2(iz,
00235         7,lev)));
00235     }
00236     }
00237 }
00238
00239 // Build a sparse format coarse grid operator
00240 if (*mgsolv == 1) {
00241     lev = *nlev;
00242
00243     Vbuidband(&key, &nxx, &nyy, &nzz,
00244         RAT(ipc, VAT2(iz, 5,lev )), RAT(rpc, VAT2(iz, 6,lev )), RAT(ac, VAT2(iz, 7,lev )),
00245         RAT(ipc, VAT2(iz, 5,lev+1)), RAT(rpc, VAT2(iz, 6,lev+1)), RAT(ac, VAT2(iz, 7,lev+1)));
00246
00247     if (key == 1) {
00248         VERRMSG0("Changing your mgsolv to iterative");
00249         *mgsolv = 0;
00250     }
00251 }
00252 }
00253 }
00254
00255
00256
00257 VPUBLIC void Vbuidstr(int *nx, int *ny, int *nz, int *nlev, int *iz) {
00258     int nxold, nyold, nzold;
00259     int nxnew, nynew, nznew;
00260     int n, lev;
00261
00262     // Utility variable
00263     int numlev;
00264
00265

```

```

00266     MAT2(iz, 50, *nlev);
00267
00268     // Setup
00269     nxnew = *nx;
00270     nynew = *ny;
00271     nznew = *nz;
00272     n      = nxnew * nynew * nznew;
00273
00274     // Start with level 1
00275     lev = 1;
00276
00277     // Mark beginning of everything at level 1 ***
00278     VAT2(iz, 1, lev) = 1;
00279     VAT2(iz, 2, lev) = 1;
00280     VAT2(iz, 3, lev) = 1;
00281     VAT2(iz, 4, lev) = 1;
00282     VAT2(iz, 5, lev) = 1;
00283     VAT2(iz, 6, lev) = 1;
00284     VAT2(iz, 7, lev) = 1;
00285     VAT2(iz, 8, lev) = 1;
00286     VAT2(iz, 9, lev) = 1;
00287     VAT2(iz, 10, lev) = 1;
00288     VAT2(iz, 11, lev) = 1;
00289
00290     // Mark beginning of everything at level 2
00291     VAT2(iz, 1, lev + 1) = VAT2(iz, 1, lev) + n;
00292     VAT2(iz, 2, lev + 1) = VAT2(iz, 2, lev) + 4 * nynew * nznew;
00293     VAT2(iz, 3, lev + 1) = VAT2(iz, 3, lev) + 4 * nxnew * nznew;
00294     VAT2(iz, 4, lev + 1) = VAT2(iz, 4, lev) + 4 * nxnew * nynew;
00295     VAT2(iz, 5, lev + 1) = VAT2(iz, 5, lev) + 100;
00296     VAT2(iz, 6, lev + 1) = VAT2(iz, 6, lev) + 100;
00297     VAT2(iz, 8, lev + 1) = VAT2(iz, 8, lev) + nxnew;
00298     VAT2(iz, 9, lev + 1) = VAT2(iz, 9, lev) + nynew;
00299     VAT2(iz, 10, lev + 1) = VAT2(iz, 10, lev) + nznew;
00300
00301     /* *****
00302     * ***NOTE: we mark operator offsets as we build the operators ***
00303     * ***VAT2(iz, 7,lev+1) = VAT2(iz, 7, lev) + 4*n ***
00304     * *****
00305     * ***NOTE: we mark prolongation operator offsets lagging a level ***
00306     * ***VAT2(iz, 11, lev) = VAT2(iz, 11,lev-1) + 27*nsmall ***
00307     * *****/
00308
00309     // Mark the beginning of everything at (nlev-1) more
00310     for (lev=2; lev<=*nlev; lev++) {
00311         nxold = nxnew;
00312         nyold = nynew;
00313         nzold = nznew;
00314         numlev = 1;
00315         Vmkcors(&numlev, &nxold, &nyold, &nzold, &nxnew, &nynew, &nznew);
00316         n = nxnew * nynew * nznew;
00317
00318         // Mark the beginning of everything at level (lev+1)
00319         VAT2(iz, 1, lev + 1) = VAT2(iz, 1, lev) + n;
00320         VAT2(iz, 2, lev + 1) = VAT2(iz, 2, lev) + 4 * nynew * nznew;
00321         VAT2(iz, 3, lev + 1) = VAT2(iz, 3, lev) + 4 * nxnew * nznew;
00322         VAT2(iz, 4, lev + 1) = VAT2(iz, 4, lev) + 4 * nxnew * nynew;
00323         VAT2(iz, 5, lev + 1) = VAT2(iz, 5, lev) + 100;
00324         VAT2(iz, 6, lev + 1) = VAT2(iz, 6, lev) + 100;
00325         VAT2(iz, 7, lev + 1) = VAT2(iz, 7, lev) + 4 * n;
00326         VAT2(iz, 8, lev + 1) = VAT2(iz, 8, lev) + nxnew;
00327         VAT2(iz, 9, lev + 1) = VAT2(iz, 9, lev) + nynew;
00328         VAT2(iz, 10, lev + 1) = VAT2(iz, 10, lev) + nznew;
00329
00330         // Mark prolongation operator storage for previous level
00331         VAT2(iz, 11, lev) = VAT2(iz, 11, lev - 1) + 27 * n;
00332
00333         /* *****
00334         * *** NOTE: we mark operator offsets as we build the operators ***
00335         * ***      VAT2(iz, 7, lev + 1) = VAT2(iz, 7, lev) + 4 * n ***
00336         * *****/
00337     }
00338 }
00339
00340
00341 VPUBLIC void Vbuildgaler0(int *nxf, int *nyf, int *nzf,
00342     int *nxc, int *nyc, int *nzc,
00343     int *ipkey, int *numdia,
00344     double *pcFF, int *ipcFF, double *rpcFF,
00345     double *acFF, double *ccFF, double *fcFF,
00346     int *ipc, double *rpc,

```

```

00347         double *ac, double *cc, double *fc) {
00348
00349     int numdia_loc;
00350
00351     // Call the algebraic galerkin routine
00352     numdia_loc = VAT(ipcFF, 11);
00353     VbuildG(nxf, nyf, nzf,
00354            nxc, nyc, nzc,
00355            &numdia_loc,
00356            pcFF, acFF, ac);
00357
00358     // Note how many nonzeros in this new discretization stencil
00359     VAT(ipc, 11) = 27;
00360     *numdia = 14;
00361
00362     // Save the problem key with this new operator
00363     VAT(ipc, 10) = *ipkey;
00364
00365     // Restrict the helmholtz term and source function
00366     Vrestrc(nxf, nyf, nzf,
00367            nxc, nyc, nzc,
00368            ccFF, cc, pcFF);
00369
00370     Vrestrc(nxf, nyf, nzf,
00371            nxc, nyc, nzc,
00372            fcFF, fc, pcFF);
00373 }
00374
00375
00376
00377 VPUBLIC void Vmkcors(int *numlev,
00378                    int *nxold, int *nyold, int *nzold,
00379                    int *nxnew, int *nynew, int *nznew) {
00380     int nxtmp, nytmp, nztmp; // Temporary variables to hold current x,y,z values
00381     int i;                  // Index used in for loops
00382
00383     // Determine the coarser grid
00384     *nxnew = *nxold;
00385     *nynew = *nyold;
00386     *nznew = *nzold;
00387
00388     for (i=1; i<=*numlev; i++) {
00389         nxtmp = *nxnew;
00390         nytmp = *nynew;
00391         nztmp = *nznew;
00392         Vcorsr(&nxtmp, nxnew);
00393         Vcorsr(&nytmp, nynew);
00394         Vcorsr(&nztmp, nznew);
00395     }
00396 }
00397
00398
00399
00400 VPUBLIC void Vcorsr(int *nold, int *nnew) {
00401
00402     // Find the coarser grid size ***
00403     *nnew = (*nold - 1) / 2 + 1;
00404
00405     // Check a few things
00406     if ((*nnew - 1) * 2 != *nold - 1) {
00407         Vnm_print(2, "Vcorsr: WARNING! The grid dimensions are not\n");
00408         Vnm_print(2, "Vcorsr: consistent with nlev! Your\n");
00409         Vnm_print(2, "Vcorsr: calculation will only work if you\n");
00410         Vnm_print(2, "Vcorsr: are performing a mg-dummy run.\n");
00411     }
00412     if (*nnew < 1) {
00413         Vnm_print(2, "Vcorsr: ERROR! The grid dimensions are not\n");
00414         Vnm_print(2, "Vcorsr: consistent with nlev!\n");
00415         Vnm_print(2, "Vcorsr: Grid coarsened below zero.\n");
00416     }
00417 }
00418 }
00419
00420
00421
00422 VPUBLIC void Vmkfine(int *numlev,
00423                    int *nxold, int *nyold, int *nzold,
00424                    int *nxnew, int *nynew, int *nznew) {
00425
00426     int nxtmp, nytmp, nztmp, i;
00427
00428     // Determine the finer grid

```

```

00429     *nxnew = *nxold;
00430     *nynew = *nyold;
00431     *nznew = *nzold;
00432
00433     for (i=1; i<=*numlev; i++) {
00434
00435         nxtmp = *nxnew;
00436         nytmp = *nynew;
00437         nztmp = *nznew;
00438
00439         Vfiner(&nxtmp, nxnew);
00440         Vfiner(&nytmp, nynew);
00441         Vfiner(&nztmp, nznew);
00442     }
00443
00444 }
00445
00446
00447
00448 VPUBLIC void Vfiner(int *nold, int *nnew) {
00449     // Find the coarser grid size ***
00450     *nnew = (*nold - 1) * 2 + 1;
00451 }
00452
00453
00454
00455 VPUBLIC int Vivariv(int *nu, int *level) {
00456     int ivariv;
00457
00458     // Variable V-cycle
00459     // ivariv = *nu * VPOW(2, level - 1);
00460
00461     // Standard V-cycle
00462     ivariv = *nu;
00463
00464     return ivariv;
00465 }
00466
00467
00468
00469
00470
00471 VPUBLIC int Vmaxlev(int n1, int n2, int n3) {
00472     int n1c;
00473     int n2c;
00474     int n3c;
00475     int lev;
00476     int iden;
00477     int idone;
00478
00479     // Fine the common level
00480     idone = 0;
00481     lev = 0;
00482     do {
00483         lev += 1;
00484         iden = (int)VPOW(2, lev - 1);
00485         n1c = (n1 - 1) / iden + 1;
00486         n2c = (n2 - 1) / iden + 1;
00487         n3c = (n3 - 1) / iden + 1;
00488         if ((n1c - 1) * iden != (n1 - 1)) || (n1c <= 2) )
00489             idone = 1;
00490         if ((n2c - 1) * iden != (n2 - 1)) || (n2c <= 2) )
00491             idone = 1;
00492         if ((n3c - 1) * iden != (n3 - 1)) || (n3c <= 2) )
00493             idone = 1;
00494     } while (idone != 1);
00495
00496     return lev - 1;
00497 }
00498
00499
00500
00501
00502
00503 VPUBLIC void Vprtstp(int iok, int iters,
00504     double rsnm, double rsden, double orsnrm) {
00505     double relres = 0.0;
00506     double contrac = 0.0;
00507
00508     // Initializing timer
00509     if (iters == -99) {

```

```

00511         // Vnm_tstart(40, "MG iteration");
00512         cputme = 0.0;
00513         return;
00514     }
00515
00516     // Setup for the iteration
00517     else if (iters == -1) {
00518         Vnm_tstop(40, "MG iteration");
00519         return;
00520     }
00521
00522     // During the iteration
00523     else {
00524
00525         // Stop the timer
00526         // Vnm_tstop(40, "MG iteration");
00527
00528         // Relative residual
00529         if (rsden == 0.0) {
00530             relres = 1.0e6;
00531             VERRMSG0("Vprtstp: avoided division by zero\n");
00532         } else {
00533             relres = rsnmr / rsden;
00534         }
00535
00536         // Contraction number
00537         if (orsnmr == 0.0) {
00538             contrac = 1.0e6;
00539             VERRMSG0("avoided division by zero\n");
00540         } else {
00541             contrac = rsnmr / orsnmr;
00542         }
00543
00544         // The i/o
00545         if (iok == 1 || iok == 2) {
00546             VMESAGE1("iteration = %d", iters);
00547             VMESAGE1("relative residual = %e", relres);
00548             VMESAGE1("contraction number = %e", contrac);
00549         }
00550     }
00551 }
00552
00553
00554
00555 VPUBLIC void Vpackmg(int *iparm, double *rparm, size_t *nrwk, int *niwk,
00556 int *nx, int *ny, int *nz, int *nlev, int *nul, int *nu2, int *mgkey,
00557 int *itmax, int *istop, int *ipcon, int *nonlin, int *mgsmoo, int *mgprol,
00558 int *mgcoar, int *mgsolv, int *mgdisc, int *iinfo, double *errtol,
00559 int *ipkey, double *omegal, double *omegan, int *irite, int *iperf) {
00560
00561
00562
00563     // Encode iparm parameters ***
00564     VAT(iparm, 1) = *nrwk;
00565     VAT(iparm, 2) = *niwk;
00566     VAT(iparm, 3) = *nx;
00567     VAT(iparm, 4) = *ny;
00568     VAT(iparm, 5) = *nz;
00569     VAT(iparm, 6) = *nlev;
00570     VAT(iparm, 7) = *nul;
00571     VAT(iparm, 8) = *nu2;
00572     VAT(iparm, 9) = *mgkey;
00573     VAT(iparm, 10) = *itmax;
00574     VAT(iparm, 11) = *istop;
00575     VAT(iparm, 12) = *iinfo;
00576     VAT(iparm, 13) = *irite;
00577     VAT(iparm, 14) = *ipkey;
00578     VAT(iparm, 15) = *ipcon;
00579     VAT(iparm, 16) = *nonlin;
00580     VAT(iparm, 17) = *mgprol;
00581     VAT(iparm, 18) = *mgcoar;
00582     VAT(iparm, 19) = *mgdisc;
00583     VAT(iparm, 20) = *mgsmoo;
00584     VAT(iparm, 21) = *mgsolv;
00585     VAT(iparm, 22) = *iperf;
00586
00587     // Encode rparm parameters
00588     VAT(rparm, 1) = *errtol;
00589     VAT(rparm, 9) = *omegal;
00590     VAT(rparm, 10) = *omegan;
00591 }
00592

```

```

00593
00594
00595 VEXTERNC void Vbuildcopy0(int *nx, int *ny, int *nz,
00596     int *nxf, int *nyf, int *nzf,
00597     double *xc, double *yc, double *zc,
00598     double *gxc, double *gyc, double *gzc,
00599     double *alc, double *a2c, double *a3c,
00600     double *cc, double *fc, double *tc,
00601     double *xf, double *yf, double *zf,
00602     double *gxcf, double *gycf, double *gzcf,
00603     double *alcf, double *a2cf, double *a3cf,
00604     double *ccf, double *fcf, double *tcf) {
00605
00606
00607     int i, j, k;
00608     int ii, jj, kk;
00609     int iadd, jadd, kadd;
00610
00611     MAT3( gxc, *ny, *nz, 4);
00612     MAT3( gyc, *nx, *nz, 4);
00613     MAT3( gzc, *nx, *ny, 4);
00614     MAT3( alc, *nx, *ny, *nz);
00615     MAT3( a2c, *nx, *ny, *nz);
00616     MAT3( a3c, *nx, *ny, *nz);
00617     MAT3( cc, *nx, *ny, *nz);
00618     MAT3( fc, *nx, *ny, *nz);
00619     MAT3( tc, *nx, *ny, *nz);
00620     MAT3(gxcf, *nyf, *nzf, 4);
00621     MAT3(gycf, *nxf, *nzf, 4);
00622     MAT3(gzcf, *nxf, *nyf, 4);
00623     MAT3(alcf, *nxf, *nyf, *nzf);
00624     MAT3(a2cf, *nxf, *nyf, *nzf);
00625     MAT3(a3cf, *nxf, *nyf, *nzf);
00626     MAT3( tcf, *nxf, *nyf, *nzf);
00627     MAT3( ccf, *nxf, *nyf, *nzf);
00628     MAT3( fcf, *nxf, *nyf, *nzf);
00629
00630     WARN_UNTESTED;
00631
00632     // How far to step into the coefficient arrays
00633     iadd = (*nxf - 1) / (*nx - 1);
00634     jadd = (*nyf - 1) / (*ny - 1);
00635     kadd = (*nzf - 1) / (*nz - 1);
00636
00637     if (iadd != 2 || jadd != 2 || kadd != 2) {
00638         Vnm_print(2, "Vbuildcopy0: Problem with grid dimensions...\n");
00639     }
00640
00641     // Compute the coarse grid pde coefficients
00642     for (k=1; k<=*nz; k++) {
00643         kk = 2 * k - 1;
00644         VAT(zc, k) = VAT(zf, kk);
00645
00646         for (j=1; j<=*ny; j++) {
00647             jj = 2 * j - 1;
00648             VAT(yc, j) = VAT(yf, jj);
00649
00650             for (i=1; i<=*nx; i++){
00651                 ii = 2 * i - 1;
00652                 VAT(xc, i) = VAT(xf, ii);
00653
00654                 // True solution
00655                 VAT3( tc, i, j, k) = VAT3( tcf, ii, jj, kk);
00656
00657                 // Helmholtz coefficient
00658                 VAT3( cc, i, j, k) = VAT3( ccf, ii, jj, kk);
00659
00660                 // Source function
00661                 VAT3( fc, i, j, k) = VAT3( fcf, ii, jj, kk);
00662
00663                 // East/West neighbor
00664                 VAT3(alc, i, j, k) = VAT3(alcf, ii, jj, kk);
00665
00666                 // North/South neighbor
00667                 VAT3(a2c, i, j, k) = VAT3(a2cf, ii, jj, kk);
00668
00669                 // Up/Down neighbor
00670                 VAT3(a3c, i, j, k) = VAT3(a3cf, ii, jj, kk);
00671             }
00672         }
00673     }

```

```

00674
00675 // The (i=1) and (i=nx) boundaries
00676 for (k=1; k<=*nz; k++) {
00677     kk = 2 * k - 1;
00678
00679     for (j=1; j<=*ny; j++) {
00680         jj = 2 * j - 1;
00681
00682         VAT3(gxc, j, k, 1) = VAT3(gxcf, jj, kk, 1);
00683         VAT3(gxc, j, k, 2) = VAT3(gxcf, jj, kk, 2);
00684         VAT3(gxc, j, k, 3) = VAT3(gxcf, jj, kk, 3);
00685         VAT3(gxc, j, k, 4) = VAT3(gxcf, jj, kk, 4);
00686     }
00687 }
00688
00689 // The (j=1) and (j=ny) boundaries
00690 for (k=1; k<=*nz; k++) {
00691     kk = 2 * k - 1;
00692
00693     for (i=1; i<=*nx; i++) {
00694         ii = 2 * i - 1;
00695
00696         VAT3(gyc, i, k, 1) = VAT3(gycf, ii, kk, 1);
00697         VAT3(gyc, i, k, 2) = VAT3(gycf, ii, kk, 2);
00698         VAT3(gyc, i, k, 3) = VAT3(gycf, ii, kk, 3);
00699         VAT3(gyc, i, k, 4) = VAT3(gycf, ii, kk, 4);
00700     }
00701 }
00702
00703 // The (k=1) and (k=nz) boundaries
00704 for (j=1; j<=*ny; j++) {
00705     jj = 2 * j - 1;
00706
00707     for (i=1; i<=*nx; i++) {
00708         ii = 2 * i - 1;
00709
00710         VAT3(gzc, i, j, 1) = VAT3(gzcf, ii, jj, 1);
00711         VAT3(gzc, i, j, 2) = VAT3(gzcf, ii, jj, 2);
00712         VAT3(gzc, i, j, 3) = VAT3(gzcf, ii, jj, 3);
00713         VAT3(gzc, i, j, 4) = VAT3(gzcf, ii, jj, 4);
00714     }
00715 }
00716 }
00717
00718 VPUBLIC void Vbuildharm0(int *nx, int *ny, int *nz,
00719     int *nxf, int *nyf, int *nzf,
00720     double *xc, double *yc, double *zc,
00721     double *gxc, double *gyc, double *gzc,
00722     double *alc, double *a2c, double *a3c,
00723     double *cc, double *fc, double *tc,
00724     double *xf, double *yf, double *zf,
00725     double *gxcf, double *gycf, double *gzcf,
00726     double *alcf, double *a2cf, double *a3cf,
00727     double *ccf, double *fcf, double *tcf) {
00728     #if 1
00729     Vnm_print(2, "WARNING: FUNCTION IS NOT FULLY IMPLEMENTED YET!!!");
00730     #else
00731     int i, j, k;
00732     int ii, jj, kk;
00733     int iadd, jadd, kadd;
00734
00735     MAT3(gxc, *ny, *nz, 4);
00736     MAT3(gyc, *nx, *nz, 4);
00737     MAT3(gzc, *nx, *ny, 4);
00738
00739     MAT3(alc, *nx, *ny, *nz);
00740     MAT3(a2c, *nx, *ny, *nz);
00741     MAT3(a3c, *nx, *ny, *nz);
00742
00743     MAT3(cc, *nx, *ny, *nz);
00744     MAT3(fc, *nx, *ny, *nz);
00745     MAT3(tc, *nx, *ny, *nz);
00746
00747     MAT3(gxcf, *nyf, *nzf, 4);
00748     MAT3(gycf, *nxf, *nzf, 4);
00749     MAT3(gzcf, *nxf, *nyf, 4);
00750     MAT3(alcf, *nxf, *nyf, *nzf);
00751     MAT3(a2cf, *nxf, *nyf, *nzf);
00752     MAT3(a3cf, *nxf, *nyf, *nzf);
00753     MAT3(tcf, *nxf, *nyf, *nzf);
00754     MAT3(ccf, *nxf, *nyf, *nzf);

```



```

00755     MAT3( fcf, *nxf, *nyf, *nzf);
00756
00757     // Statement functions
00759     double a, b, c, d, e, f, g, h;
00760
00761     // How far to step into the coefficient arrays
00762     iadd = (*nxf - 1) / (*nx - 1);
00763     jadd = (*nyf - 1) / (*ny - 1);
00764     kadd = (*nzf - 1) / (*nz - 1);
00765     if (iadd != 2 || jadd != 2 || kadd != 2) {
00766         Vnm_print(2, "BUILDHARM0: problem with grid dimensions...\n");
00767     }
00768
00769     // Compute the coarse grid pde coefficients
00770     for (k=1; k<=*nz; k++) {
00771         kk = 2 * k - 1;
00772         VAT(zc, k) = VAT(zf, kk);
00773
00774         for (j=1; j<=*ny; j++) {
00775             jj = 2 * j - 1;
00776             VAT(yc, j) = VAT(yf, jj);
00777
00778             for (i=1; i<=*nx; i++) {
00779                 ii = 2 * i - 1;
00780                 VAT(xc, i) = VAT(xf, ii);
00781
00782                 // True solution
00783                 VAT3(tc, i, j, k) = VAT3(tcf, ii, jj, kk);
00784
00785                 // Helmholtz coefficient
00786                 VAT3(cc, i, j, k) = VAT3(ccf, ii, jj, kk);
00787
00788                 /* Commented out in original fortran code
00789                 cc(i,j,k) = (
00790                     +0.5e0 * ccf(ii,jj,kk)
00791                     +0.5e0 * ARITH6( ccf(max0(1,ii-1),jj,kk),
00792                         ccf(min0(nxf,ii+1),jj,kk),
00793                         ccf(ii,max0(1,jj-1),kk),
00794                         ccf(ii,min0(nyf,jj+1),kk),
00795                         ccf(ii,jj,max0(nzf,kk-1)),
00796                         ccf(ii,jj,min0(nzf,kk+1))) )
00797                 )
00798                 */
00799
00800                 // Source function
00801                 VAT3(fc, i, j, k) = VAT3(fcf, ii, jj, kk);
00802                 /*
00803                 fc(i,j,k) = (
00804                     +0.5e0 * fcf(ii,jj,kk)
00805                     +0.5e0 * ARITH6( fcf(max0(1,ii-1),jj,kk),
00806                         fcf(min0(nxf,ii+1),jj,kk),
00807                         fcf(ii,max0(1,jj-1),kk),
00808                         fcf(ii,min0(nyf,jj+1),kk),
00809                         fcf(ii,jj,max0(nzf,kk-1)),
00810                         fcf(ii,jj,min0(nzf,kk+1))) )
00811                 )
00812                 */
00813
00814                 // East/West neighbor
00815                 VAT3(alc, i, j, k) = (
00816                     +0.500 * HARMO2(VAT3(alcf, ii, jj, kk),
00817                         VAT3(alcf, VMIN2(*nxf, ii+1), jj, kk))
00818                     +0.125 * HARMO2(VAT3(alcf, ii, jj, VMAX2(1, kk-1)),
00819                         VAT3(alcf, VMIN2(*nxf, ii+1), jj, VMAX2(1, kk-1)))
00820                     +0.125 * HARMO2(VAT3(alcf, ii, jj, VMIN2(*nzf, kk+1)),
00821                         VAT3(alcf, VMIN2(*nxf, ii+1), jj, VMIN2(*nzf, kk+1)))
00822                     +0.125 * HARMO2(VAT3(alcf, ii, VMAX2(1, jj-1), kk),
00823                         VAT3(alcf, VMIN2(*nxf, ii+1), VMAX2(1, jj-1), kk))
00824                     +0.125 * HARMO2(VAT3(alcf, ii, VMIN2(*nyf, jj+1), kk),
00825                         VAT3(alcf, VMIN2(*nxf, ii+1), VMIN2(*nyf, jj+1), kk))
00826                 );
00827
00828                 // North/South neighbor
00829                 VAT3(a2c, i, j, k) = (
00830                     +0.500 * HARMO2(VAT3(a2cf, ii, jj, kk),
00831                         VAT3(a2cf, ii, VMIN2(*nyf, jj+1), kk))
00832                     +0.125 * HARMO2(VAT3(a2cf, ii, jj, VMAX2(1, kk-1)),
00833                         VAT3(a2cf, ii, VMIN2(*nyf, jj+1), VMAX2(1, kk-1)))
00834                     +0.125 * HARMO2(VAT3(a2cf, ii, jj, VMIN2(*nzf, kk+1)),
00835                         VAT3(a2cf, ii, VMIN2(*nyf, jj+1), VMIN2(*nzf, kk+1)))
00836                     +0.125 * HARMO2(VAT3(a2cf, VMAX2(1, ii-1), jj, kk),

```

```

00837             VAT3(a2cf, VMAX2(1, ii-1), VMIN2(nyf, jj+1), kk))
00838         +0.125 * HARMO2(VAT3(a2cf, VMIN2(*nxf, ii+1), jj, kk),
00839             VAT3(a2cf, VMIN2(*nxf, ii+1), VMIN2(*nyf, jj+1), kk))
00840     );
00841
00842     // Up/Down neighbor
00843     VAT3(a3c, i, j, k) = (
00844         +0.500 * HARMO2(VAT3(a3cf, ii, jj, kk),
00845             VAT3(a3cf, ii, jj, VMIN2(*nzf, kk+1)))
00846         +0.125 * HARMO2(VAT3(a3cf, ii, VMAX2(1, jj-1), kk),
00847             VAT3(a3cf, ii, VMAX2(1, jj-1), VMIN2(*nzf, kk+1)))
00848         +0.125 * HARMO2(VAT3(a3cf, ii, VMIN2(*nyf, jj+1), kk),
00849             VAT3(a3cf, ii, VMIN2(*nyf, jj+1), VMIN2(*nzf, kk+1)))
00850         +0.125 * HARMO2(VAT3(a3cf, VMAX2(1, ii-1), jj, kk),
00851             VAT3(a3cf, VMAX2(1, ii-1), jj, VMIN2(*nzf, kk+1)))
00852         +0.125 * HARMO2(VAT3(a3cf, VMIN2(*nxf, ii+1), jj, kk),
00853             VAT3(a3cf, VMIN2(*nxf, ii+1), jj, VMIN2(*nzf, kk+1)))
00854     );
00855 }
00856 }
00857 }
00858
00859 // The (i=1) and (i=nx) boundaries ***
00860 for (k=1; k<=*nz; k++) {
00861     kk = 2 * k - 1;
00862
00863     for (j=1; j<=*ny; j++) {
00864         jj = 2 * j - 1;
00865
00866         VAT3(gxc, j, k, 1) = VAT3(gxcf, jj, kk, 1);
00867         VAT3(gxc, j, k, 2) = VAT3(gxcf, jj, kk, 2);
00868         VAT3(gxc, j, k, 3) = VAT3(gxcf, jj, kk, 3);
00869         VAT3(gxc, j, k, 4) = VAT3(gxcf, jj, kk, 4);
00870     }
00871 }
00872
00873 // The (j=1) and (j=ny) boundaries
00874 for (k=1; k<=*nz; k++) {
00875     kk = 2 * k - 1;
00876
00877     for (i=1; i<=*nx; i++) {
00878         ii = 2 * i - 1;
00879         VAT3(gyc, i, k, 1) = VAT3(gycf, ii, kk, 1);
00880         VAT3(gyc, i, k, 2) = VAT3(gycf, ii, kk, 2);
00881         VAT3(gyc, i, k, 3) = VAT3(gycf, ii, kk, 3);
00882         VAT3(gyc, i, k, 4) = VAT3(gycf, ii, kk, 4);
00883     }
00884 }
00885
00886 // The (k=1) and (k=nz) boundaries
00887 for (j=1; j<=*ny; j++) {
00888     jj = 2 * j - 1;
00889
00890     for (i=1; i<=*nx; i++) {
00891         ii = 2 * i - 1;
00892
00893         VAT3(gzc, i, j, 1) = VAT3(gzcf, ii, jj, 1);
00894         VAT3(gzc, i, j, 2) = VAT3(gzcf, ii, jj, 2);
00895         VAT3(gzc, i, j, 3) = VAT3(gzcf, ii, jj, 3);
00896         VAT3(gzc, i, j, 4) = VAT3(gzcf, ii, jj, 4);
00897     }
00898 }
00899 #endif
00900 }
00901
00902
00903
00904 VPUBLIC void Vbuildalg(int *nx, int *ny, int *nz,
00905     int *mode, int *nlev, int *iz,
00906     int *ipc, double *rpc,
00907     double *ac, double *cc, double *fc,
00908     double *x, double *y, double *tmp) {
00909
00910     int nxx, nyy, nzz;
00911     int nxold, nyold, nzold;
00912     int lev, numlev;
00913
00914     MAT2(iz, 50, *nlev);
00915
00916     // Setup
00917     nxx = *nx;

```

```

00918     nyy = *ny;
00919     nzz = *nz;
00920
00921     // Build the rhs the finest level
00922     lev = 1;
00923     if ((*mode == 1) || (*mode == 2)) {
00924         Vnmatvec(&nxx, &nyy, &nzz,
00925                 RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00926                 RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00927                 RAT(x, VAT2(iz, 1, lev)), RAT(y, VAT2(iz, 1, lev)),
00928                 tmp);
00929     } else {
00930         Vmatvec(&nxx, &nyy, &nzz,
00931                RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00932                RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00933                RAT(x, VAT2(iz, 1, lev)), RAT(y, VAT2(iz, 1, lev)));
00934     }
00935
00936     // Build the (nlev-1) level rhs function
00937     for (lev=2; lev <= *nlev; lev++) {
00938         nxold = nxx;
00939         nyold = nyy;
00940         nzold = nzz;
00941
00942         numlev = 1;
00943         Vmkcors(&numlev, &nxold, &nyold, &nzold, &nxx, &nyy, &nzz);
00944
00945         // Build the rhs on this level
00946         if ((*mode == 1) || (*mode == 2)) {
00947             Vnmatvec(&nxx, &nyy, &nzz,
00948                     RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00949                     RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00950                     RAT(x, VAT2(iz, 1, lev)), RAT(y, VAT2(iz, 1, lev)),
00951                     tmp);
00952         } else {
00953             Vmatvec(&nxx, &nyy, &nzz,
00954                    RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00955                    RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00956                    RAT(x, VAT2(iz, 1, lev)), RAT(y, VAT2(iz, 1, lev)));
00957         }
00958     }
00959 }

```

9.135 mgsubd.h

```

00001
00050 #ifndef _MGSUBD_H_
00051 #define _MGSUBD_H_
00052
00053 #include "apbscfg.h"
00054
00055 #include "malloc/malloc.h"
00056
00057 #include "generic/vhal.h"
00058 #include "generic/vmatrix.h"
00059 #include "pmgc/matvecd.h"
00060 #include "pmgc/buildAd.h"
00061 #include "pmgc/buildPd.h"
00062 #include "pmgc/buildBd.h"
00063 #include "pmgc/buildGd.h"
00064
00065 #define HARMO2(a, b) ((2.0 * (a) * (b) / ((a) + (b)))
00066 #define HARMO4(a, b, c, d) (1.0 / ( 0.25 * ( 1.0/(a) + 1.0/(b) + 1.0/(c) + 1.0/(d))))
00067 #define ARITH2(a, b) ((a) + (b)) / 2.0
00068 #define ARITH4(a, b, c, d) ((a) + (b) + (c) + (d)) / 4.0
00069 #define ARITH6(a, b, c, d, e, f) ((a) + (b) + (c) + (d) + (e) + (f)) / 6.0
00070 #define ARITH8(a, b, c, d, e, f, g, h) ((a) + (b) + (c) + (d) + (e) + (f) + (g) + (h)) / 8.0
00071
00084 VEXTERNC void Vbuildops(
00085     int    *nx,
00086     int    *ny,
00087     int    *nz,
00088     int    *nlev,
00089     int    *ipkey,
00090     int    *iinfo,
00091     int    *ido,
00092     int    *iz,
00093     int    *mgprol,

```

```
00094         int      *mgcoar,
00095         int      *mgsolv,
00096         int      *mgdisc,
00097         int      *ipc,
00098         double   *rpc,
00099         double   *pc,
00100         double   *ac,
00101         double   *cc,
00102         double   *fc,
00103         double   *xf,
00104         double   *yf,
00105         double   *zf,
00106         double   *gxcf,
00107         double   *gycf,
00108         double   *gzcf,
00109         double   *alcf,
00110         double   *a2cf,
00111         double   *a3cf,
00112         double   *ccf,
00113         double   *fcf,
00114         double   *tcf
00115     );
00116
00136 VEXTERNC void Vbuildstr(
00137     int *nx,
00138     int *ny,
00139     int *nz,
00140     int *nlev,
00141     int *iz
00142 );
00143
00152 VEXTERNC void Vbuildgaler0(
00153     int *nxf,
00154     int *nyf,
00155     int *nzf,
00156     int *nxc,
00157     int *nyc,
00158     int *nzc,
00159     int *ipkey,
00160     int *numdia,
00161     double *pcFF,
00162     int *ipcFF,
00163     double *rpcFF,
00164     double *acFF,
00165     double *ccFF,
00166     double *fcFF,
00167     int *ipc,
00168     double *rpc,
00169     double *ac,
00170     double *cc,
00171     double *fc
00172 );
00173
00174
00175
00182 VEXTERNC void Vmkcors(
00183     int *numlev,
00184     int *nxold,
00185     int *nyold,
00186     int *nzold,
00187     int *nxnew,
00188     int *nynew,
00189     int *nznew
00190 );
00191
00198 VEXTERNC void Vcorsr(
00199     int *nold,
00200     int *nnew
00201 );
00202
00203
00204
00211 VEXTERNC void Vmkfine(
00212     int *numlev,
00213     int *nxold,
00214     int *nyold,
00215     int *nzold,
00216     int *nxnew,
00217     int *nynew,
00218     int *nznew
00219 );
```

```
00220
00227 VEXTERNC void Vfiner(
00228     int *nold,
00229     int *nnew
00230 );
00231
00232
00233
00240 VEXTERNC int Vivariv(
00241     int *nu,
00242     int *level
00243 );
00244
00250 VEXTERNC int Vmaxlev(
00251     int n1,
00252     int n2,
00253     int n3
00254 );
00255
00256
00258 double bf, oh, cputme;
00259
00264 VEXTERNC void Vprtstp(
00265     int iok,
00266     int iters,
00267     double rsnm,
00268     double rsden,
00269     double orsnrm
00270 );
00271
00272
00273
00280 VEXTERNC void Vpackmg(
00281     int *iparm,
00282     double *rparm,
00283     size_t *nrwk,
00284     int *niwk,
00285     int *nx,
00286     int *ny,
00287     int *nz,
00288     int *nlev,
00289     int *nul,
00290     int *nu2,
00291     int *mgkey,
00292     int *itmax,
00293     int *istop,
00294     int *ipcon,
00295     int *nonlin,
00296     int *mgsmoo,
00297     int *mgprol,
00298     int *mgcoar,
00299     int *mgsolv,
00300     int *mgdisc,
00301     int *iinfo,
00302     double *errtol,
00303     int *ipkey,
00304     double *omegal,
00305     double *omegan,
00306     int *irite,
00307     int *iperf
00308 );
00309
00310
00311
00317 VEXTERNC void Vbuildharm0(
00318     int *nx,
00319     int *ny,
00320     int *nz,
00321     int *nxf,
00322     int *nyf,
00323     int *nzf,
00324     double *xc,
00325     double *yc,
00326     double *zc,
00327     double *gxc,
00328     double *gyc,
00329     double *gzc,
00330     double *alc,
00331     double *a2c,
00332     double *a3c,
00333     double *cc,
```

```

00334         double *fc,
00335         double *tc,
00336         double *xf,
00337         double *yf,
00338         double *zf,
00339         double *gxcf,
00340         double *gycf,
00341         double *gzcf,
00342         double *alcf,
00343         double *a2cf,
00344         double *a3cf,
00345         double *ccf,
00346         double *fcf,
00347         double *tcf
00348     );
00349
00350
00351
00357 VEXTERNC void Vbuildcopy0(
00358     int     *nx,
00359     int     *ny,
00360     int     *nz,
00361     int     *nxf,
00362     int     *nyf,
00363     int     *nzf,
00364     double *xc,
00365     double *yc,
00366     double *zc,
00367     double *gxc,
00368     double *gyc,
00369     double *gzc,
00370     double *alc,
00371     double *a2c,
00372     double *a3c,
00373     double *cc,
00374     double *fc,
00375     double *tc,
00376     double *xf,
00377     double *yf,
00378     double *zf,
00379     double *gxcf,
00380     double *gycf,
00381     double *gzcf,
00382     double *alcf,
00383     double *a2cf,
00384     double *a3cf,
00385     double *ccf,
00386     double *fcf,
00387     double *tcf
00388 );
00389
00390
00391
00397 VEXTERNC void Vbuildalg(
00398     int     *nx,
00399     int     *ny,
00400     int     *nz,
00401     int     *mode,
00402     int     *nlev,
00403     int     *iz,
00404     int     *ipc,
00405     double *rpc,
00406     double *ac,
00407     double *cc,
00408     double *fc,
00409     double *x,
00410     double *y,
00411     double *tmp
00412 );
00413
00414
00415
00416 #endif // _MGSUBD_H_

```

9.136 mikpckd.c

```

00001
00055 #include "mikpckd.h"

```

```

00056
00057 VPUBLIC void Vxcopy(int *nx, int *ny, int *nz, double *x, double *y) {
00058
00059     MAT3(x, *nx, *ny, *nz);
00060     MAT3(y, *nx, *ny, *nz);
00061
00062     // The indices used to traverse the matrices
00063     int i, j, k;
00064
00065     #pragma omp parallel for private(i,j,k)
00066     for(k=2; k<=*nz-1; k++)
00067         for(j=2; j<=*ny-1; j++)
00068             for(i=2; i<=*nx-1; i++)
00069                 VAT3(y, i, j, k) = VAT3(x, i, j, k);
00070 }
00071
00072
00073
00074
00075 VPUBLIC void Vxcopy_small(int *nx, int *ny, int *nz, double *x, double *y) {
00076
00077     MAT3(x, *nx, *ny, *nz);
00078     MAT3(y, *nx - 2, *ny - 2, *nz - 2);
00079
00080     // The indices used to traverse the matrices
00081     int i, j, k;
00082
00083     for(k=2; k<=*nz-1; k++)
00084         for(j=2; j<=*ny-1; j++)
00085             for(i=2; i<=*nx-1; i++)
00086                 VAT3(y, i - 1, j - 1, k - 1) = VAT3(x, i, j, k);
00087 }
00088
00089
00090
00091 VPUBLIC void Vxcopy_large(int *nx, int *ny, int *nz, double *x, double *y) {
00092
00093     MAT3(x, *nx - 2, *ny - 2, *nz - 2);
00094     MAT3(y, *nx, *ny, *nz);
00095
00096     // The indices used to traverse the matrices
00097     int i, j, k;
00098
00099     for(k=2; k<=*nz-1; k++)
00100         for(j=2; j<=*ny-1; j++)
00101             for(i=2; i<=*nx-1; i++)
00102                 VAT3(y, i, j, k) = VAT3(x, i - 1, j - 1, k - 1);
00103 }
00104
00105
00106
00107
00108
00109
00110
00111
00112 VPUBLIC void Vxaxpy(int *nx, int *ny, int *nz,
00113     double *alpha, double *x, double *y) {
00114
00115     // Create the wrappers
00116     MAT3(x, *nx, *ny, *nz);
00117     MAT3(y, *nx, *ny, *nz);
00118
00119     // The indices used to traverse the matrices
00120     int i, j, k;
00121
00122     for(k=2; k<=*nz-1; k++)
00123         for(j=2; j<=*ny-1; j++)
00124             for(i=2; i<=*nx-1; i++)
00125                 VAT3(y, i, j, k) += *alpha * VAT3(x, i, j, k);
00126 }
00127
00128
00129
00130
00131 VPUBLIC double Vxnrm1(int *nx, int *ny, int *nz,
00132     double *x) {
00133
00134     double xnm1 = 0.0;
00135
00136     MAT3(x, *nx, *ny, *nz);
00137
00138     // The indices used to traverse the matrices
00139     int i, j, k;
00140
00141     for(k=2; k<=*nz-1; k++)
00142         for(j=2; j<=*ny-1; j++)
00143             for(i=2; i<=*nx-1; i++)

```

```

00145             xnrml += VABS(VAT3(x, i, j, k));
00146
00147     return xnrml;
00148 }
00149
00150
00151
00152 VPUBLIC double Vxnm2(int *nx, int *ny, int *nz,
00153     double *x) {
00154
00155     double xnm2 = 0.0;
00156
00157     MAT3(x, *nx, *ny, *nz);
00158
00159     // The indices used to traverse the matrices
00160     int i, j, k;
00161
00162     for(k=2; k<=*nz-1; k++)
00163         for(j=2; j<=*ny-1; j++)
00164             for(i=2; i<=*nx-1; i++)
00165                 xnm2 += VAT3(x, i, j, k) * VAT3(x, i, j, k);
00166
00167     return VSQRT(xnm2);
00168 }
00169
00170
00171
00172
00173 VPUBLIC double Vxdot(int *nx, int *ny, int *nz,
00174     double *x, double *y) {
00175
00176     int i, j, k;
00177
00178     // Initialize
00179     double xdot = 0.0;
00180
00181     MAT3(x, *nx, *ny, *nz);
00182     MAT3(y, *nx, *ny, *nz);
00183
00184     // Do it
00185     for(k=2; k<=*nz-1; k++)
00186         for(j=2; j<=*ny-1; j++)
00187             for(i=2; i<=*nx-1; i++)
00188                 xdot += VAT3(x, i, j, k) * VAT3(y, i, j, k);
00189
00190     return xdot;
00191 }
00192
00193
00194
00195 VPUBLIC void Vazeros(int *nx, int *ny, int *nz, double *x) {
00196
00197     int i, n;
00198     int nproc = 1;
00199
00200     n = *nx * *ny * *nz;
00201
00202     #pragma omp parallel for private(i)
00203     for (i=1; i<=n; i++)
00204         VAT(x, i) = 0.0;
00205 }
00206
00207
00208
00209 VPUBLIC void VfboundPMG(int *ibound, int *nx, int *ny, int *nz,
00210     double *x, double *gxc, double *gyc, double *gzc) {
00211
00212     int i, j, k;
00213
00214     // Create and bind the wrappers for the source data
00215     MAT3( x, *nx, *ny, *nz);
00216     MAT3(gxc, *ny, *nz, 2);
00217     MAT3(gyc, *nx, *nz, 2);
00218     MAT3(gzc, *nx, *ny, 2);
00219
00220     // Dirichlet test
00221     if (ibound == 0) {
00222
00223         // Dero dirichlet
00224         VfboundPMG00(nx, ny, nz, x);
00225
00226     } else {

```



```

00227
00228     // Nonzero dirichlet
00229
00230     // The (i=1) and (i=nx) boundaries
00231     for (k=1; k<=*nz; k++) {
00232         for (j=1; j<=*ny; j++) {
00233             VAT3(x, 1, j, k) = VAT3(gxc, j, k, 1);
00234             VAT3(x, *nx, j, k) = VAT3(gxc, j, k, 2);
00235         }
00236     }
00237
00238     // The (j=1) and (j=ny) boundaries
00239     for (k=1; k<=*nz; k++) {
00240         for (i=1; i<=*nx; i++) {
00241             VAT3(x, i, 1, k) = VAT3(gyc, i, k, 1);
00242             VAT3(x, i, *ny, k) = VAT3(gyc, i, k, 2);
00243         }
00244     }
00245
00246     // The (k=1) and (k=nz) boundaries
00247     for (j=1; j<=*ny; j++) {
00248         for (i=1; i<=*nx; i++) {
00249             VAT3(x, i, j, 1) = VAT3(gzc, i, j, 1);
00250             VAT3(x, i, j, *nz) = VAT3(gzc, i, j, 2);
00251         }
00252     }
00253 }
00254 }
00255
00256
00257
00258 VPUBLIC void VfboundPMG00(int *nx, int *ny, int *nz, double *x) {
00259
00260     int i, j, k;
00261
00262     MAT3( x, *nx, *ny, *nz);
00263
00264     // The (i=1) and (i=nx) boundaries
00265     for (k=1; k<=*nz; k++) {
00266         for (j=1; j<=*ny; j++) {
00267             VAT3(x, 1, j, k) = 0.0;
00268             VAT3(x, *nx, j, k) = 0.0;
00269         }
00270     }
00271
00272     // The (j=1) and (j=ny) boundaries
00273     for (k=1; k<=*nz; k++) {
00274         for(i=1; i<=*nx; i++) {
00275             VAT3(x, i, 1, k) = 0.0;
00276             VAT3(x, i, *ny, k) = 0.0;
00277         }
00278     }
00279
00280     // The (k=1) and (k=nz) boundaries
00281     for (j=1; j<=*ny; j++) {
00282         for (i=1; i<=*nx; i++) {
00283             VAT3(x, i, j, 1) = 0.0;
00284             VAT3(x, i, j, *nz) = 0.0;
00285         }
00286     }
00287 }
00288
00289
00290
00291 VPUBLIC void Vaxrand(int *nx, int *ny, int *nz, double *x) {
00292
00293     int n, i, ii, ipara, ivect, iflag;
00294     int nproc = 1;
00295     double xdum;
00296
00297     WARN_UNTESTED;
00298
00299     // Find parallel loops (ipara), remainder (ivect)
00300     n = *nx * *ny * *nz;
00301     ipara = n / nproc;
00302     ivect = n % nproc;
00303     iflag = 1;
00304     xdum = (double) (VRAND);
00305
00306     // Do parallel loops
00307     for (ii=1; ii<=nproc; ii++)

```

```

00308         for (i=1+(ipara*(ii-1)); i<=ipara*ii; i++)
00309             VAT(x, i) = (double)(VRAND);
00310
00311         // Do vector loops
00312         for (i=ipara*nproc+1; i<=n; i++)
00313             VAT(x, i) = (double)(VRAND);
00314     }
00315
00316
00317
00318 VPUBLIC void Vxscal(int *nx, int *ny, int *nz, double *fac, double *x) {
00319
00320     int i, j, k;
00321
00322     MAT3(x, *nx, *ny, *nz);
00323
00324     for (k=2; k<=*nz-1; k++)
00325         for (j=2; j<=*ny-1; j++)
00326             for (i=2; i<=*nx-1; i++)
00327                 VAT3(x, i, j, k) *= *fac;
00328 }
00329
00330
00331
00332 VPUBLIC void Vprtmatd(int *nx, int *ny, int *nz,
00333     int *ipc, double *rpc, double *ac) {
00334
00335     int numdia;
00336
00337     MAT2(ac, *nx * *ny * *nz, 1);
00338
00339     WARN_UNTESTED;
00340
00341     // Do the printing
00342     numdia = VAT(ipc, 11);
00343     if (numdia == 7) {
00344         Vprtmatd7(nx, ny, nz,
00345             ipc, rpc,
00346             RAT2(ac, 1, 1), RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4));
00347     } else if (numdia == 27) {
00348         Vprtmatd27(nx, ny, nz,
00349             ipc, rpc,
00350             RAT2(ac, 1, 1), RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
00351             RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00352             RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1, 10),
00353             RAT2(ac, 1, 11), RAT2(ac, 1, 12), RAT2(ac, 1, 13), RAT2(ac, 1, 14));
00354     } else {
00355         Vnm_print(2, "Vprtmatd: invalid stencil type given: %d\n", numdia);
00356     }
00357 }
00358
00359
00360
00361 VPUBLIC void Vprtmatd7(int *nx, int *ny, int *nz,
00362     int *ipc, double *rpc,
00363     double *oC, double *oE, double *oN, double *uC) {
00364
00365     int n, i, j, k;
00366
00367     MAT3(oC, *nx, *ny, *nz);
00368     MAT3(oE, *nx, *ny, *nz);
00369     MAT3(oN, *nx, *ny, *nz);
00370     MAT3(uC, *nx, *ny, *nz);
00371
00372     WARN_UNTESTED;
00373
00374     // Recover matrix dimension
00375     n = (*nx - 2) * (*ny - 2) * (*nz - 2);
00376
00377     Vnm_print(2, "Vprtmatd7: Dimension of matrix = %d\n", n);
00378     Vnm_print(2, "Vprtmatd7: Begin diagonal matrix\n");
00379
00380     // Handle first block
00381     for (k=2; k<=*nz-1; k++)
00382         for (j=2; j<=*ny-1; j++)
00383             for (i=2; i<=*nx-1; i++)
00384                 Vnm_print(2, "Vprtmatd7: (%d,%d,%d) - oC=%g, oE=%g, oN=%g, uC=%g\n",
00385                     VAT3(oC,i,j,k), VAT3(oE,i,j,k), VAT3(oN,i,j,k), VAT3(uC,i,j,k));
00386
00387     // Finish up
00388     Vnm_print(2, "Vprtmatd7: End diagonal matrix\n");

```

```

00389 }
00390
00391
00392
00393 VEXTERNC void Vprtmtd27(int *nx, int *ny, int *nz,
00394     int *ipc, double *rpc,
00395     double *oC, double *oE, double *oN, double *uC,
00396     double *oNE, double *oNW,
00397     double *uE, double *uW, double *uN, double *uS,
00398     double *uNE, double *uNW, double *uSE, double *uSW) {
00399
00400     int n, i, j, k;
00401
00402     MAT3( oC, *nx, *ny, *nz);
00403     MAT3( oE, *nx, *ny, *nz);
00404     MAT3( oN, *nx, *ny, *nz);
00405     MAT3( uC, *nx, *ny, *nz);
00406     MAT3( oNE, *nx, *ny, *nz);
00407     MAT3( oNW, *nx, *ny, *nz);
00408     MAT3( uE, *nx, *ny, *nz);
00409     MAT3( uW, *nx, *ny, *nz);
00410     MAT3( uN, *nx, *ny, *nz);
00411     MAT3( uS, *nx, *ny, *nz);
00412     MAT3( uNE, *nx, *ny, *nz);
00413     MAT3( uNW, *nx, *ny, *nz);
00414     MAT3( uSE, *nx, *ny, *nz);
00415     MAT3( uSW, *nx, *ny, *nz);
00416
00417     WARN_UNTESTED;
00418
00419     // Recover matrix dimension
00420     n = (*nx - 2) * (*ny - 2) * (*nz - 2);
00421
00422     Vnm_print(2, "Vprtmtd27: Dimension of matrix = %d\n", n);
00423     Vnm_print(2, "Vprtmtd27: Begin diagonal matrix\n");
00424
00425     // Handle first block
00426     for (k=2; k<=*nz-1; k++)
00427         for (j=2; j<=*ny-1; j++)
00428             for (i=2; i<=*nx-1; i++)
00429                 Vnm_print(2, "Vprtmtd7: (%d,%d,%d) - oC = %g, oE = %g, "
00430                     "oNW = %g, oN = %g, oNE = %g, uSW = %g, uS = %g, "
00431                     "uSE = %g, uW = %g, uC = %g, uE = %g, uNW = %g, "
00432                     "uN = %g, uNE = %g\n",
00433                     VAT3( oC, i, j, k), VAT3( oE, i, j, k),
00434                     VAT3( oNW, i, j, k), VAT3( oN, i, j, k),
00435                     VAT3( oNE, i, j, k), VAT3( uSW, i, j, k),
00436                     VAT3( uS, i, j, k), VAT3( uSE, i, j, k),
00437                     VAT3( uW, i, j, k), VAT3( uC, i, j, k),
00438                     VAT3( uE, i, j, k), VAT3( uNW, i, j, k),
00439                     VAT3( uN, i, j, k), VAT3( uNE, i, j, k) );
00440
00441     // Finish up
00442     Vnm_print(2, "Vprtmtd27: End diagonal matrix\n");
00443 }
00444
00445 VPUBLIC void Vlinesearch(int *nx, int *ny, int *nz,
00446     double *alpha,
00447     int *ipc, double *rpc,
00448     double *ac, double *cc, double *fc,
00449     double *p, double *x, double *r,
00450     double *ap, double *zk, double *zkp1) {
00451     VABORT_MSG0("Not translated yet");
00452 }

```

9.137 mikpckd.h

```

00001
00050 #ifndef MIKPCCKD_H_
00051 #define MIKPCCKD_H_
00052
00053 #include "apbscfg.h"
00054
00055 #include "malloc/malloc.h"
00056
00057 #include "generic/vhal.h"
00058 #include "generic/vmatrix.h"
00059

```

```
00067 VEXTERNC void Vxcopy(  
00068     int *nx,  
00069     int *ny,  
00070     int *nz,  
00071     double *x,  
00072     double *y  
00073 );  
00074  
00075  
00076  
00084 VEXTERNC void Vxcopy_small(  
00085     int *nx,  
00086     int *ny,  
00087     int *nz,  
00088     double *x,  
00089     double *y  
00090 );  
00091  
00092  
00093  
00101 VEXTERNC void Vxcopy_large(  
00102     int *nx,  
00103     int *ny,  
00104     int *nz,  
00105     double *x,  
00106     double *y  
00107 );  
00108  
00109  
00110  
00117 VEXTERNC void Vxaxpy(  
00118     int *nx,  
00119     int *ny,  
00120     int *nz,  
00121     double *alpha,  
00122     double *x,  
00123     double *y  
00124 );  
00125  
00132 VEXTERNC double Vxnrm1(  
00133     int *nx,  
00134     int *ny,  
00135     int *nz,  
00136     double *x  
00137 );  
00138  
00139  
00140  
00147 VEXTERNC double Vxnrm2(  
00148     int *nx,  
00149     int *ny,  
00150     int *nz,  
00151     double *x  
00152 );  
00153  
00160 VEXTERNC double Vxdot(  
00161     int *nx,  
00162     int *ny,  
00163     int *nz,  
00164     double *x,  
00165     double *y  
00166 );  
00167  
00174 VEXTERNC void Vazeros(  
00175     int *nx,  
00176     int *ny,  
00177     int *nz,  
00178     double *x  
00179 );  
00180  
00187 VEXTERNC void VfboundPMG(  
00188     int *ibound,  
00189     int *nx,  
00190     int *ny,  
00191     int *nz,  
00192     double *x,  
00193     double *gxc,  
00194     double *gyc,  
00195     double *gzc  
00196 );  
00197
```

```
00204 VEXTERNC void VfboundPMG00 (
00205     int    *nx,
00206     int    *ny,
00207     int    *nz,
00208     double *x
00209 );
00210
00217 VEXTERNC void Vaxrand(
00218     int    *nx,
00219     int    *ny,
00220     int    *nz,
00221     double *x
00222 );
00223
00230 VEXTERNC void Vxscal (
00231     int    *nx,
00232     int    *ny,
00233     int    *nz,
00234     double *fac,
00235     double *x
00236 );
00237
00244 VEXTERNC void Vprtmatd(
00245     int    *nx,
00246     int    *ny,
00247     int    *nz,
00248     int    *ipc,
00249     double *rpc,
00250     double *ac
00251 );
00252
00253 VEXTERNC void Vprtmatd7(
00254     int *nx,
00255     int *ny,
00256     int *nz,
00257     int *ipc,
00258     double *rpc,
00259     double *oC,
00260     double *oE,
00261     double *oN,
00262     double *uC
00263 );
00264
00265 VEXTERNC void Vprtmatd27(
00266     int *nx,
00267     int *ny,
00268     int *nz,
00269     int *ipc,
00270     double *rpc,
00271     double *oC,
00272     double *oE,
00273     double *oN,
00274     double *uC,
00275     double *oNE,
00276     double *oNW,
00277     double *uE,
00278     double *uW,
00279     double *uN,
00280     double *uS,
00281     double *uNE,
00282     double *uNW,
00283     double *uSE,
00284     double *uSW
00285 );
00286
00287 VEXTERNC void Vlinesearch(
00288     int    *nx,
00289     int    *ny,
00290     int    *nz,
00291     double *alpha,
00292     int    *ipc,
00293     double *rpc,
00294     double *ac,
00295     double *cc,
00296     double *fc,
00297     double *p,
00298     double *x,
00299     double *r,
00300     double *ap,
00301     double *zk,
00302     double *zkp1
```

```

00303     );
00304
00305 #endif /* MIKPCKD_H_ */

```

9.138 mlinpckd.c

```

00001
00055 #include "mlinpckd.h"
00056
00057 VPUBLIC void Vdpbs1(double *abd, int *lda, int *n, int *m, double *b) {
00058     double t;
00059     int k, kb, la, lb, lm;
00061
00062     MAT2(abd, *lda, 1);
00063
00064     for (k=1; k<=*n; k++) {
00065         lm = VMIN2(k-1, *m);
00066         la = *m + 1 - lm;
00067         lb = k - lm;
00068         t = Vddot(lm, RAT2(abd, la, k), 1, RAT(b, lb), 1);
00069         VAT(b, k) = (VAT(b, k) - t) / VAT2(abd, *m+1, k);
00070     }
00071
00072     // Solve R*X = Y
00073     for (kb=1; kb<=*n; kb++) {
00074         k = *n + 1 - kb;
00075         lm = VMIN2(k-1, *m);
00076         la = *m + 1 - lm;
00077         lb = k - lm;
00078         VAT(b, k) /= VAT2(abd, *m+1, k);
00080         t = -VAT(b, k);
00081         Vdaxpy(lm, t, RAT2(abd, la, k), 1, RAT(b, lb), 1);
00082     }
00083 }
00084
00085 VPUBLIC void Vdaxpy(int n, double da,
00086     double *dx, int incx,
00087     double *dy, int incy) {
00088
00089     int i, ix, iy, m, mpl;
00090
00091     if (n <= 0)
00092         return;
00093
00094     if (da == 0)
00095         return;
00096
00097     if (incx == 1 && incy == 1) {
00098         m = n % 4;
00099         if (m != 0) {
00100             for (i=1; i<=m; i++)
00101                 VAT(dy, i) += da * VAT(dx, i);
00102         }
00103
00104         if (n < 4)
00105             return;
00106
00107         mpl = m + 1;
00108
00109         for (i=mpl; i<=n; i+=4) {
00110             VAT(dy, i) += da * VAT(dx, i);
00111             VAT(dy, i+1) += da * VAT(dx, i+1);
00112             VAT(dy, i+2) += da * VAT(dx, i+2);
00113             VAT(dy, i+3) += da * VAT(dx, i+3);
00114         }
00115     } else {
00116         ix = 1;
00117         if (incx < 0)
00118             ix = (-n + 1) * incx + 1;
00119
00120         iy = 1;
00121         if (incy < 0)

```

```

00126         iy = (-n + 1) * incy + 1;
00127
00128         for (i=1; i<=n; i++) {
00129             VAT(dy, iy) += da * VAT(dx, ix);
00130             ix += incx;
00131             iy += incy;
00132         }
00133     }
00134 }
00135 }
00136
00137
00138 VPUBLIC double Vddot(int n, double *dx, int incx, double *dy, int incy) {
00139     double dtemp;
00140     int i, ix, iy, m, mpl;
00141
00142     double ddot = 0.0;
00143     dtemp = 0.0;
00144
00145     if (n <= 0)
00146         return ddot;
00147
00148     if (incx == 1 && incy == 1) {
00149         m = n % 5;
00150
00151         if (m != 0) {
00152             for (i=1; i<=m; i++)
00153                 dtemp += VAT(dx, i) * VAT(dy, i);
00154
00155             if (n < 5) {
00156                 ddot = dtemp;
00157                 return ddot;
00158             }
00159         }
00160
00161         mpl = m + 1;
00162
00163         for (i=mpl; i<=n; i+=5)
00164             dtemp += VAT(dx, i) * VAT(dy, i)
00165                 + VAT(dx, i+1) * VAT(dy, i+1)
00166                 + VAT(dx, i+2) * VAT(dy, i+2)
00167                 + VAT(dx, i+3) * VAT(dy, i+3)
00168                 + VAT(dx, i+4) * VAT(dy, i+4);
00169     } else {
00170         ix = 1;
00171         if (incx < 0)
00172             ix = (-n + 1) * incx + 1;
00173
00174         iy = 1;
00175         if (incy < 0)
00176             iy = (-n + 1) * incy + 1;
00177
00178         for (i=1; i<=n; i++) {
00179             ix += incx;
00180             iy += incy;
00181         }
00182     }
00183
00184     ddot = dtemp;
00185     return ddot;
00186 }
00187
00188
00189 VPUBLIC void Vdpbfa(double *abd, int *lda, int *n, int *m, int *info) {
00190     double t, s;
00191     int ik, j, jk, k, mu;
00192
00193     MAT2(abd, *lda, 1);
00194
00195     *info = 0;
00196
00197     for(j = 1; j <= *n; j++) {
00198         s = 0.0;
00199         ik = *m + 1;

```

```

00207         jk = VMAX2(j - *m, 1);
00208         mu = VMAX2(*m + 2 - j, 1);
00209
00210         if (*m >= mu ) {
00211
00212             for(k = mu; k <= *m; k++) {
00213                 t = VAT2(abd, k, j) - Vddot(k - mu,
00214                     RAT2(abd, ik, jk), 1,
00215                     RAT2(abd, mu, j), 1);
00216                 t /= VAT2(abd, *m + 1, jk);
00217                 VAT2(abd, k, j) = t;
00218                 s += t * t;
00219                 ik--;
00220                 jk++;
00221             }
00222         }
00223
00224         s = VAT2(abd, *m + 1, j) - s;
00225
00226         if (s <= 0.0) {
00227             *info = j;
00228             break;
00229         }
00230
00231         VAT2(abd, *m + 1, j) = VSQRT(s);
00232     }
00233 }

```

9.139 mlinpckd.h

```

00001
00049 #ifndef MLINPCKD_H_
00050 #define MLINPCKD_H_
00051
00052 #include "apbscfg.h"
00053
00054 #include "malloc/malloc.h"
00055
00056 #include "generic/vhal.h"
00057 #include "generic/vmatrix.h"
00058
00069 VEXTERNC void Vdpbsl(
00070     double *abd,
00071     int *lda,
00072     int *n,
00073     int *m,
00074     double *b
00075 );
00076
00080 VEXTERNC void Vdaxpy(int n, double da,
00081     double *dx, int incx,
00082     double *dy, int incy);
00083
00087 VEXTERNC double Vddot(int n, double *dx, int incx, double *dy, int incy);
00088
00092 VEXTERNC void Vdpbfa(double *abd, int *lda, int *n, int *m, int *info);
00093
00094 #endif /* MLINPCKD_H_ */

```

9.140 mypdec.c

```

00001
00055 #include "mypdec.h"
00056
00057 VPUBLIC void Vmyndefinitlpbe(int *tnion, double *tcharge, double *tsconc) {
00058
00059     int i;
00060
00061     nion = *tnion;
00062     if (nion > MAXIONS) {
00063         Vnm_print(2, "Vmypde: Warning: Ignoring extra ion species\n");
00064         nion = MAXIONS;
00065     }
00066
00067     for (i=1; i<=nion; i++) {
00068         VAT(charge, i) = VAT(tcharge, i);

```



```

00069     VAT(sconc, i) = VAT(tsconc, i);
00070 }
00071 }
00072
00073
00074
00075 VPUBLIC void Vmypdefinitnpbe(int *tnion, double *tcharge, double *tsconc) {
00076
00077     int i;
00078
00079     nion = *tnion;
00080     if (nion > MAXIONS) {
00081         Vnm_print(2, "Vmypde: Warning: Ignoring extra ion species\n");
00082         nion = MAXIONS;
00083     }
00084
00085     for (i=1; i<=nion; i++) {
00086         VAT(charge, i) = VAT(tcharge, i);
00087         VAT(sconc, i) = VAT(tsconc, i);
00088     }
00089 }
00090
00091
00092
00093 VPUBLIC void Vmypdefinitmpbe(int *tnion, double *tcharge, double *tsconc,
00094     double *smvolume, double *smsize) {
00095
00096     int i;
00097
00098     WARN_UNTESTED;
00099
00100     VABORT_MSG0("Not tested");
00101
00102     if (*tnion > 3) {
00103         Vnm_print(2, "SMPBE: modified theory handles only three ion species.\n");
00104         Vnm_print(2, "      Ignoring the rest of the ions!\n");
00105         Vnm_print(2, "      (mypde.f::mypdefinit)\n");
00106     }
00107
00108     v1 = VAT(tcharge, 1);
00109     v2 = VAT(tcharge, 2);
00110     v3 = VAT(tcharge, 3);
00111     conc1 = VAT(tsconc, 1);
00112     conc2 = VAT(tsconc, 2);
00113     conc3 = VAT(tsconc, 3);
00114
00115     vol = *smvolume;
00116     relSize = *smsize;
00117 }
00118
00119
00120
00121 VPUBLIC void Vc_vec(double *coef, double *uin, double *uout,
00122     int *nx, int *ny, int *nz, int *ipkey) {
00123
00124     if (*ipkey == -2) {
00125         Vc_vecsmpbe(coef, uin, uout, nx, ny, nz, ipkey);
00126     } else {
00127         Vc_vecpmg(coef, uin, uout, nx, ny, nz, ipkey);
00128     }
00129 }
00130
00131
00132
00133 VPUBLIC void Vc_vecpmg(double *coef, double *uin, double *uout,
00134     int *nx, int *ny, int *nz, int *ipkey) {
00135
00136     double zcf2;
00137     double zu2;
00138     double am_zero;
00139     double am_neg;
00140     double am_pos;
00141     double argument;
00142     int ichopped;
00143     int ichopped_neg;
00144     int ichopped_pos;
00145     int iion;
00146
00147     int n, i;
00148
00149     n = *nx * *ny * *nz;

```

```

00150
00151     for (i=1; i<=n; i++) {
00152         VAT(uout, i) = 0;
00153     }
00154
00155     for (iion=1; iion<=nion; iion++) {
00156
00157         // Assemble the ion-specific coefficient
00158         zcf2 = -1.0 * VAT(sconc, iion) * VAT(charge, iion);
00159
00160         // Assemble the ion-specific potential value
00161         zu2 = -1.0 * VAT(charge, iion);
00162
00163         if (*ipkey == 0) {
00164             ichopped = 0;
00165
00166             #pragma omp parallel for \
00167             default(shared) \
00168             private(i, ichopped_neg, ichopped_pos, am_zero, am_neg, am_pos, argument) \
00169             reduction(+ : ichopped)
00170             for (i=1; i<=n; i++) {
00171
00172                 // am_zero is 0 if coef zero, and 1 if coef nonzero
00173                 am_zero = VMIN2(ZSMALL, VABS(zcf2 * VAT(coef, i))) * ZLARGE;
00174
00175                 // am_neg is chopped u if u negative, 0 if u positive
00176                 am_neg = VMAX2(VMIN2(zu2 * VAT(uin, i), 0.0), SINH_MIN);
00177
00178                 // am_pos is chopped u if u positive, 0 if u negative
00179                 am_pos = VMIN2(VMAX2(zu2 * VAT(uin, i), 0.0), SINH_MAX);
00180
00181                 // Finally determine the function value
00182                 argument = am_zero * (am_neg + am_pos);
00183
00184                 VAT(uout, i) = VAT(uout, i) + zcf2 * VAT(coef, i) * exp(argument);
00185
00186                 // Count chopped values
00187                 ichopped_neg = (int)(am_neg / SINH_MIN);
00188                 ichopped_pos = (int)(am_pos / SINH_MAX);
00189                 ichopped += (int)(floor(am_zero+0.5)) * (ichopped_neg + ichopped_pos);
00190             }
00191
00192             // Info
00193             if (ichopped > 0) {
00194                 Vnm_print(2, "Vc_vecpmg: trapped exp overflows: %d\n", ichopped);
00195             }
00196
00197         } else if (*ipkey > 1 && *ipkey % 2 == 1 && *ipkey <= MAXPOLY) {
00198
00199             // Polynomial requested
00200             Vnm_print(2, "Vc_vecpmg: POLYNOMIAL APPROXIMATION UNAVAILABLE\n");
00201             abort();
00202         } else {
00203
00204             // Return linear approximation !***
00205             Vnm_print(2, "Vc_vecpmg: LINEAR APPROXIMATION UNAVAILABLE\n");
00206             abort();
00207         }
00208     }
00209 }
00210
00211
00212
00213 VPUBLIC void Vc_vecsmpbe(double *coef, double *uin, double *uout,
00214     int *nx, int *ny, int *nz, int *ipkey) {
00215
00216     int ideg;
00217     double zcf2, zu2;
00218     double am_zero, am_neg, am_pos;
00219     double argument, poly, fact;
00220
00221     int ichopped, ichopped_neg, ichopped_pos;
00222     int iion;
00223     int n, i, ii, ipara, ivect;
00224
00225     int nproc = 1;
00226
00227     // Added by DG SMPBE variables and common blocks
00228     double fracOccA, fracOccB, fracOccC, phi, ionStr;
00229     double z1, z2, z3, ca, cb, cc, a, k;
00230     double a1_neg, a1_pos, a2_neg, a2_pos;

```

```

00231     double a3_neg, a3_pos, a1, a2, a3;
00232     double f, g, gpark, alpha;
00233
00234     WARN_UNTESTED;
00235
00236     Vnm_print(2, "Vc_vecsmpbe: v1      = %f\n", v1);
00237     Vnm_print(2, "Vc_vecsmpbe: v2      = %f\n", v2);
00238     Vnm_print(2, "Vc_vecsmpbe: v3      = %f\n", v3);
00239     Vnm_print(2, "Vc_vecsmpbe: conc1   = %f\n", conc1);
00240     Vnm_print(2, "Vc_vecsmpbe: conc2   = %f\n", conc2);
00241     Vnm_print(2, "Vc_vecsmpbe: conc3   = %f\n", conc3);
00242     Vnm_print(2, "Vc_vecsmpbe: vol     = %f\n", vol);
00243     Vnm_print(2, "Vc_vecsmpbe: relSize = %f\n", relSize);
00244
00245     Vnm_print(2, "Vc_vecsmpbe: nion    = %d\n", nion);
00246
00247     Vnm_print(2, "Vc_vecsmpbe: charge = [");
00248     for (i=1; i<=nion; i++)
00249         Vnm_print(2, "%f ", VAT(charge, i));
00250     Vnm_print(2, "]\n");
00251
00252     Vnm_print(2, "Vc_vecsmpbe: sconc  = [");
00253     for (i=1; i<=nion; i++)
00254         Vnm_print(2, "%f ", VAT(sconc, i));
00255     Vnm_print(2, "]\n");
00256
00257
00258
00259     // Find parallel loops (ipara), remainder (ivect)
00260     n = *nx * *ny * *nz;
00261     ipara = n / nproc;
00262     ivect = n % nproc;
00263
00264     for (i=1; i<=n; i++)
00265         VAT(uout, i) = 0;
00266
00267     // Initialize the chopped counter
00268     ichopped = 0;
00269
00270     z1 = v1;
00271     z2 = v2;
00272     z3 = v3;
00273     ca = conc1;
00274     cb = conc2;
00275     cc = conc3;
00276     a  = vol;
00277     k  = relSize;
00278
00279     if (k - 1 < ZSMALL)
00280         Vnm_print(2, "Vc_vecsmpbe: k=1, using special routine\n");
00281
00282     // Derived quantities
00283     fracOccA = Na * ca * VPOW(a, 3.0);
00284     fracOccB = Na * cb * VPOW(a, 3.0);
00285     fracOccC = Na * cc * VPOW(a, 3.0);
00286
00287     phi      = (fracOccA / k) + fracOccB + fracOccC;
00288     alpha    = (fracOccA / k) / (1 - phi);
00289     ionStr   = 0.5 * (ca * VPOW(z1, 2.0) + cb * VPOW(z2, 2.0) + cc * VPOW(z3, 2.0));
00290
00291     for (i=1; i<=n; i++) {
00292
00293         am_zero = VMIN2(ZSMALL, VABS(VAT(coef, i))) * ZLARGE;
00294
00295         // Compute the arguments for exp(-z*u) term
00296         a1_neg = VMAX2(VMIN2(-1.0 * z1 * VAT(uin, i), 0.0), SINH_MIN);
00297         a1_pos = VMIN2(VMAX2(-1.0 * z1 * VAT(uin, i), 0.0), SINH_MAX);
00298
00299         // Compute the arguments for exp(-u) term
00300         a2_neg = VMAX2(VMIN2(-1.0 * z2 * VAT(uin, i), 0.0), SINH_MIN);
00301         a2_pos = VMIN2(VMAX2(-1.0 * z2 * VAT(uin, i), 0.0), SINH_MAX);
00302
00303         // Compute the arguments for exp(u) term
00304         a3_neg = VMAX2(VMIN2(-1.0 * z3 * VAT(uin, i), 0.0), SINH_MIN);
00305         a3_pos = VMIN2(VMAX2(-1.0 * z3 * VAT(uin, i), 0.0), SINH_MAX);
00306
00307         a1 = am_zero * (a1_neg + a1_pos);
00308         a2 = am_zero * (a2_neg + a2_pos);
00309         a3 = am_zero * (a3_neg + a3_pos);
00310
00311         gpark = (1 + alpha * exp(a1)) / (1 + alpha);

```

```

00312
00313     if (k - 1 < ZSMALL) {
00314         f = z1 * ca * exp(a1) + z2 * cb * exp(a2) + z3 * cc * exp(a3);
00315         g = 1 - phi + fracOccA * exp(a1)
00316             + fracOccB * exp(a2)
00317             + fracOccC * exp(a3);
00318     } else {
00319         f = z1 * ca * exp(a1) * VPOW(gpark, k-1)
00320             + z2 * cb * exp(a2)
00321             + z3 * cc * exp(a3);
00322         g = (1 - phi + fracOccA / k) * VPOW(gpark, k)
00323             + fracOccB * exp(a2)
00324             + fracOccC * exp(a3);
00325     }
00326
00327     VAT(uout, i) = -1.0 * VAT(coef, i) * (0.5 / ionStr) * (f / g);
00328
00329     // Count chopped values
00330     ichopped_neg = (int)((a1_neg + a2_neg+a3_neg) / SINH_MIN);
00331     ichopped_pos = (int)((a1_pos + a2_pos+a3_pos) / SINH_MAX);
00332     ichopped += (int)floor(am_zero+0.5) * (ichopped_neg + ichopped_pos);
00333 }
00334
00335 // Info
00336 if (ichopped > 0)
00337     Vnm_print(2, "Vc_vecsmpbe: trapped exp overflows: %d\n", ichopped);
00338
00339 }
00340
00341 VPUBLIC void Vdc_vec(double *coef, double *uin, double *uout,
00342     int *nx, int *ny, int *nz, int *ipkey) {
00343
00344     int i;
00345     int n = *nx * *ny * *nz;
00346
00347     if(*ipkey == -2) {
00348         Vdc_vecsmpbe(coef, uin, uout, nx, ny, nz, ipkey);
00349     } else {
00350         Vdc_vecpmg(coef, uin, uout, nx, ny, nz, ipkey);
00351     }
00352 }
00353
00354 VPUBLIC void Vdc_vecpmg(double *coef, double *uin, double *uout,
00355     int *nx, int *ny, int *nz, int *ipkey) {
00356
00357     int ideg, iion;
00358     double zcf2, zu2;
00359     double am_zero, am_neg, am_pos;
00360     double argument, poly, fact;
00361
00362     int ichopped, ichopped_neg, ichopped_pos;
00363     int n, i;
00364
00365     // Find parallel loops (ipara), remainder (ivect)
00366     n = *nx * *ny * *nz;
00367
00368     for (i=1; i<=n; i++) {
00369         VAT(uout, i) = 0.0;
00370     }
00371
00372     for (iion=1; iion<=nion; iion++) {
00373
00374         zcf2 = VAT(sconc, iion) * VAT(charge, iion) * VAT(charge, iion);
00375         zu2 = -1.0 * VAT(charge, iion);
00376
00377         // Check if full exp requested
00378         if (*ipkey == 0) {
00379
00380             // Initialize chopped counter
00381             ichopped = 0;
00382
00383             #pragma omp parallel for \
00384                 default(shared) \
00385                 private(i, ichopped_neg, ichopped_pos, \
00386                     am_zero, am_neg, am_pos, argument) \
00387                 reduction(+:ichopped)
00388             for (i=1; i<=n; i++) {
00389
00390                 // am_zero is 0 if coef zero, and 1 if coef nonzero
00391                 am_zero = VMIN2(ZSMALL, VABS(zcf2 * VAT(coef, i))) * ZLARGE;
00392

```

```

00393         // am_neg is chopped u if u negative, 0 if u positive
00394         am_neg = VMAX2(VMIN2(zu2 * VAT(uin, i), 0.0), SINH_MIN);
00395
00396         // am_neg is chopped u if u positive, 0 if u negative
00397         am_pos = VMIN2(VMAX2(zu2 * VAT(uin, i), 0.0), SINH_MAX);
00398
00399         // Finally determine the function value
00400         argument = am_zero * (am_neg + am_pos);
00401         VAT(uout, i) += zcf2 * VAT(coef, i) * exp( argument );
00402
00403         // Count chopped values
00404         ichopped_neg = (int)(am_neg / SINH_MIN);
00405         ichopped_pos = (int)(am_pos / SINH_MAX);
00406         ichopped += (int)floor(am_zero+0.5) * (ichopped_neg + ichopped_pos);
00407     }
00408
00409     // Info
00410     if (ichopped > 0)
00411         Vnm_print(2, "Vdc_vec: trapped exp overflows: %d\n", ichopped);
00412
00413     } else if ((*ipkey) > 1 && (*ipkey) % 2 == 1 && (*ipkey) <= MAXPOLY) {
00414         VABORT_MSG0("Vdc_vec: Polynomial approximation unavailable\n");
00415     } else {
00416         VABORT_MSG0("Vdc_vec: Linear approximation unavailable\n");
00417     }
00418 }
00419 }
00420
00421
00422
00423 VPUBLIC void Vdc_vecsmpbe(double *coef, double *uin, double *uout,
00424     int *nx, int *ny, int *nz, int *ipkey) {
00425
00426     int ideg, iion;
00427     double zcf2, zu2;
00428     double am_zero, am_neg, am_pos;
00429     double argument, poly, fact;
00430     int ichopped, ichopped_neg, ichopped_pos;
00431
00432     int n, i, ii;
00433     int ipara, ivect;
00434
00435     int nproc = 1;
00436
00437     // Added by DG SMPBE variables and common blocks
00438     double fracOccA, fracOccB, fracOccC, phi, ionStr;
00439     double z1, z2, z3, ca, cb, cc, a, k;
00440     double a1_neg, a1_pos, a2_neg, a2_pos;
00441     double a3_neg, a3_pos, a1, a2, a3;
00442     double f, g, fprime, gprime, gpark, alpha;
00443
00444     WARN_UNTESTED;
00445
00446     // Find parallel loops (ipara), remainder (ivect)
00447     n = *nx * *ny * *nz;
00448     ipara = n / nproc;
00449     ivect = n % nproc;
00450
00451     for (i=1; i<=n; i++)
00452         VAT(uout, i) = 0.0;
00453
00454     // Initialize the chopped counter
00455     ichopped = 0;
00456
00457     z1 = v1;
00458     z2 = v2;
00459     z3 = v3;
00460     ca = conc1;
00461     cb = conc2;
00462     cc = conc3;
00463     a = vol;
00464     k = relSize;
00465
00466     if (k - 1 < ZSMALL)
00467         Vnm_print(2, "Vdc_vecsmpbe: k=1, using special routine\n");
00468
00469     // Derived quantities
00470     fracOccA = Na * ca * VPOW(a, 3.0);
00471     fracOccB = Na * cb * VPOW(a, 3.0);
00472     fracOccC = Na * cc * VPOW(a, 3.0);
00473     phi = fracOccA / k + fracOccB + fracOccC;

```

```

00474     alpha = (fracOccA / k) / (1 - phi);
00475     ionStr = 0.5*(ca * VPOW(z1, 2) + cb * VPOW(z2, 2) + cc * VPOW(z3, 2));
00476
00477     for (i=1; i<=n; i++) {
00478
00479         am_zero = VMIN2(ZSMALL, VABS(VAT(coef, i))) * ZLARGE;
00480
00481         // Compute the arguments for exp(-z*u) term
00482         a1_neg = VMAX2(VMIN2(-1.0 * z1 * VAT(uin, i), 0.0), SINH_MIN);
00483         a1_pos = VMIN2(VMAX2(-1.0 * z1 * VAT(uin, i), 0.0), SINH_MAX);
00484
00485         // Compute the arguments for exp(-u) term
00486         a2_neg = VMAX2(VMIN2(-1.0 * z2 * VAT(uin, i), 0.0), SINH_MIN);
00487         a2_pos = VMIN2(VMAX2(-1.0 * z2 * VAT(uin, i), 0.0), SINH_MAX);
00488
00489         // Compute the arguments for exp(u) term
00490         a3_neg = VMAX2(VMIN2(-1.0 * z3 * VAT(uin, i), 0.0), SINH_MIN);
00491         a3_pos = VMIN2(VMAX2(-1.0 * z3 * VAT(uin, i), 0.0), SINH_MAX);
00492
00493         a1 = am_zero * (a1_neg + a1_pos);
00494         a2 = am_zero * (a2_neg + a2_pos);
00495         a3 = am_zero * (a3_neg + a3_pos);
00496
00497         gpark = (1 + alpha * exp(a1)) / (1 + alpha);
00498
00499         if (k - 1 < ZSMALL) {
00500             f = z1 * ca * exp(a1) + z2 * cb * exp(a2) + z3 * cc * exp(a3);
00501             g = 1 - phi + fracOccA * exp(a1)
00502                 + fracOccB * exp(a2)
00503                 + fracOccC * exp(a3);
00504
00505             fprime =
00506                 - VPOW(z1, 2) * ca * exp(a1)
00507                 - VPOW(z2, 2) * cb * exp(a2)
00508                 - VPOW(z3, 2) * cc * exp(a3);
00509
00510             gprime =
00511                 - z1 * fracOccA * exp(a1)
00512                 - z2 * fracOccB * exp(a2)
00513                 - z3 * fracOccC * exp(a3);
00514         } else {
00515             f = z1 * ca * exp(a1) * VPOW(gpark, k - 1)
00516                 + z2 * cb * exp(a2)
00517                 + z3 * cc * exp(a3);
00518             g = (1 - phi + fracOccA / k) * VPOW(gpark, k)
00519                 + fracOccB * exp(a2)
00520                 + fracOccC * exp(a3);
00521
00522             fprime =
00523                 - VPOW(z1, 2) * ca * exp(a1) * VPOW(gpark, k - 2)
00524                 * (gpark + (k - 1) * (alpha / (1 + alpha)) * exp(a1))
00525                 - VPOW(z2, 2) * cb * exp(a2)
00526                 - VPOW(z3, 2) * cc * exp(a3);
00527
00528             gprime =
00529                 - k * z1 * (alpha / (1 + alpha)) * exp(a1)
00530                 * (1 - phi + fracOccA / k) * VPOW(gpark, k - 1)
00531                 - z2 * fracOccB * exp(a2)
00532                 - z3 * fracOccC * exp(a3);
00533         }
00534     }
00535
00536     VAT(uout, i) = -1.0 * VAT(coef, i) * (0.5 / ionStr)
00537         * (fprime * g - gprime * f) / VPOW(g, 2.0);
00538
00539     // Count chopped values
00540     ichopped_neg = (int)((a1_neg + a2_neg + a3_neg) / SINH_MIN);
00541     ichopped_pos = (int)((a1_pos + a2_pos + a3_pos) / SINH_MAX);
00542     ichopped += (int)floor(am_zero+0.5) * (ichopped_neg + ichopped_pos);
00543 }
00544
00545 // Info
00546 if (ichopped > 0)
00547     Vnm_print(2, "Vdc_vecsmpbe: trapped exp overflows: %d\n", ichopped);
00548 }

```

9.141 mypdec.h

```

00001
00050 #ifndef _MYPDE_H_
00051 #define _MYPDE_H_
00052
00053 #include "math.h"
00054
00055 #include "apbscfg.h"
00056
00057 #include "malloc/malloc.h"
00058
00059 #include "generic/vhal.h"
00060 #include "pmgc/mypdec.h"
00061
00062 #define MAXIONS 50
00063 #define MAXPOLY 50
00064 #define ZSMALL 1.0e-20
00065 #define ZLARGE 1.0e20
00066 #define SINH_MIN -85.0
00067 #define SINH_MAX 85.0
00068
00070 double v1, v2, v3, conc1, conc2, conc3, vol, relSize;
00071 int nion;
00072 double charge[MAXIONS];
00073 double sconc[MAXIONS];
00074
00075 #define Na 6.022045000e-04
00076
00084 VEXTERNC void Vmypdefinitlpbe(
00085     int *tnion,
00086     double *tcharge,
00087     double *tsconc
00091 );
00092
00093
00094
00102 VEXTERNC void Vmypdefinitnpbe(
00103     int *tnion,
00104     double *tcharge,
00105     double *tsconc
00109 );
00110
00111
00112
00120 VEXTERNC void Vmypdefinitmpbe(
00121     int *tnion,
00122     double *tcharge,
00123     double *tsconc,
00127     double *smvolume,
00128     double *smsize
00129 );
00130
00131
00132
00139 VEXTERNC void Vc_vec(
00140     double *coef,
00141     double *uin,
00142     double *uout,
00143     int *nx,
00144     int *ny,
00145     int *nz,
00146     int *ipkey
00147 );
00148
00149
00150
00157 VEXTERNC void Vdc_vec(
00158     double *coef,
00159     double *uin,
00160     double *uout,
00161     int *nx,
00162     int *ny,
00163     int *nz,
00164     int *ipkey
00165 );
00166
00167 VEXTERNC void Vdc_vecpmg(
00168     double *coef,
00169     double *uin,

```

```

00170         double *uout,
00171         int      *nx,
00172         int      *ny,
00173         int      *nz,
00174         int      *ipkey
00175     );
00176
00177 VEXTERNC void Vdc_vecsmpbe(
00178     double *coef,
00179     double *uin,
00180     double *uout,
00181     int     *nx,
00182     int     *ny,
00183     int     *nz,
00184     int     *ipkey
00185 );
00186
00187
00188
00195 VEXTERNC void Vc_vecpmg(
00196     double *coef,
00197     double *uin,
00198     double *uout,
00199     int     *nx,
00200     int     *ny,
00201     int     *nz,
00202     int     *ipkey
00203 );
00204
00205
00206
00213 VEXTERNC void Vc_vecsmpbe(
00214     double *coef,
00215     double *uin,
00216     double *uout,
00217     int     *nx,
00218     int     *ny,
00219     int     *nz,
00220     int     *ipkey
00221 );
00222
00223 #endif /* _MYPDE_H_ */

```

9.142 newdrvd.c

```

00001
00055 #include "newdrvd.h"
00056
00057 VEXTERNC void Vnewdriv(
00058     int *iparm, double *rparm,
00059     int *iwork, double *rwork,
00060     double *u,
00061     double *xf, double *yf, double *zf,
00062     double *gxcf, double *gycf, double *gzcf,
00063     double *alcf, double *a2cf, double *a3cf,
00064     double *ccf, double *fcf, double *tcf) {
00065
00066     int nxc;
00067     int nyc;
00068     int nzc;
00069     int nf;
00070     int nc;
00071     int narr;
00072     int narrc;
00073     int n_rpc;
00074     int n_iz;
00075     int n_ipc;
00076     int iretot;
00077     int iintot;
00078
00079     int nrwk;
00080     int niwk;
00081     int nx;
00082     int ny;
00083     int nz;
00084     int nlev;
00085     int ierror;
00086     int maxlev;

```



```

00087     int mxlv;
00088     int mgcoar;
00089     int mgdisc;
00090     int mgsolv;
00091     int k_iz;
00092     int k_w1;
00093     int k_w2;
00094     int k_ipc;
00095     int k_rpc;
00096     int k_ac;
00097     int k_cc;
00098     int k_fc;
00099     int k_pc;
00100
00101     // Decode some parameters
00102     nrwk  = VAT(iparm, 1);
00103     niwk  = VAT(iparm, 2);
00104     nx    = VAT(iparm, 3);
00105     ny    = VAT(iparm, 4);
00106     nz    = VAT(iparm, 5);
00107     nlev  = VAT(iparm, 6);
00108
00109     // Some checks on input ***
00110     VASSERT_MSG0(nlev > 0, "The nlev parameter must be positive");
00111     VASSERT_MSG0(nx > 0, "The nx parameter must be positive");
00112     VASSERT_MSG0(ny > 0, "The ny parameter must be positive");
00113     VASSERT_MSG0(nz > 0, "The nz parameter must be positive");
00114
00115     mxlv = Vmaxlev(nx,ny,nz);
00116
00117     VASSERT_MSG1(nlev <= mxlv, "Max lev for your grid size is: %d", mxlv);
00118
00119     // Basic grid sizes, etc.
00120     mgcoar = VAT(iparm, 18);
00121     mgdisc = VAT(iparm, 19);
00122     mgsolv = VAT(iparm, 21);
00123
00124     Vmgpsz(&mgcoar, &mgdisc, &mgsolv,
00125           &nx, &ny, &nz,
00126           &nlev,
00127           &nxc, &nyc, &nzc,
00128           &nf, &nc,
00129           &narr, &narrc,
00130           &n_rpc, &n_iz, &n_ipc,
00131           &ioretot, &iintot);
00132
00133     // Allocate space for two additional work vectors ***
00134     ioretot = ioretot + 2 * nf;
00135
00136     // Some more checks on input
00137     VASSERT_MSG1( nrwk >= ioretot, "Real work space must be: %d", ioretot );
00138     VASSERT_MSG1( niwk >= iintot, "Integer work space must be: %d", iintot );
00139
00140     // Split up the integer work array
00141     k_iz = 1;
00142     k_ipc = k_iz + n_iz;
00143
00144     // Split up the real work array
00145     k_rpc = 1;
00146     k_cc = k_rpc + n_rpc;
00147     k_fc = k_cc + narr;
00148     k_w1 = k_fc + narr;
00149     k_w2 = k_w1 + nf;
00150     k_pc = k_w2 + nf;
00151     k_ac = k_pc + 27 * narrc;
00152     // k_ac_after = 4*nf + 14*narrc;
00153
00154     // Call the Newton Driver
00155     Vnewdrv2(iparm, rparam,
00156             &nx, &ny, &nz,
00157             u, RAT(iwork, k_iz),
00158             RAT(rwork, k_w1), RAT(rwork, k_w2),
00159             RAT(iwork, k_ipc), RAT(rwork, k_rpc),
00160             RAT(rwork, k_pc), RAT(rwork, k_ac), RAT(rwork, k_cc), RAT(rwork, k_fc),
00161             xf, yf, zf,
00162             gxcf, gycf, gzcf,
00163             alcf, a2cf, a3cf,
00164             ccf, fcf, tcf);
00165 }
00166
00167

```

```

00168
00169 VPUBLIC void Vnewdriv2(int *iparm, double *rparm,
00170     int *nx, int *ny, int *nz,
00171     double *u, int *iz,
00172     double *w1, double *w2,
00173     int *ipc, double *rpc,
00174     double *pc, double *ac, double *cc, double *fc,
00175     double *xf, double *yf, double *zf,
00176     double *gxcf, double *gycf, double *gzcf,
00177     double *alcf, double *a2cf, double *a3cf,
00178     double *ccf, double *fcf, double *tcf) {
00179
00180     int mgkey;
00181     int nlev;
00182     int itmax;
00183     int iok;
00184     int iinfo;
00185     int istop;
00186     int ipkey;
00187     int nul;
00188     int nu2;
00189     int ilev;
00190     int ido;
00191     int iters;
00192     int ierror;
00193     int nlev_real;
00194     int ibound;
00195     int mgprol;
00196     int mgcoar;
00197     int mgsolv;
00198     int mgdisc;
00199     int mgsmoo;
00200     int mode;
00201     double epsiln;
00202     double epsmac;
00203     double errtol;
00204     double omegal;
00205     double omegan;
00206     double bf;
00207     double oh;
00208     double tsetupf;
00209     double tsetupc;
00210     double tsolve;
00211
00212
00213
00214     // Utility variables
00215     int numlev;
00216
00217     int iok_t;
00218     int iters_t;
00219     double rsnrm_t;
00220     double rsden_t;
00221     double orsnrm_t;
00222
00223     int i;
00224
00225
00226
00227     // Decode the iparm array
00228     nlev = VAT(iparm, 6);
00229     nul = VAT(iparm, 7);
00230     nu2 = VAT(iparm, 8);
00231     mgkey = VAT(iparm, 9);
00232     itmax = VAT(iparm, 10);
00233     istop = VAT(iparm, 11);
00234     iinfo = VAT(iparm, 12);
00235     ipkey = VAT(iparm, 14);
00236     mgprol = VAT(iparm, 17);
00237     mgcoar = VAT(iparm, 18);
00238     mgdisc = VAT(iparm, 19);
00239     mgsmoo = VAT(iparm, 20);
00240     mgsolv = VAT(iparm, 21);
00241
00242     errtol = VAT(rparm, 1);
00243     omegal = VAT(rparm, 9);
00244     omegan = VAT(rparm, 10);
00245
00246     Vprtstp(0, -99, 0.0, 0.0, 0.0);
00247
00248     // Build the multigrid data structure in iz

```

```

00249     Vbuildstr(nx, ny, nz, &nlev, iz);
00250
00251     // Start the timer
00252     Vnm_tstart(30, "Vnewdrv2: fine problem setup");
00253
00254     // Build op and rhs on fine grid ***
00255     ido = 0;
00256     Vbuildops(nx, ny, nz,
00257               &nlev, &ipkey, &iinfo, &ido, iz,
00258               &mgprol, &mgcoar, &mgsovl, &mgdisc,
00259               ipc, rpc,
00260               pc, ac, cc, fc,
00261               xf, yf, zf,
00262               gxcf, gycf, gzcf,
00263               alcf, a2cf, a3cf,
00264               ccf, fcf, tcf);
00265
00266     // Stop the timer
00267     Vnm_tstop(30, "Vnewdrv2: fine problem setup");
00268
00269     // Start the timer
00270     Vnm_tstart(30, "Vnewdrv2: coarse problem setup");
00271
00272     // Build op and rhs on all coarse grids
00273     ido = 1;
00274     Vbuildops(nx, ny, nz,
00275               &nlev, &ipkey, &iinfo, &ido, iz,
00276               &mgprol, &mgcoar, &mgsovl, &mgdisc,
00277               ipc, rpc,
00278               pc, ac, cc, fc,
00279               xf, yf, zf,
00280               gxcf, gycf, gzcf,
00281               alcf, a2cf, a3cf,
00282               ccf, fcf, tcf);
00283
00284     // Stop the timer
00285     Vnm_tstop(30, "Vnewdrv2: coarse problem setup");
00286
00287
00288
00289     /* *****
00290     * *** this overwrites the rhs array provided by pde specification ***
00291     * ***** compute an algebraically produced rhs for the given tcf *****
00292     * *****
00293     mode = 1;
00294
00295     if (istop == 4 || istop == 5) {
00296         WARN_UNTESTED;
00297         Vbuildalg(nx, ny, nz,
00298                   &mode, &nlev, iz,
00299                   ipc, rpc, ac, cc, ccf, tcf, fc, fcf);
00300     }
00301
00302
00303
00304     // Determine machine epsilon
00305     epsiln = Vnm_epsmac();
00306
00307     // Impose zero dirichlet boundary conditions (now in source fcn)
00308     VfboundPMG00(nx, ny, nz, u);
00309
00310     // Start the timer
00311     Vnm_tstart(30, "Vnewdrv2: solve");
00312
00313     // Call specified multigrid method
00314     nlev_real = nlev;
00315     iok = 1;
00316     ilev = 1;
00317     if (mgkey == 0) {
00318         Vnewton(nx, ny, nz,
00319                u, iz,
00320                ccf, fcf, w1, w2,
00321                &istop, &itmax, &iters, &ierror,
00322                &nlev, &ilev, &nlev_real, &mgsovl,
00323                &iok, &iinfo,
00324                &epsiln, &errtol, &omegan,
00325                &nu1, &nu2, &mgsmoo,
00326                alcf, a2cf, a3cf,
00327                ipc, rpc,
00328                pc, ac, cc, fc, tcf);
00329     } else if (mgkey == 1) {

```

```

00330         Vfnwton(nx, ny, nz,
00331                 u, iz, ccf, fcf, w1, w2,
00332                 &istop, &itmax, &iters, &ierror,
00333                 &nlev, &ilev, &nlev_real, &mgsolv,
00334                 &iok, &iinfo,
00335                 &epsiln, &errtol, &omegan,
00336                 &nul, &nu2, &mgs moo,
00337                 alcf, a2cf, a3cf,
00338                 ipc, rpc,
00339                 pc, ac, cc, fc, tcf);
00340     } else {
00341         VABORT_MSG1("Bad mgkey given: %d", mgkey);
00342     }
00343
00344     // Stop the timer
00345     Vnm_tstop(30, "Vnewdrv2: solve");
00346
00347     // Restore boundary conditions
00348     ibound = 1;
00349     VfboundPMG(&ibound, nx, ny, nz, u, gxcf, gycf, gzcf);
00350 }

```

9.143 newdrv2.h

```

00001
00050 #ifndef _NEWDRV2_H_
00051 #define _NEWDRV2_H_
00052
00053 #include "apbscfg.h"
00054
00055 #include "malloc/malloc.h"
00056
00057 #include "generic/vhal.h"
00058 #include "pmgc/mgs subd.h"
00059 #include "pmgc/mikpckd.h"
00060 #include "pmgc/newtond.h"
00061 #include "pmgc/mgdrv2.h"
00062
00069 VEXTERN void Vnewdrv(
00070     int      *iparm,
00071     double   *rparm,
00072     int      *iwork,
00073     double   *rwork,
00074     double   *u,
00075     double   *xf,
00076     double   *yf,
00077     double   *zf,
00078     double   *gxcf,
00079     double   *gycf,
00080     double   *gzcf,
00081     double   *alcf,
00082     double   *a2cf,
00083     double   *a3cf,
00084     double   *ccf,
00085     double   *fcf,
00086     double   *tcf
00087 );
00088
00125 VEXTERN void Vnewdrv2(
00126     int      *iparm,
00127     double   *rparm,
00128     int      *nx,
00129     int      *ny,
00130     int      *nz,
00131     double   *u,
00132     int      *iz,
00133     double   *w1,
00134     double   *w2,
00135     int      *ipc,
00136     double   *rpc,
00137     double   *pc,
00138     double   *ac,
00139     double   *cc,
00140     double   *fc,
00141     double   *xf,
00142     double   *yf,
00143     double   *zf,
00144     double   *gxcf,

```

```

00145         double *gycf,
00146         double *gzcf,
00147         double *alcf,
00148         double *a2cf,
00149         double *a3cf,
00150         double *ccf,
00151         double *fcf,
00152         double *tcf
00153     );
00154
00155 #endif /* _NEWDRVD_H_ */

```

9.144 newtond.c

```

00001
00056 #include "newtond.h"
00057
00058 VPUBLIC void Vfnewton(int *nx,int *ny,int *nz,
00059     double *x, int *iz,
00060     double *w0, double *w1, double *w2, double *w3,
00061     int *istop, int *itmax, int *iters, int *ierror,
00062     int *nlev, int *ilev, int *nlev_real,
00063     int *mgsolv, int *iok, int *iinfo,
00064     double *epsiln, double *errtol, double *omega,
00065     int *nul, int *nu2, int *mgsmoo,
00066     double *cprime, double *rhs, double *xtmp,
00067     int *ipc, double *rpc,
00068     double *pc, double *ac, double *cc, double *fc, double *tru) {
00069
00070     int level, itmx, nlevd, iterd, iokd;
00071     int nxf, nyf, nzf;
00072     int nxc, nyc, nzc;
00073     int istpd;
00074     int numlev;
00075     double errd;
00076
00077     MAT2( iz, 50, 1);
00078
00079     // Recover gridsizes ***
00080     nxf = *nx;
00081     nyf = *ny;
00082     nzf = *nz;
00083
00084     numlev = *nlev - 1;
00085     Vmkcors(&numlev, &nxf, &nyf, &nzf, &nxc, &nyc, &nzc);
00086
00087     // Move up grids: interpolate solution to finer, do newton
00088     if (*iinfo > 1) {
00089         VMESAGE0("Starting");
00090         VMESAGE3("Fine Grid Size: (%d, %d, %d)", nxf, nyf, nzf);
00091         VMESAGE3("Course Grid Size: (%d, %d, %d)", nxc, nyc, nzc);
00092     }
00093
00094     for (level=*nlev_real; level<=*ilev+1; level--) {
00095
00096         // Call mv cycle
00097         errd = *errtol;
00098         itmx = 1000;
00099         nlevd = *nlev_real - level + 1;
00100         iterd = 0;
00101         iokd = *iok;
00102         istpd = *istop;
00103
00104         Vnewton(&nxc, &nyc, &nzc,
00105             x, iz,
00106             w0, w1, w2, w3,
00107             &istpd, &itmx, &iterd, ierror,
00108             &nlevd, &level, nlev_real,
00109             mgsolv, &iokd, iinfo,
00110             epsiln, &errd, omega,
00111             nul, nu2, mgsmoo,
00112             cprime, rhs, xtmp,
00113             ipc, rpc,
00114             pc, ac, cc, fc, tru);
00115
00116
00117         // Find new grid size ***
00118         numlev = 1;

```

```

00119         Vmkfine(&numlev, &nxc, &nyc, &nzc, &nxf, &nyf, &nzf);
00120
00121         // Interpolate to next finer grid (use correct bc's)
00122         VinterpPMG(&nxc, &nyc, &nzc,
00123                 &nxf, &nyf, &nzf,
00124                 RAT( x, VAT2(iz, 1, level )),
00125                 RAT( x, VAT2(iz, 1, level-1)),
00126                 RAT(pc, VAT2(iz, 11, level-1)));
00127
00128         /*
00129         Commented out fortran code. May need to implement later
00130         call ninterpPMG(nxc,nyc,nzc,nxf,nyf,nzf,
00131                 x(iz(1,level)),x(iz(1,level-1)),pc(iz(11,level-1)),
00132                 ipc(iz(5,level-1)),rpc(iz(6,level-1)),
00133                 ac(iz(7,level-1)),cc(iz(1,level-1)),fc(iz(1,level-1)))
00134         */
00135
00136         // New grid size
00137         nxc = nxf;
00138         nyc = nyf;
00139         nzc = nzf;
00140     }
00141
00142
00143     // Call mv cycle
00144     level = *ilev;
00145
00146     Vnewton(nx, ny, nz,
00147            x, iz,
00148            w0, w1, w2, w3,
00149            istop, itmax, iters, ierror,
00150            nlev, &level, nlev_real,
00151            mgsolv, iok, iinfo,
00152            epsiln, errtol, omega,
00153            nul, nu2, mgsmoo,
00154            cprime, rhs, xtmp,
00155            ipc, rpc,
00156            pc, ac, cc, fc, tru);
00157 }
00158
00159
00160
00161
00162 VPUBLIC void Vnewton(int *nx, int *ny, int *nz,
00163         double *x, int *iz,
00164         double *w0, double *w1, double *w2, double *w3,
00165         int *istop, int *itmax, int *iters, int *ierror,
00166         int *nlev, int *ilev, int *nlev_real,
00167         int *mgsolv, int *iok, int *iinfo,
00168         double *epsiln, double *errtol, double *omega,
00169         int *nul, int *nu2, int *mgsmoo,
00170         double *cprime, double *rhs, double *xtmp,
00171         int *ipc, double *rpc,
00172         double *pc, double *ac, double *cc, double *fc, double *tru) {
00173
00174     int level, lev;
00175     int itmax_s, iters_s, ierror_s, iok_s, iinfo_s, istop_s;
00176     double errtol_s, ord, bigc;
00177     double rsden, rsnm, orsnrm;
00178
00179     double xnorm_old, xnorm_new, damp, xnorm_med, xnorm_den;
00180     double rho_max, rho_min, rho_max_mod, rho_min_mod, errtol_p;
00181     int iter_d, itmax_d, mode, idamp, ipkey;
00182     int itmax_p, iters_p, iok_p, iinfo_p;
00183
00184     // Utility and temporary parameters
00185     double alpha;
00186
00187     MAT2(iz, 50, 1);
00188
00189     // Recover level information
00190     level = 1;
00191     lev = (*ilev - 1) + level;
00192
00193     // Do some i/o if requested
00194     if (*iinfo > 1) {
00195         VMESSAGE3("Starting: (%d, %d, %d)", *nx, *ny, *nz);
00196     }
00197
00198     if (*iok != 0) {
00199         Vprtstp(*iok, -1, 0.0, 0.0, 0.0);

```

```

00200     }
00201
00202     /*****
00203     *** note: if (iok!=0) then: use a stopping test.      ***
00204     ***     else: use just the itmax to stop iteration.    ***
00205     *****/
00206     *** istop=0 most efficient (whatever it is)          ***
00207     *** istop=1 relative residual                        ***
00208     *** istop=2 rms difference of successive iterates    ***
00209     *** istop=3 relative true error (provided for testing) ***
00210     *****/
00211
00212     // Compute denominator for stopping criterion
00213     if (*istop == 0) {
00214         rsden = 1.0;
00215     } else if (*istop == 1) {
00216
00217         // Compute initial residual with zero initial guess
00218         // this is analogous to the linear case where one can
00219         // simply take norm of rhs for a zero initial guess
00220
00221         Vazeros(nx, ny, nz, w1);
00222
00223         Vnmresid(nx, ny, nz,
00224                 RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00225                 RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00226                 RAT(fc, VAT2(iz, 1, lev)),
00227                 w1, w2, w3);
00228         rsden = Vxnrm1(nx, ny, nz, w2);
00229     } else if (*istop == 2) {
00230         rsden = VSQRT(*nx * *ny * *nz);
00231     } else if (*istop == 3) {
00232         rsden = Vxnrm2(nx, ny, nz, RAT(tru, VAT2(iz, 1, lev)));
00233     } else if (*istop == 4) {
00234         rsden = Vxnrm2(nx, ny, nz, RAT(tru, VAT2(iz, 1, lev)));
00235     } else if (*istop == 5) {
00236         Vnmatvec(nx, ny, nz,
00237                 RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00238                 RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00239                 RAT(tru, VAT2(iz, 1, lev)),
00240                 w1, w2);
00241         rsden = VSQRT(Vxdot(nx, ny, nz, RAT(tru, VAT2(iz, 1, lev)), w1));
00242     } else {
00243         VABORT_MSG1("Bad istop value: %d\n", *istop);
00244     }
00245
00246     if (rsden == 0.0) {
00247         rsden = 1.0;
00248         VWARN_MSG0(rsden != 0, "rhs is zero");
00249     }
00250     rsnrm = rsden;
00251     orsnrm = rsnrm;
00252
00253     if (*iok != 0) {
00254         Vprtstp(*iok, 0, rsnrm, rsden, orsnrm);
00255     }
00256
00257     /*****
00258     *** begin newton iteration
00259     *****/
00260
00261     // Now compute residual with the initial guess
00262
00263     Vnmresid(nx, ny, nz,
00264             RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00265             RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00266             RAT(fc, VAT2(iz, 1, lev)), RAT(x, VAT2(iz, 1, lev)),
00267             w0, w2);
00268     xnorm_old = Vxnrm1(nx, ny, nz, w0);
00269     if (*iok != 0) {
00270         xnorm_den = rsden;
00271     } else {
00272         xnorm_den = xnorm_old;
00273     }
00274
00275
00276
00277     /*****
00278     *** begin the loop
00279     *****/
00280

```

```

00281 // Setup for the looping
00282 VMESAGE0("Damping enabled");
00283 idamp = 1;
00284 *iters = 0;
00285
00286 //30
00287 while(1) {
00288     (*iters)++;
00289
00290     // Save iterate if stop test will use it on next iter
00291     if (*istop == 2) {
00292         Vxcopy(nx, ny, nz,
00293             RAT(x, VAT2(iz, 1, lev)), RAT(tru, VAT2(iz, 1, lev)));
00294     }
00295
00296     // Compute the current jacobian system and rhs
00297     ipkey = VAT(ipc, 10);
00298     Vgetjac(nx, ny, nz, nlev_real, iz, ilev, &ipkey,
00299         x, w0, cprime, rhs, cc, pc);
00300
00301     // Determine number of correct digits in current residual
00302     // Algorithm 5.3 in the thesis, test version (1')
00303     // Global-superlinear convergence
00304     bigc = 1.0;
00305     ord = 2.0;
00306
00307     /* NAB 06-18-01: If complex problems are not converging, set this to
00308     * machine epsilon. This makes it use the exact jacobian rather than
00309     * the appropriate form (as here)
00310     */
00311     errtol_s = VMIN2((0.9 * xnorm_old), (bigc * VPOW(xnorm_old, ord)));
00312     VMESAGE1("Using errtol_s: %f", errtol_s);
00313
00314     // Do a linear multigrid solve of the newton equations
00315     Vazeros(nx, ny, nz, RAT(xtmp, VAT2(iz, 1, lev)));
00316
00317     itmax_s = 1000;
00318     istop_s = 0;
00319     iters_s = 0;
00320     ierror_s = 0;
00321
00322     // NAB 06-18-01 -- What this used to be:
00323     iok_s = 0;
00324     iinfo_s = 0;
00325     if ((*iinfo >= 2) && (*ilev == 1))
00326         iok_s = 2;
00327
00328     // What it's changed to:
00329     if (*iinfo >= 2)
00330         iinfo_s = *iinfo;
00331     iok_s = 2;
00332
00333     // End of NAB hack.
00334
00335     Vmvcs(nx, ny, nz,
00336         xtmp, iz,
00337         w0, w1, w2, w3,
00338         &istop_s, &itmax_s, &iters_s, &ierror_s,
00339         nlev, ilev, nlev_real, mgsolv,
00340         &iok_s, &iinfo_s,
00341         epsiln, &errtol_s, omega,
00342         nu1, nu2, mgsmoo,
00343         ipc, rpc, pc, ac, cprime, rhs, tru);
00344
00345     /*****
00346     *** note: rhs and cprime are now available as temp vectors ***
00347     *****/
00348
00349     // If damping is still enabled -- doit
00350     if (idamp == 1) {
00351         // Try the correction
00352         Vxcopy(nx, ny, nz,
00353             RAT(x, VAT2(iz, 1, lev)), w1);
00354         damp = 1.0;
00355         Vxaxpy(nx, ny, nz, &damp, RAT(xtmp, VAT2(iz, 1, lev)), w1);
00356
00357         Vnmresid(nx, ny, nz,
00358             RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00359             RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00360

```



```

00362         RAT( fc, VAT2(iz, 1, lev)),
00363         w1, w0,
00364         RAT(rhs, VAT2(iz, 1, lev)));
00365     xnorm_new = Vxnrm1(nx, ny, nz, w0);
00366
00367     // Damping is still enabled -- doit
00368     damp = 1.0;
00369     iter_d = 0;
00370     itmax_d = 10;
00371     mode = 0;
00372
00373     VMESAGE1("Attempting damping, relres = %f", xnorm_new / xnorm_den);
00374
00375     while(iter_d < itmax_d) {
00376         if (mode == 0) {
00377             if (xnorm_new < xnorm_old) {
00378                 mode = 1;
00379             }
00380             } else if (xnorm_new > xnorm_med) {
00381                 break;
00382             }
00383
00384             // Keep old soln and residual around, and its norm
00385             Vxcopy(nx, ny, nz, w1, w2);
00386             Vxcopy(nx, ny, nz, w0, w3);
00387             xnorm_med = xnorm_new;
00388
00389             // New damped correction, residual, and its norm
00390             Vxcopy(nx, ny, nz,
00391                 RAT(x, VAT2(iz, 1, lev)), w1);
00392             damp = damp / 2.0;
00393             Vxaxpy(nx, ny, nz, &damp, RAT(xtmp, VAT2(iz, 1, lev)), w1);
00394
00395             Vnmresid(nx, ny, nz,
00396                 RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00397                 RAT( ac, VAT2(iz, 7, lev)), RAT( cc, VAT2(iz, 1, lev)),
00398                 RAT( fc, VAT2(iz, 1, lev)),
00399                 w1, w0,
00400                 RAT(rhs, VAT2(iz, 1, lev)));
00401             xnorm_new = Vxnrm1(nx, ny, nz, w0);
00402
00403             // Next iter...
00404             iter_d = iter_d + 1;
00405             VMESAGE1("Attempting damping, relres = %f",
00406                 xnorm_new / xnorm_den);
00407         }
00408
00409         Vxcopy(nx, ny, nz, w2, RAT(x, VAT2(iz, 1, lev)));
00410         Vxcopy(nx, ny, nz, w3, w0);
00411         xnorm_new = xnorm_med;
00412         xnorm_old = xnorm_new;
00413
00414         VMESAGE1("Damping accepted, relres = %f", xnorm_new / xnorm_den);
00415
00416         // Determine whether or not to disable damping
00417         if ((iter_d - 1) == 0) {
00418             VMESAGE0("Damping disabled");
00419             idamp = 0;
00420         }
00421     } else {
00422
00423         // Damping is disabled -- accept the newton step
00424         damp = 1.0;
00425
00426         Vxaxpy(nx, ny, nz, &damp,
00427             RAT(xtmp, VAT2(iz, 1, lev)), RAT(x, VAT2(iz, 1, lev)));
00428
00429         Vnmresid(nx, ny, nz,
00430             RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00431             RAT( ac, VAT2(iz, 7, lev)), RAT( cc, VAT2(iz, 1, lev)),
00432             RAT( fc, VAT2(iz, 1, lev)), RAT( x, VAT2(iz, 1, lev)),
00433             w0,
00434             RAT(rhs, VAT2(iz, 1, lev)));
00435
00436         xnorm_new = Vxnrm1(nx, ny, nz, w0);
00437         xnorm_old = xnorm_new;
00438     }
00439
00440     // Compute/check the current stopping test ***
00441     if (iok != 0) {

```

```

00443         orsnrm = rsnm;
00444
00445     if (*istop == 0) {
00446         rsnm = xnorm_new;
00447     } else if (*istop == 1) {
00448         rsnm = xnorm_new;
00449     } else if (*istop == 2) {
00450         Vxcopy(nx, ny, nz, RAT(tru, VAT2(iz, 1, lev)), w1);
00451         alpha = -1.0;
00452         Vxaxpy(nx, ny, nz, &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00453         rsnm = Vxnorm1(nx, ny, nz, w1);
00454     } else if (*istop == 3) {
00455         Vxcopy(nx, ny, nz, RAT(tru, VAT2(iz, 1, lev)), w1);
00456         alpha = -1.0;
00457         Vxaxpy(nx, ny, nz, &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00458         rsnm = Vxnorm2(nx, ny, nz, w1);
00459     } else if (*istop == 4) {
00460         Vxcopy(nx, ny, nz, RAT(tru, VAT2(iz, 1, lev)), w1);
00461         alpha = -1.0;
00462         Vxaxpy(nx, ny, nz, &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00463         rsnm = Vxnorm2(nx, ny, nz, w1);
00464     } else if (*istop == 5) {
00465         Vxcopy(nx, ny, nz, RAT(tru, VAT2(iz, 1, lev)), w1);
00466         alpha = -1.0;
00467         Vxaxpy(nx, ny, nz, &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00468         Vnmatvec(nx, ny, nz,
00469                 RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00470                 RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00471                 w1, w2, w3);
00472         rsnm = VSQRT(Vxdot(nx, ny, nz, w1, w2));
00473     } else {
00474         VABORT_MSG1("Bad istop value: %d", *istop);
00475     }
00476
00477     Vprtstp(*iok, *iters, rsnm, rsden, orsnrm);
00478
00479     if ((rsnm/rsden) <= *errtol)
00480         break;
00481 }
00482
00483 // Check iteration count ***
00484 if (*iters >= *itmax)
00485     break;
00486 }
00487
00488 // Condition estimate of final jacobian
00489 if (*iinfo > 2) {
00490     Vnm_print(2, "%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%\n");
00491     Vnm_print(2, "% Vnewton: JACOBIAN ANALYSIS ==> (%d, %d, %d)\n",
00492             *nx, *ny, *nz );
00493
00494     // Largest eigenvalue of the jacobian matrix
00495     Vnm_print(2, "% Vnewton: Power calculating rho(JAC)\n");
00496     itmax_p = 1000;
00497     errtol_p = 1.0e-4;
00498     iters_p = 0;
00499     iinfo_p = *iinfo;
00500
00501     Vpower(nx, ny, nz,
00502           iz, ilev,
00503           ipc, rpc, ac, cprime,
00504           w0, w1, w2, w3,
00505           &rho_max, &rho_max_mod,
00506           &errtol_p, &itmax_p, &iters_p, &iinfo_p);
00507
00508     Vnm_print(2, "% Vnewton: power iters = %d\n", iters_p);
00509     Vnm_print(2, "% Vnewton: power eigmax = %d\n", rho_max);
00510     Vnm_print(2, "% Vnewton: power (MODEL) = %d\n", rho_max_mod);
00511
00512     // Smallest eigenvalue of the system matrix A ***
00513     Vnm_print(2, "% Vnewton: ipower calculating lambda_min(JAC)...\n");
00514     itmax_p = 1000;
00515     errtol_p = 1.0e-4;
00516     iters_p = 0;
00517     iinfo_p = *iinfo;
00518
00519     Vazeros(nx, ny, nz, xtmp);
00520
00521     Vipower(nx, ny, nz,

```

```

00524         xtmp, iz,
00525         w0, w1, w2, w3,
00526         rhs, &rho_min, &rho_min_mod,
00527         &errtol_p, &itmax_p, &iters_p,
00528         nlev, ilev, nlev_real, mgsolv,
00529         &iok_p, &iinfo_p,
00530         epsilon, errtol, omega,
00531         nu1, nu2, mgsmoo,
00532         ipc, rpc,
00533         pc, ac, cprime, tru);
00534
00535     Vnm_print(2, "% Vnewton: ipower iters   = %d\n", iters_p);
00536     Vnm_print(2, "% Vnewton: ipower eigmin = %d\n", rho_min);
00537     Vnm_print(2, "% Vnewton: ipower (MODEL) = %d\n", rho_min_mod);
00538
00539     // Condition number estimate
00540     Vnm_print(2, "% Vnewton: condition number = %f\n",
00541             (double)rho_max / rho_min);
00542     Vnm_print(2, "% Vnewton: condition (MODEL) = %f\n",
00543             (double)rho_max_mod / rho_min_mod);
00544     Vnm_print(2, "%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%\n");
00545 }
00546 }
00547
00548
00549
00550 VPUBLIC void Vgetjac(int *nx, int *ny, int *nz,
00551     int *nlev_real, int *iz, int *lev, int *ipkey,
00552     double *x, double *r,
00553     double *cprime, double *rhs,
00554     double *cc, double *pc) {
00555
00556     int nxx, nyy, nzz;
00557     int nxold, nyold, nzold;
00558     int level, numlev;
00559
00560     MAT2(iz, 50, 1);
00561
00562     // Setup
00563     nxx = *nx;
00564     nyy = *ny;
00565     nzz = *nz;
00566
00567     // Form the rhs of the newton system -- just current residual
00568     Vxcopy(nx, ny, nz, r, RAT(rhs, VAT2(iz, 1,*lev)));
00569
00570     // Get nonlinear part of the jacobian operator
00571     Vdc_vec(RAT(cc, VAT2(iz, 1,*lev)), RAT(x, VAT2(iz, 1,*lev)),
00572         RAT(cprime, VAT2(iz, 1,*lev)),
00573         nx, ny, nz, ipkey);
00574
00575     // Build the (nlev-1) level operators
00576     for (level=*lev+1; level<=*nlev_real; level++) {
00577         nxold = nxx;
00578         nyold = nyy;
00579         nzold = nzz;
00580
00581         numlev = 1;
00582         Vmkcors(&numlev, &nxold, &nyold, &nzold, &nxx, &nyy, &nzz);
00583
00584         // Make the coarse grid rhs functions
00585         Vrestrc(&nxold, &nyold, &nzold,
00586             &nxx, &nyy, &nzz,
00587             RAT(rhs, VAT2(iz, 1,level-1)),
00588             RAT(rhs, VAT2(iz, 1,level )),
00589             RAT(pc, VAT2(iz, 11,level-1)));
00590
00591         // Make the coarse grid helmholtz terms
00592         Vrestrc(&nxold, &nyold, &nzold,
00593             &nxx, &nyy, &nzz,
00594             RAT(cprime, VAT2(iz, 1, level-1)),
00595             RAT(cprime, VAT2(iz, 1, level )),
00596             RAT(pc, VAT2(iz, 11, level-1)));
00597     }
00598 }

```

9.145 newtond.h

```
00001
00049 #ifndef _NEWTOND_H_
00050 #define _NEWTOND_H_
00051
00052 #include "apbscfg.h"
00053
00054 #include "malloc/malloc.h"
00055
00056 #include "generic/vhal.h"
00057 #include "generic/vmatrix.h"
00058 #include "pmgc/matvecd.h"
00059 #include "pmgc/mikpckd.h"
00060 #include "pmgc/mgcsd.h"
00061 #include "pmgc/mgsudd.h"
00062 #include "pmgc/powerd.h"
00063
00070 VPUBLIC void Vfnewton(
00071     int *nx,
00072     int *ny,
00073     int *nz,
00074     double *x,
00075     int *iz,
00076     double *w0,
00077     double *w1,
00078     double *w2,
00079     double *w3,
00080     int *istop,
00081     int *itmax,
00082     int *iters,
00083     int *ierror,
00084     int *nlev,
00085     int *ilev,
00086     int *nlev_real,
00087     int *mgsolv,
00088     int *iok,
00089     int *iinfo,
00090     double *epsiln,
00091     double *errtol,
00092     double *omega,
00093     int *nul,
00094     int *nu2,
00095     int *mgs moo,
00096     double *cprime,
00097     double *rhs,
00098     double *xtmp,
00099     int *ipc,
00100     double *rpc,
00101     double *pc,
00102     double *ac,
00103     double *cc,
00104     double *fc,
00105     double *tru
00106 );
00107
00114 VEXTERN void Vnewton(
00115     int *nx,
00116     int *ny,
00117     int *nz,
00118     double *x,
00119     int *iz,
00120     double *w0,
00121     double *w1,
00122     double *w2,
00123     double *w3,
00124     int *istop,
00125     int *itmax,
00126     int *iters,
00127     int *ierror,
00128     int *nlev,
00129     int *ilev,
00130     int *nlev_real,
00131     int *mgsolv,
00132     int *iok,
00133     int *iinfo,
00134     double *epsiln,
00135     double *errtol,
00136     double *omega,
00137     int *nul,
```

```

00138         int *nu2,
00139         int *mgsmoo,
00140         double *cprime,
00141         double *rhs,
00142         double *xtmp,
00143         int *ipc,
00144         double *rpc,
00145         double *pc,
00146         double *ac,
00147         double *cc,
00148         double *fc,
00149         double *tru
00150     );
00151
00152
00159 VEXTERNC void Vgetjac(
00160     int *nx,
00161     int *ny,
00162     int *nz,
00163     int *nlev_real,
00164     int *iz,
00165     int *lev,
00166     int *ipkey,
00167     double *x,
00168     double *r,
00169     double *cprime,
00170     double *rhs,
00171     double *cc,
00172     double *pc
00173 );
00174
00175 #endif /* _NEWTOND_H_ */

```

9.146 powerd.c

```

00001
00055 #include "powerd.h"
00056
00057 VPUBLIC void Vpower(int *nx, int *ny, int *nz,
00058     int *iz, int *ilev,
00059     int *ipc, double *rpc, double *ac, double *cc,
00060     double *w1, double *w2, double *w3, double *w4,
00061     double *eigmax, double *eigmax_model, double *tol,
00062     int *itmax, int *iters, int *iinfo) {
00063
00064     int lev, level;
00065     double denom, fac, rho, oldrho, error, relerr;
00066
00068     double pi = 4.0 * atan( 1.0 );
00069
00070     // Utility variables
00071     int skipIters = 0;
00072     double alpha;
00073
00074     MAT2(iz, 50, 1);
00075
00076     WARN_UNTESTED;
00077
00078     // Recover level information
00079     level = 1;
00080     lev = (*ilev - 1) + level;
00081
00082     // Seed vector: random to contain all components
00083
00084     Vaxrand(nx, ny, nz, w1);
00085
00086     Vazeros(nx, ny, nz, w2);
00087     Vazeros(nx, ny, nz, w3);
00088     Vazeros(nx, ny, nz, w4);
00089
00090     // Compute raleigh quotient with the seed vector
00091     denom = Vxnorm2(nx, ny, nz, w1);
00092     fac = 1.0 / denom;
00093     Vxscal(nx, ny, nz, &fac, w1);
00094     Vmatvec(nx, ny, nz,
00095         RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00096         RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)), w1, w2);
00097     oldrho = Vxdot(nx, ny, nz, w1, w2);

```

```

00098
00099 // I/O
00100 if (oldrho == 0.0) {
00101     if (*iinfo > 3) {
00102         Vnm_print(2, "POWER: iter: estimate = %d %g\n", *iters, oldrho);
00103     }
00104     rho = oldrho;
00105 } else {
00106
00107     // Main iteration
00108     *iters = 0;
00109     while(1) {
00110         (*iters)++;
00111
00112         // Apply the matrix A
00113         Vmatvec(nx, ny, nz,
00114             RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00115             RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)), w1, w2);
00116
00117         Vxcopy(nx, ny, nz, w2, w1);
00118
00119         // Normalize the new vector
00120         denom = Vxnorm2(nx, ny, nz, w1);
00121         fac = 1.0 / denom;
00122         Vxscal(nx, ny, nz, &fac, w1);
00123
00124         // Compute the new raleigh quotient
00125         Vmatvec(nx, ny, nz,
00126             RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00127             RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)), w1, w2);
00128         rho = Vxdot(nx, ny, nz, w1, w2);
00129
00130         // Stopping test ***
00131         // w2=A*x, w1=x, stop = 2-norm(A*x-lamda*x)
00132
00133         Vxcopy(nx, ny, nz, w1, w3);
00134         Vxcopy(nx, ny, nz, w2, w4);
00135         Vxscal(nx, ny, nz, &rho, w3);
00136         alpha = -1.0;
00137         Vxaxpy(nx, ny, nz, &alpha, w3, w4);
00138         error = Vxnorm2(nx, ny, nz, w4);
00139         relerr = VABS(rho - oldrho) / VABS(rho);
00140
00141         // I/O
00142         if (*iinfo > 3) {
00143
00144             Vnm_print(2, "POWER:  iters  =%d\n", *iters);
00145             Vnm_print(2, "          error  =%g\n", error);
00146             Vnm_print(2, "          relerr =%g\n", relerr);
00147             Vnm_print(2, "          rho   =%g\n", rho);
00148         }
00149
00150         if( relerr < *tol || *iters == *itmax)
00151             break;
00152
00153         oldrho = rho;
00154     }
00155 }
00156
00157 // Return some stuff ***
00158 *eigmax = rho;
00159 fac = VPOW(2.0, *ilev - 1);
00160 *eigmax_model = fac * (6.0 - 2.0 * VCOS((nx - 2) * pi / (nx - 1))
00161     - 2.0 * VCOS((ny - 2) * pi / (ny - 1)));
00162 }
00163
00164
00165 VPUBLIC void Vipower(int *nx,int *ny,int *nz,
00166     double *u, int *iz,
00167     double *w0, double *w1, double *w2, double *w3, double *w4,
00168     double *eigmin, double *eigmin_model, double *tol,
00169     int *itmax, int *iters,
00170     int *nlev, int *ilev, int *nlev_real, int *mgsolv,
00171     int *iok, int *iinfo, double *epsiln, double *errtol, double *omega,
00172     int *nu1, int *nu2, int *mgs moo,
00173     int *ipc, double *rpc,
00174     double *pc, double *ac, double *cc, double *tru) {
00175
00176     int level, lev;
00177     double denom, fac, rho, oldrho;
00178     double error, relerr, errtol_s;

```

```

00179     int itmax_s, iters_s, ierror_s, iok_s, iinfo_s, istop_s;
00180     int nul_s, nu2_s, mgsmoo_s;
00181
00182     double pi = 4.0 * atan( 1.0 );
00183
00184     // Utility variables
00185     double alpha;
00186
00187     MAT2(iz, 50, 1);
00188
00189     WARN_UNTESTED;
00190
00191     // Recover level information
00192     level = 1;
00193     lev   = (*ilev - 1) + level;
00194
00195     // Seed vector: random to contain all components
00196     Vaxrand(nx, ny, nz, w1);
00197     Vazeros(nx, ny, nz, w2);
00198     Vazeros(nx, ny, nz, w3);
00199     Vazeros(nx, ny, nz, w4);
00200     Vazeros(nx, ny, nz, RAT(w0, VAT2(iz, 1, lev)));
00201     Vazeros(nx, ny, nz, RAT( u, VAT2(iz, 1, lev)));
00202
00203     // Compute raleigh quotient with the seed vector ***
00204     denom = Vxnorm2(nx, ny, nz, w1);
00205     fac = 1.0 / denom;
00206     Vxscal(nx, ny, nz, &fac, w1);
00207     Vmatvec(nx, ny, nz,
00208             RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00209             RAT( ac, VAT2(iz, 7, lev)), RAT( cc, VAT2(iz, 1, lev)), w1, w2);
00210     oldrho = Vxdot(nx, ny, nz, w1, w2);
00211
00212     // I/O
00213     if (oldrho == 0.0) {
00214         if (*iinfo > 3) {
00215             Vnm_print(2, "Vipower: iters=%d\n", *iters);
00216             Vnm_print(2, "          estimate=%f\n", oldrho);
00217         }
00218         rho = oldrho;
00219     } else {
00220         //main iteration
00221         *iters = 0;
00222         while (1) {
00223             (*iters)++;
00224
00225             // Apply the matrix A^{-1} (using MG solver)
00226             itmax_s = 100;
00227             iters_s = 0;
00228             ierror_s = 0;
00229             iok_s = 0;
00230             iinfo_s = 0;
00231             istop_s = 0;
00232             mgsmoo_s = 1;
00233             nul_s = 1;
00234             nu2_s = 1;
00235             errtol_s = *epsiln;
00236
00237             Vxcopy(nx, ny, nz, w1, RAT(w0, VAT2(iz, 1, lev)));
00238             Vmvcs(nx, ny, nz, u, iz,
00239                 w1, w2, w3, w4,
00240                 &istop_s, &itmax_s, &iters_s, &ierror_s,
00241                 nlev, ilev, nlev_real, mgsolv,
00242                 &iok_s, &iinfo_s, epsiln,
00243                 &errtol_s, omega, &nul_s, &nu2_s, &mgsmoo_s,
00244                 ipc, rpc, pc, ac, cc, w0, tru);
00245             Vxcopy(nx, ny, nz, RAT(u, VAT2(iz, 1, lev)), w1);
00246
00247             // Normalize the new vector
00248             denom = Vxnorm2(nx, ny, nz, w1);
00249             fac = 1.0 / denom;
00250             Vxscal(nx, ny, nz, &fac, w1);
00251
00252             // Compute the new raleigh quotient
00253             Vmatvec(nx, ny, nz,
00254                 RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00255                 RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)), w1, w2);
00256             rho = Vxdot(nx, ny, nz, w1, w2);
00257
00258             // Stopping test
00259
00260

```

```

00261         // w2=A*x, w1=x, stop = 2-norm(A*x-lamda*x) ***
00262         Vxcopy(nx, ny, nz, w1, w3);
00263         Vxcopy(nx, ny, nz, w2, w4);
00264         Vxscal(nx, ny, nz, &rho, w3);
00265         alpha = -1.0;
00266         Vxaxpy(nx, ny, nz, &alpha, w3, w4);
00267         error = Vxnrm2(nx, ny, nz, w4);
00268         relerr = VABS(rho - oldrho) / VABS(rho);
00269
00270         // I/O
00271         if (*iinfo > 3) {
00272
00273             Vnm_print(2, "POWER:  iters  =%d\n", *iters);
00274             Vnm_print(2, "          error  =%g\n", error);
00275             Vnm_print(2, "          relerr =%g\n", relerr);
00276             Vnm_print(2, "          rho   =%g\n", rho);
00277         }
00278
00279         if (relerr < *tol || *iters == *itmax)
00280             break;
00281
00282         oldrho = rho;
00283     }
00284 }
00285
00286 // Return some stuff
00287 *eigmin = rho;
00288 fac = VPOW(2.0, *ilev - 1);
00289 *eigmin_model = fac * (6.0 - 2.0 * VCOS(pi / (*nx - 1))
00290                      - 2.0 * VCOS(pi / (*ny - 1))
00291                      - 2.0 * VCOS(pi / (*nz - 1)));
00292 }
00293
00294 VEXTERNC void Vmpower(int *nx, int *ny, int *nz,
00295                      double *u, int *iz,
00296                      double *w0, double *w1, double *w2, double *w3, double *w4,
00297                      double *eigmax, double *tol,
00298                      int *itmax, int *iters, int *nlev, int *ilev, int *nlev_real,
00299                      int *mgsolv, int *iok, int *iinfo,
00300                      double *epsiln, double *errtol, double *omega,
00301                      int *nul, int *nu2, int *mgsmoo, int *ipc, double *rpc,
00302                      double *pc, double *ac, double *cc, double *fc, double *tru) {
00303
00304     // Local variables
00305     int lev, level;
00306     double denom, fac, rho, oldrho, error;
00307     double relerr;
00308     int itmax_s, iters_s, ierror_s, iok_s, iinfo_s, istop_s;
00309     double alpha;
00310
00311     MAT2(iz, 50, 1);
00312
00313     // Recover level information
00314     level = 1;
00315     lev = (*ilev - 1) + level;
00316
00317     // Seed vector: random to contain all components
00318     Vaxrand(nx, ny, nz, w1);
00319     Vazeros(nx, ny, nz, w2);
00320     Vazeros(nx, ny, nz, w3);
00321     Vazeros(nx, ny, nz, w4);
00322     Vazeros(nx, ny, nz, RAT(u, VAT2(iz, 1, lev)));
00323
00324     // NOTE: we destroy "fc" on this level due to lack of vectors... ***
00325     Vazeros(nx, ny, nz, RAT(fc, VAT2(iz, 1, lev)));
00326
00327     // Normalize the seed vector
00328     denom = Vxnrm2(nx, ny, nz, w1);
00329     fac = 1.0 / denom;
00330     Vxscal(nx, ny, nz, &fac, w1);
00331
00332     // Compute raleigh quotient with the seed vector
00333     Vxcopy(nx, ny, nz, w1, RAT(u, VAT2(iz, 1, lev)));
00334     itmax_s = 1;
00335     iters_s = 0;
00336     ierror_s = 0;
00337     iok_s = 0;
00338     iinfo_s = 0;
00339     istop_s = 1;
00340     Vmvcs(nx, ny, nz,
00341          u, iz, w0, w2, w3, w4,

```



```

00342         &istop_s, &itmax_s, &iters_s, &ierror_s,
00343         nlev, ilev, nlev_real, mgsolv,
00344         &iok_s, &iinfo_s,
00345         epsiln, errtol, omega, nul, nu2, mgsmoo,
00346         ipc, rpc,
00347         pc, ac, cc, fc, tru);
00348     oldrho = Vxdot(nx, ny, nz, w1, RAT(u, VAT2(iz, 1, lev)));
00349
00350     // I/O
00351     if (oldrho == 0.0) {
00352         if (*iinfo > 3) {
00353             Vnm_print(2, "Vmp0ower: iter=%d, estimate=%f", *iters, oldrho);
00354         }
00355         rho = oldrho;
00356     } else {
00357         // Main iteration
00358         *iters = 0;
00359         while (1) {
00360             (*iters)++;
00361
00362             // Apply the matrix M
00363             Vxcopy(nx, ny, nz, w1, RAT(u, VAT2(iz, 1, lev)));
00364             itmax_s = 1;
00365             iters_s = 0;
00366             ierror_s = 0;
00367             iok_s = 0;
00368             iinfo_s = 0;
00369             istop_s = 1;
00370             Vmvcs(nx, ny, nz,
00371                 u, iz, w1, w2, w3, w4,
00372                 &istop_s, &itmax_s, &iters_s, &ierror_s,
00373                 nlev, ilev, nlev_real, mgsolv,
00374                 &iok_s, &iinfo_s,
00375                 epsiln, errtol, omega, nul, nu2, mgsmoo,
00376                 ipc, rpc,
00377                 pc, ac, cc, fc, tru);
00378             Vxcopy(nx, ny, nz, RAT(u, VAT2(iz, 1, lev)), w1);
00379
00380             // Normalize the new vector
00381             denom = Vxnorm2(nx, ny, nz, w1);
00382             fac = 1.0 / denom;
00383             Vxscal(nx, ny, nz, &fac, w1);
00384
00385             // Compute the new raleigh quotient
00386             Vxcopy(nx, ny, nz, w1, RAT(u, VAT2(iz, 1, lev)));
00387             itmax_s = 1;
00388             iters_s = 0;
00389             ierror_s = 0;
00390             iok_s = 0;
00391             iinfo_s = 0;
00392             istop_s = 1;
00393             Vmvcs(nx, ny, nz,
00394                 u, iz, w0, w2, w3, w4,
00395                 &istop_s, &itmax_s, &iters_s, &ierror_s,
00396                 nlev, ilev, nlev_real, mgsolv,
00397                 &iok_s, &iinfo_s,
00398                 epsiln, errtol, omega, nul, nu2, mgsmoo,
00399                 ipc, rpc,
00400                 pc, ac, cc, fc, tru);
00401             Vxcopy(nx, ny, nz, RAT(u, VAT2(iz, 1, lev)), w2);
00402             rho = Vxdot(nx, ny, nz, w1, w2);
00403
00404             // Stopping test
00405             // w2=A*x, w1=x, stop = 2-norm(A*x-lamda*x)
00406             alpha = -1.0;
00407             Vxcopy(nx, ny, nz, w1, w3);
00408             Vxcopy(nx, ny, nz, w2, w4);
00409             Vxscal(nx, ny, nz, &rho, w3);
00410             Vxaxpy(nx, ny, nz, &alpha, w3, w4);
00411             error = Vxnorm2(nx, ny, nz, w4);
00412             relerr = VABS( rho - oldrho ) / VABS( rho );
00413
00414             // I/O
00415             if (*iinfo > 3) {
00416                 Vnm_print(2, "Vmpower: iter=%d; error=%f; relerr=%f; estimate=%f",
00417                     *iters, error, relerr, rho);
00418             }
00419
00420             if ((relerr < *tol) || (*iters == *itmax)) {

```

```
00423         break;
00424     }
00425
00426     oldrho = rho;
00427 }
00428 }
00429
00430 *eigmax = rho;
00431 }
```

9.147 powerd.h

```
00001
00049 #ifndef _POWERD_H_
00050 #define _POWERD_H_
00051
00052 #include "apbscfg.h"
00053
00054 #include "malloc/malloc.h"
00055
00056 #include "generic/vhal.h"
00057 #include "generic/vmatrix.h"
00058 #include "pmgc/mikpckd.h"
00059 #include "pmgc/mgcsd.h"
00060
00078 VEXTERNC void Vpower(
00079     int *nx,
00080     int *ny,
00081     int *nz,
00082     int *iz,
00083     int *ilev,
00084     int *ipc,
00085     double *rpc,
00086     double *ac,
00087     double *cc,
00088     double *w1,
00089     double *w2,
00090     double *w3,
00091     double *w4,
00092     double *eigmax,
00093     double *eigmax_model,
00094     double *tol,
00095     int *itmax,
00096     int *iters,
00097     int *iinfo
00098 );
00099
00100
00101
00119 VEXTERNC void Vipower(
00120     int *nx,
00121     int *ny,
00122     int *nz,
00123     double *u,
00124     int *iz,
00125     double *w0,
00126     double *w1,
00127     double *w2,
00128     double *w3,
00129     double *w4,
00130     double *eigmin,
00131     double *eigmin_model,
00132     double *tol,
00133     int *itmax,
00134     int *iters,
00135     int *nlev,
00136     int *ilev,
00137     int *nlev_real,
00138     int *mgsolv,
00139     int *iok,
00140     int *iinfo,
00141     double *epsiln,
00142     double *errtol,
00143     double *omega,
00144     int *nul,
00145     int *nu2,
00146     int *mgsmoo,
00147     int *ipc,
```

```

00148         double *rpc,
00149         double *pc,
00150         double *ac,
00151         double *cc,
00152         double *tru
00153     );
00154
00155
00156
00157 VEXTERNC void Vmpower(
00158     int     *nx,
00159     int     *ny,
00160     int     *nz,
00161     double  *u,
00162     int     *iz,
00163     double  *w0,
00164     double  *w1,
00165     double  *w2,
00166     double  *w3,
00167     double  *w4,
00168     double  *eigmax,
00169     double  *tol,
00170     int     *itmax,
00171     int     *iters,
00172     int     *nlev,
00173     int     *ilev,
00174     int     *nlev_real,
00175     int     *mgsolv,
00176     int     *iok,
00177     int     *iinfo,
00178     double  *epsiln,
00179     double  *errtol,
00180     double  *omega,
00181     int     *nul,
00182     int     *nu2,
00183     int     *mgsmoo,
00184     int     *ipc,
00185     double  *rpc,
00186     double  *pc,
00187     double  *ac,
00188     double  *cc,
00189     double  *fc,
00190     double  *tru
00191 );
00192
00193 #endif /* _POWERD_H_ */

```

9.148 smoothd.c

```

00001
00056 #include "smoothd.h"
00057
00058 VEXTERNC void Vsmooth(int *nx, int *ny, int *nz,
00059     int *ipc, double *rpc,
00060     double *ac, double *cc, double *fc,
00061     double *x, double *w1, double *w2, double *r,
00062     int *itmax, int *iters,
00063     double *errtol, double *omega,
00064     int *iresid, int *iadjoint, int *meth) {
00065
00066     // Do in one step
00067     if (*meth == 0) {
00068         VABORT_MSG0( "wjac not yet translated" );
00069         //wjac(nx,ny,nz,ipc,rpc,ac,cc,fc,x,w1,w2,r,itmax,iters,errtol,omega,iresid,iadjoint);
00070     } else if (*meth == 1) {
00071         Vgsrb(nx, ny, nz,
00072             ipc, rpc,
00073             ac, cc, fc,
00074             x, w1, w2, r,
00075             itmax, iters,
00076             errtol, omega,
00077             iresid, iadjoint);
00078     } else if (*meth == 2) {
00079         VABORT_MSG0( "sor not yet translated" );
00080         //sor(nx,ny,nz,ipc,rpc,ac,cc,fc,x,w1,w2,r,itmax,iters,errtol,omega,iresid,iadjoint);
00081     } else if (*meth == 3) {
00082         VABORT_MSG0( "rich not yet translated" );
00083         //rich(nx,ny,nz,ipc,rpc,ac,cc,fc,x,w1,w2,r,itmax,iters,errtol,omega,iresid,iadjoint);

```

```

00084     } else if (*meth == 4) {
00085         Vcghs(nx, ny, nz,
00086             ipc, rpc,
00087             ac, cc, fc,
00088             x, w1, w2, r,
00089             itmax, iters,
00090             errtol, omega,
00091             iresid, iadjoint);
00092     } else {
00093         VABORT_MSG1("Bad smoothing routine specified = %d", *meth);
00094     }
00095 }
00096
00097
00098 VEXTERNC void Vnsmooth(int *nx, int *ny, int *nz,
00099     int *ipc, double *rpc,
00100     double *ac, double *cc, double *fc,
00101     double *x, double *w1, double *w2, double *r,
00102     int *itmax, int *iters,
00103     double *errtol, double *omega,
00104     int *iresid, int *iadjoint, int *meth) {
00105
00106     WARN_UNTESTED;
00107
00108     // Do in one step
00109     if (*meth == 0) {
00110         VABORT_MSG0("nwjac not yet translated");
00111         //nwjac(nx,ny,nz,ipc,rpc,ac,cc,fc,x,w1,w2,r,itmax,iters,errtol,omega,iresid,iadjoint)
00112     } else if (*meth == 1) {
00113         VABORT_MSG0("ngsrb not yet translated");
00114         //ngsrb(nx,ny,nz,ipc,rpc,ac,cc,fc,x,w1,w2,r,itmax,iters,errtol,omega,iresid,iadjoint)
00115     } else if (*meth == 2) {
00116         VABORT_MSG0("nsor not yet translated");
00117         //nsor(nx,ny,nz,ipc,rpc,ac,cc,fc,x,w1,w2,r,itmax,iters,errtol,omega,iresid,iadjoint)
00118     } else if (*meth == 3) {
00119         VABORT_MSG0("nrich not yet translated");
00120         //nrich(nx,ny,nz,ipc,rpc,ac,cc,fc,x,w1,w2,r,itmax,iters,errtol,omega,iresid,iadjoint)
00121     } else {
00122         VABORT_MSG1("Bad smoothing routine specified: %d", *meth);
00123     }
00124 }

```

9.149 smoothd.h

```

00001
00049 #ifndef _SMOOTHD_H_
00050 #define _SMOOTHD_H_
00051
00052 #include "apbscfg.h"
00053
00054 #include "malloc/malloc.h"
00055
00056 #include "generic/vhal.h"
00057 #include "generic/vmatrix.h"
00058 #include "pmgc/gsd.h"
00059 #include "pmgc/cgd.h"
00060
00067 VEXTERNC void Vsmooth(
00068     int *nx,
00069     int *ny,
00070     int *nz,
00071     int *ipc,
00072     double *rpc,
00073     double *ac,
00074     double *cc,
00075     double *fc,
00076     double *x,
00077     double *w1,
00078     double *w2,
00079     double *r,
00080     int *itmax,
00081     int *iters,
00082     double *errtol,
00083     double *omega,
00084     int *iresid,
00085     int *iadjoint,
00086     int *meth
00087 );

```

```

00088
00095 VEXTERNC void Vnsmooth(
00096     int    *nx,
00097     int    *ny,
00098     int    *nz,
00099     int    *ipc,
00100     double *rpc,
00101     double *ac,
00102     double *cc,
00103     double *fc,
00104     double *x,
00105     double *wl,
00106     double *w2,
00107     double *r,
00108     int    *itmax,
00109     int    *iters,
00110     double *errtol,
00111     double *omega,
00112     int    *iresid,
00113     int    *iadjoint,
00114     int    *meth
00115 );
00116
00117
00118 #endif /* _SMOOTH_H_ */

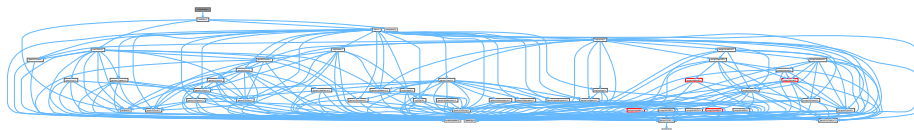
```

9.150 src/routines.c File Reference

Supporting routines for APBS front end.

```
#include "routines.h"
```

Include dependency graph for routines.c:



Functions

- VPUBLIC void [startVio](#) ()
Wrapper to start MALOC Vio layer.
- VPUBLIC [Vparam](#) * [loadParameter](#) ([NOsh](#) *nosh)
Loads and returns parameter object.
- VPUBLIC int [loadMolecules](#) ([NOsh](#) *nosh, [Vparam](#) *param, [Valist](#) *alist[[NOSH_MAXMOL](#)])
Load the molecules given in NOsh into atom lists.
- VPUBLIC void [killMolecules](#) ([NOsh](#) *nosh, [Valist](#) *alist[[NOSH_MAXMOL](#)])
Destroy the loaded molecules.
- VPUBLIC int [loadDielMaps](#) ([NOsh](#) *nosh, [Vgrid](#) *dielXMap[[NOSH_MAXMOL](#)], [Vgrid](#) *dielYMap[[NOSH_MAXMOL](#)], [Vgrid](#) *dielZMap[[NOSH_MAXMOL](#)])
Load the dielectric maps given in NOsh into grid objects.
- VPUBLIC void [killDielMaps](#) ([NOsh](#) *nosh, [Vgrid](#) *dielXMap[[NOSH_MAXMOL](#)], [Vgrid](#) *dielYMap[[NOSH_MAXMOL](#)], [Vgrid](#) *dielZMap[[NOSH_MAXMOL](#)])
Destroy the loaded dielectric.
- VPUBLIC int [loadKappaMaps](#) ([NOsh](#) *nosh, [Vgrid](#) *map[[NOSH_MAXMOL](#)])
Load the kappa maps given in NOsh into grid objects.
- VPUBLIC void [killKappaMaps](#) ([NOsh](#) *nosh, [Vgrid](#) *map[[NOSH_MAXMOL](#)])
Destroy the loaded kappa maps.

- VPUBLIC int [loadPotMaps](#) (NOSH *nosh, Vgrid *map[NOSH_MAXMOL])
Load the potential maps given in NOSH into grid objects.
- VPUBLIC void [killPotMaps](#) (NOSH *nosh, Vgrid *map[NOSH_MAXMOL])
Destroy the loaded potential maps.
- VPUBLIC int [loadChargeMaps](#) (NOSH *nosh, Vgrid *map[NOSH_MAXMOL])
Load the charge maps given in NOSH into grid objects.
- VPUBLIC void [killChargeMaps](#) (NOSH *nosh, Vgrid *map[NOSH_MAXMOL])
Destroy the loaded charge maps.
- VPUBLIC void [printPBEPARM](#) (PBEParm *pbeparm)
Print out generic PBE params loaded from input.
- VPUBLIC void [printMGPARAM](#) (MGparm *mgparm, double realCenter[3])
Print out MG-specific params loaded from input.
- VPUBLIC int [initMG](#) (int icalc, NOSH *nosh, MGparm *mgparm, PBEParm *pbeparm, double realCenter[3], Vpbe *pbe[NOSH_MAXCALC], Valist *alist[NOSH_MAXMOL], Vgrid *dielXMap[NOSH_MAXMOL], Vgrid *dielYMap[NOSH_MAXMOL], Vgrid *dielZMap[NOSH_MAXMOL], Vgrid *kappaMap[NOSH_MAXMOL], Vgrid *chargeMap[NOSH_MAXMOL], Vpmgp *pmgp[NOSH_MAXCALC], Vpmg *pmg[NOSH_MAXCALC], Vgrid *potMap[NOSH_MAXMOL])
Initialize an MG calculation.
- VPUBLIC void [killIMG](#) (NOSH *nosh, Vpbe *pbe[NOSH_MAXCALC], Vpmgp *pmgp[NOSH_MAXCALC], Vpmg *pmg[NOSH_MAXCALC])
Kill structures initialized during an MG calculation.
- VPUBLIC int [solveMG](#) (NOSH *nosh, Vpmg *pmg, MGparm_CalcType type)
Solve the PBE with MG.
- VPUBLIC int [setPartMG](#) (NOSH *nosh, MGparm *mgparm, Vpmg *pmg)
Set MG partitions for calculating observables and performing I/O.
- VPUBLIC int [energyMG](#) (NOSH *nosh, int icalc, Vpmg *pmg, int *nenergy, double *totEnergy, double *qfEnergy, double *qmEnergy, double *dielEnergy)
Calculate electrostatic energies from MG solution.
- VPUBLIC int [forceMG](#) (Vmem *mem, NOSH *nosh, PBEParm *pbeparm, MGparm *mgparm, Vpmg *pmg, int *nforce, AtomForce **atomForce, Valist *alist[NOSH_MAXMOL])
Calculate forces from MG solution.
- VPUBLIC void [killEnergy](#) ()
Kill arrays allocated for energies.
- VPUBLIC void [killForce](#) (Vmem *mem, NOSH *nosh, int nforce[NOSH_MAXCALC], AtomForce *atomForce[NOSH_MAXCALC])
Free memory from MG force calculation.
- VPUBLIC int [writematMG](#) (int rank, NOSH *nosh, PBEParm *pbeparm, Vpmg *pmg)
Write out operator matrix from MG calculation to file.
- VPUBLIC void [storeAtomEnergy](#) (Vpmg *pmg, int icalc, double **atomEnergy, int *nenergy)
Store energy in arrays for future use.
- VPUBLIC int [writedataFlat](#) (NOSH *nosh, Vcom *com, const char *fname, double totEnergy[NOSH_MAXCALC], double qfEnergy[NOSH_MAXCALC], double qmEnergy[NOSH_MAXCALC], double dielEnergy[NOSH_MAXCALC], int nenergy[NOSH_MAXCALC], double *atomEnergy[NOSH_MAXCALC], int nforce[NOSH_MAXCALC], AtomForce *atomForce[NOSH_MAXCALC])
Write out information to a flat file.
- VPUBLIC int [writedataXML](#) (NOSH *nosh, Vcom *com, const char *fname, double totEnergy[NOSH_MAXCALC], double qfEnergy[NOSH_MAXCALC], double qmEnergy[NOSH_MAXCALC], double dielEnergy[NOSH_MAXCALC], int nenergy[NOSH_MAXCALC], double *atomEnergy[NOSH_MAXCALC], int nforce[NOSH_MAXCALC], AtomForce *atomForce[NOSH_MAXCALC])

- Write out information to an XML file.*

 - VPUBLIC int [writedataMG](#) (int rank, [NOsh](#) *nosh, [PBEparm](#) *pbeparm, [Vpmg](#) *pmg)
- Write out observables from MG calculation to file.*

 - VPUBLIC double [returnEnergy](#) (Vcom *com, [NOsh](#) *nosh, double totEnergy[[NOSH_MAXCALC](#)], int iprint)
- Access net local energy.*

 - VPUBLIC int [printEnergy](#) (Vcom *com, [NOsh](#) *nosh, double totEnergy[[NOSH_MAXCALC](#)], int iprint)
- Combine and pretty-print energy data (deprecated...see [printElecEnergy](#))*

 - VPUBLIC int [printElecEnergy](#) (Vcom *com, [NOsh](#) *nosh, double totEnergy[[NOSH_MAXCALC](#)], int iprint)
- Combine and pretty-print energy data.*

 - VPUBLIC int [printApolEnergy](#) ([NOsh](#) *nosh, int iprint)
- Combine and pretty-print energy data.*

 - VPUBLIC int [printForce](#) (Vcom *com, [NOsh](#) *nosh, int nforce[[NOSH_MAXCALC](#)], [AtomForce](#) *atom←Force[[NOSH_MAXCALC](#)], int iprint)
- Combine and pretty-print force data (deprecated...see [printElecForce](#))*

 - VPUBLIC int [printElecForce](#) (Vcom *com, [NOsh](#) *nosh, int nforce[[NOSH_MAXCALC](#)], [AtomForce](#) *atom←Force[[NOSH_MAXCALC](#)], int iprint)
- Combine and pretty-print force data.*

 - VPUBLIC int [printApolForce](#) (Vcom *com, [NOsh](#) *nosh, int nforce[[NOSH_MAXCALC](#)], [AtomForce](#) *atom←Force[[NOSH_MAXCALC](#)], int iprint)
- Combine and pretty-print force data.*

 - VPUBLIC void [killFE](#) ([NOsh](#) *nosh, [Vpbe](#) *pbe[[NOSH_MAXCALC](#)], [Vfetk](#) *fetk[[NOSH_MAXCALC](#)], Gem *gm[[NOSH_MAXMOL](#)])
- Kill structures initialized during an FE calculation.*

 - VPUBLIC Vrc_Codes [initFE](#) (int icalc, [NOsh](#) *nosh, [FEMparm](#) *feparm, [PBEparm](#) *pbeparm, [Vpbe](#) *pbe[[NOSH_MAXCALC](#)], [Valist](#) *alist[[NOSH_MAXMOL](#)], [Vfetk](#) *fetk[[NOSH_MAXCALC](#)])
- Initialize FE solver objects.*

 - VPUBLIC void [printFEPARM](#) (int icalc, [NOsh](#) *nosh, [FEMparm](#) *feparm, [Vfetk](#) *fetk[[NOSH_MAXCALC](#)])
- Print out FE-specific params loaded from input.*

 - VPUBLIC int [partFE](#) (int icalc, [NOsh](#) *nosh, [FEMparm](#) *feparm, [Vfetk](#) *fetk[[NOSH_MAXCALC](#)])
- Partition mesh (if applicable)*

 - VPUBLIC int [preRefineFE](#) (int icalc, [FEMparm](#) *feparm, [Vfetk](#) *fetk[[NOSH_MAXCALC](#)])
- Pre-refine mesh before solve.*

 - VPUBLIC int [solveFE](#) (int icalc, [PBEparm](#) *pbeparm, [FEMparm](#) *feparm, [Vfetk](#) *fetk[[NOSH_MAXCALC](#)])
- Solve-estimate-refine.*

 - VPUBLIC int [energyFE](#) ([NOsh](#) *nosh, int icalc, [Vfetk](#) *fetk[[NOSH_MAXCALC](#)], int *nenergy, double *totEnergy, double *qfEnergy, double *qmEnergy, double *dielEnergy)
- Calculate electrostatic energies from FE solution.*

 - VPUBLIC int [postRefineFE](#) (int icalc, [FEMparm](#) *feparm, [Vfetk](#) *fetk[[NOSH_MAXCALC](#)])
- Estimate error, mark mesh, and refine mesh after solve.*

 - VPUBLIC int [writedataFE](#) (int rank, [NOsh](#) *nosh, [PBEparm](#) *pbeparm, [Vfetk](#) *fetk)
- Write FEM data to files.*

 - VPUBLIC int [initAPOL](#) ([NOsh](#) *nosh, Vmem *mem, [Vparam](#) *param, [APOLparm](#) *apolparm, int *nforce, [AtomForce](#) **atomForce, [Valist](#) *alist)
- Upperlevel routine to the non-polar energy and force routines.*

 - VPUBLIC int [energyAPOL](#) ([APOLparm](#) *apolparm, double sasa, double sav, double atomsasa[], double atomwcaEnergy[], int numatoms)
- Calculate non-polar energies.*

 - VPUBLIC int [forceAPOL](#) ([Vacc](#) *acc, Vmem *mem, [APOLparm](#) *apolparm, int *nforce, [AtomForce](#) **atomForce, [Valist](#) *alist, [Vclist](#) *clist)
- Calculate non-polar forces.*

9.150.1 Detailed Description

Supporting routines for APBS front end.

Author

Nathan Baker

Version

\$Id\$

Attention

```
* APBS -- Adaptive Poisson-Boltzmann Solver
*
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*
* Additional contributing authors listed in the code documentation.
*
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*
```

Definition in file [routines.c](#).

9.151 routines.c

[Go to the documentation of this file.](#)

00001


```

00054 #include "routines.h"
00055
00056 VEMBED(rcsid="$Id$")
00057
00058 VPUBLIC void startVio() { Vio_start(); }
00059
00060 VPUBLIC Vparam* loadParameter(NOsh *nosh) {
00061     Vparam *param = VNULL;
00062
00063     if (nosh->gotparm) {
00064         param = Vparam_ctor();
00065         switch (nosh->parmfmt) {
00066             case NPF_FLAT:
00067                 Vnm_tprint(1, "Reading parameter data from %s.\n",
00068                     nosh->parmpath);
00069                 if (Vparam_readFlatFile(param, "FILE", "ASC", VNULL,
00070                     nosh->parmpath) != 1) {
00071                     Vnm_tprint(2, "Error reading parameter file (%s)!\n", nosh->parmpath);
00072                     return VNULL;
00073                 }
00074                 break;
00075             case NPF_XML:
00076                 Vnm_tprint(1, "Reading parameter data from %s.\n",
00077                     nosh->parmpath);
00078                 if (Vparam_readXMLFile(param, "FILE", "ASC", VNULL,
00079                     nosh->parmpath) != 1) {
00080                     Vnm_tprint(2, "Error reading parameter file (%s)!\n", nosh->parmpath);
00081                     return VNULL;
00082                 }
00083                 break;
00084             default:
00085                 Vnm_tprint(2, "Error! Undefined parameter file type (%d)!\n", nosh->parmfmt);
00086                 return VNULL;
00087         } /* switch parmfmt */
00088     }
00089     return param;
00090 }
00091
00092 VPUBLIC int loadMolecules(NOsh *nosh, Vparam *param, Valist *alist[NOSH_MAXMOL]) {
00093     int i;
00094     int use_params = 0;
00095     Vrc_Codes rc;
00096
00097     Vio *sock = VNULL;
00098
00099     Vnm_tprint(1, "Got paths for %d molecules\n", nosh->nmol);
00100     if (nosh->nmol <= 0) {
00101         Vnm_tprint(2, "You didn't specify any molecules (correctly)!\n");
00102         Vnm_tprint(2, "Bailing out!\n");
00103         return 0;
00104     }
00105     if (nosh->gotparm) {
00106         if (param == VNULL) {
00107             Vnm_tprint(2, "Error! You don't have a valid parameter object!\n");
00108             return 0;
00109         }
00110         use_params = 1;
00111     }
00112     for (i=0; i<nosh->nmol; i++) {
00113         if (alist[i] == VNULL) {
00114             alist[i] = Valist_ctor();
00115         } else {
00116             alist[i] = VNULL;
00117             alist[i] = Valist_ctor();
00118         }
00119     }
00120     switch (nosh->molfmt[i]) {
00121         case NMF_PQR:
00122             /* Print out a warning to the user letting them know that we are overriding PQR
00123              * values for charge, radius and epsilon */
00124             if (use_params) {
00125                 Vnm_print(2, "\nWARNING!! Radius/charge information from PQR file %s\n",
00126                     nosh->molpath[i]);
00127                 Vnm_print(2, "will be replaced with data from parameter file (%s)!\n",
00128                     nosh->parmpath);
00129             }
00130     }

```

```

00133     }
00134     Vnm_tprint( 1, "Reading PQR-format atom data from %s.\n",
00135         nosh->molpath[i]);
00136     sock = Vio_ctor("FILE", "ASC", VNULL, nosh->molpath[i], "r");
00137     if (sock == VNULL) {
00138         Vnm_print(2, "Problem opening virtual socket %s!\n",
00139             nosh->molpath[i]);
00140         return 0;
00141     }
00142     if (Vio_accept(sock, 0) < 0) {
00143         Vnm_print(2, "Problem accepting virtual socket %s!\n",
00144             nosh->molpath[i]);
00145         return 0;
00146     }
00147     if(use_params){
00148         rc = Valist_readPQR(alist[i], param, sock);
00149     }else{
00150         rc = Valist_readPQR(alist[i], VNULL, sock);
00151     }
00152     if(rc == 0) return 0;
00153
00154     Vio_acceptFree(sock);
00155     Vio_dtor(&sock);
00156     break;
00157 case NMF_PDB:
00158     /* Load parameters */
00159     if (!nosh->gotparm) {
00160         Vnm_tprint(2, "Nosh: Error! Can't read PDB without specifying PARM file!\n");
00161         return 0;
00162     }
00163     Vnm_tprint( 1, "Reading PDB-format atom data from %s.\n",
00164         nosh->molpath[i]);
00165     sock = Vio_ctor("FILE", "ASC", VNULL, nosh->molpath[i], "r");
00166     if (sock == VNULL) {
00167         Vnm_print(2, "Problem opening virtual socket %s!\n",
00168             nosh->molpath[i]);
00169         return 0;
00170     }
00171     if (Vio_accept(sock, 0) < 0) {
00172         Vnm_print(2, "Problem accepting virtual socket %s!\n", nosh->molpath[i]);
00173         return 0;
00174     }
00175     rc = Valist_readPDB(alist[i], param, sock);
00176     /* If we are looking for an atom/residue that does not exist
00177      * then abort and return 0 */
00178     if(rc == 0)
00179         return 0;
00180
00181     Vio_acceptFree(sock);
00182     Vio_dtor(&sock);
00183     break;
00184 case NMF_XML:
00185     Vnm_tprint( 1, "Reading XML-format atom data from %s.\n",
00186         nosh->molpath[i]);
00187     sock = Vio_ctor("FILE", "ASC", VNULL, nosh->molpath[i], "r");
00188     if (sock == VNULL) {
00189         Vnm_print(2, "Problem opening virtual socket %s!\n",
00190             nosh->molpath[i]);
00191         return 0;
00192     }
00193     if (Vio_accept(sock, 0) < 0) {
00194         Vnm_print(2, "Problem accepting virtual socket %s!\n",
00195             nosh->molpath[i]);
00196         return 0;
00197     }
00198     if(use_params){
00199         rc = Valist_readXML(alist[i], param, sock);
00200     }else{
00201         rc = Valist_readXML(alist[i], VNULL, sock);
00202     }
00203     if(rc == 0)
00204         return 0;
00205
00206     Vio_acceptFree(sock);
00207     Vio_dtor(&sock);
00208     break;
00209 default:
00210     Vnm_tprint(2, "Nosh: Error! Undefined molecule file type \
00211 (%d)!\n", nosh->molfmt[i]);
00212     return 0;
00213 } /* switch molfmt */

```

```

00214
00215     if (rc != 1) {
00216         Vnm_tprint( 2, "Error while reading molecule from %s\n",
00217                     nosh->molpath[i]);
00218         return 0;
00219     }
00220
00221     Vnm_tprint( 1, " %d atoms\n", Valist_getNumberAtoms(alist[i]));
00222     Vnm_tprint( 1, "   Centered at (%4.3e, %4.3e, %4.3e)\n",
00223                 alist[i]->center[0], alist[i]->center[1],
00224                 alist[i]->center[2]);
00225     Vnm_tprint( 1, "   Net charge %3.2e e\n", alist[i]->charge);
00226
00227 }
00228
00229 return 1;
00230
00231 }
00232
00233 VPUBLIC void killMolecules(NOsh *nosh, Valist *alist[NOSH_MAXMOL]) {
00234     int i;
00235
00236 #ifndef VAPBSQUIET
00237     Vnm_tprint( 1, "Destroying %d molecules\n", nosh->nmol);
00238 #endif
00239     for (i=0; i<nosh->nmol; i++)
00240         Valist_dtor(&(alist[i]));
00241 }
00242
00243
00244
00245
00250 VPUBLIC int loadDielMaps(NOsh *nosh, Vgrid *dielXMap[NOSH_MAXMOL], Vgrid *dielYMap[NOSH_MAXMOL], Vgrid
    *dielZMap[NOSH_MAXMOL]) {
00251     int i, ii, nx, ny, nz;
00252     double sum, hx, hy, hzed, xmin, ymin, zmin;
00253
00254     // Check to be sure we have dielectric map paths; if not, return.
00255     if (nosh->ndiel > 0)
00256         Vnm_tprint( 1, "Got paths for %d dielectric map sets\n", nosh->ndiel);
00257     else
00258         return 1;
00259
00260     // For each dielectric map path, read the data and calculate needed values.
00261     for (i=0; i<nosh->ndiel; i++) {
00262         Vnm_tprint( 1, "Reading x-shifted dielectric map data from %s:\n", nosh->dielXpath[i]);
00263         dielXMap[i] = Vgrid_ctor(0, 0, 0, 0.0, 0.0, 0.0, 0.0, 0.0, VNULL);
00264
00265         // Determine the format and read data if the format is valid.
00266         switch (nosh->dielfmt[i]) {
00267             // OpenDX (Data Explorer) format
00268             case VDF_DX:
00269                 if (Vgrid_readDX(dielXMap[i], "FILE", "ASC", VNULL,
00270                                 nosh->dielXpath[i]) != 1) {
00271                     Vnm_tprint( 2, "Fatal error while reading from %s\n",
00272                                 nosh->dielXpath[i]);
00273                     return 0;
00274                 }
00275
00276                 // Set grid sizes
00277                 nx = dielXMap[i]->nx;
00278                 ny = dielXMap[i]->ny;
00279                 nz = dielXMap[i]->nz;
00280
00281                 // Set spacings
00282                 hx = dielXMap[i]->hx;
00283                 hy = dielXMap[i]->hy;
00284                 hzed = dielXMap[i]->hzed;
00285
00286                 // Set minimum lower corner
00287                 xmin = dielXMap[i]->xmin;
00288                 ymin = dielXMap[i]->ymin;
00289                 zmin = dielXMap[i]->zmin;
00290                 Vnm_tprint(1, " %d x %d x %d grid\n", nx, ny, nz);
00291                 Vnm_tprint(1, " (%g, %g, %g) A spacings\n", hx, hy, hzed);
00292                 Vnm_tprint(1, " (%g, %g, %g) A lower corner\n",
00293                             xmin, ymin, zmin);
00294                 sum = 0;
00295                 for (ii=0; ii<(nx*ny*nz); ii++)
00296                     sum += (dielXMap[i]->data[ii]);
00297

```

```

00298         sum = sum*hx*hy*hzed;
00299         Vnm_tprint(1, " Volume integral = %3.2e A^3\n", sum);
00300         break;
00301
00302         //DX binary file (.dxbn)
00303         case VDF_DXBIN:
00304             //TODO: add this method and maybe change the if stmt.
00305             if (Vgrid_readDXBIN(dielXMap[i], "FILE", "ASC", VNULL,
00306                                nosh->dielXpath[i]) != 1) {
00307                 Vnm_tprint( 2, "Fatal error while reading from %s\n",
00308                             nosh->dielXpath[i]);
00309                 return 0;
00310             }
00311
00312             // Set grid sizes
00313             nx = dielXMap[i]->nx;
00314             ny = dielXMap[i]->ny;
00315             nz = dielXMap[i]->nz;
00316
00317             // Set spacings
00318             hx = dielXMap[i]->hx;
00319             hy = dielXMap[i]->hy;
00320             hzed = dielXMap[i]->hzed;
00321
00322             // Set minimum lower corner
00323             xmin = dielXMap[i]->xmin;
00324             ymin = dielXMap[i]->ymin;
00325             zmin = dielXMap[i]->zmin;
00326             Vnm_tprint(1, " %d x %d x %d grid\n", nx, ny, nz);
00327             Vnm_tprint(1, " (%g, %g, %g) A spacings\n", hx, hy, hzed);
00328             Vnm_tprint(1, " (%g, %g, %g) A lower corner\n",
00329                         xmin, ymin, zmin);
00330             sum = 0;
00331             for (ii=0; ii<(nx*ny*nz); ii++)
00332                 sum += (dielXMap[i]->data[ii]);
00333             sum = sum*hx*hy*hzed;
00334             Vnm_tprint(1, " Volume integral = %3.2e A^3\n", sum);
00335             break;
00336
00337         // Binary file (GZip)
00338         case VDF_GZ:
00339             if (Vgrid_readGZ(dielXMap[i], nosh->dielXpath[i]) != 1) {
00340                 Vnm_tprint( 2, "Fatal error while reading from %s\n",
00341                             nosh->dielXpath[i]);
00342                 return 0;
00343             }
00344
00345             // Set grid sizes
00346             nx = dielXMap[i]->nx;
00347             ny = dielXMap[i]->ny;
00348             nz = dielXMap[i]->nz;
00349
00350             // Set spacings
00351             hx = dielXMap[i]->hx;
00352             hy = dielXMap[i]->hy;
00353             hzed = dielXMap[i]->hzed;
00354
00355             // Set minimum lower corner
00356             xmin = dielXMap[i]->xmin;
00357             ymin = dielXMap[i]->ymin;
00358             zmin = dielXMap[i]->zmin;
00359             Vnm_tprint(1, " %d x %d x %d grid\n", nx, ny, nz);
00360             Vnm_tprint(1, " (%g, %g, %g) A spacings\n", hx, hy, hzed);
00361             Vnm_tprint(1, " (%g, %g, %g) A lower corner\n",
00362                         xmin, ymin, zmin);
00363             sum = 0;
00364             for (ii=0; ii<(nx*ny*nz); ii++)
00365                 sum += (dielXMap[i]->data[ii]);
00366             sum = sum*hx*hy*hzed;
00367             Vnm_tprint(1, " Volume integral = %3.2e A^3\n", sum);
00368             break;
00369         // UHBD format
00370         case VDF_UHBD:
00371             Vnm_tprint( 2, "UHBD input not supported yet!\n");
00372             return 0;
00373         // AVS UCD format
00374         case VDF_AVS:
00375             Vnm_tprint( 2, "AVS input not supported yet!\n");
00376             return 0;
00377         // FEtk MC Simplex Format (MCSF)
00378         case VDF_MCSF:

```

```

00379         Vnm_tprint( 2, "MCSF input not supported yet!\n");
00380         return 0;
00381     default:
00382         Vnm_tprint( 2, "Invalid data format (%d)!\n",
00383                 nosh->dielfmt[i]);
00384         return 0;
00385     }
00386     Vnm_tprint( 1, "Reading y-shifted dielectric map data from \
00387 %s:\n", nosh->dielYpath[i]);
00388     dielYMap[i] = Vgrid_ctor(0, 0, 0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, VNULL);
00389
00390     // Determine the format and read data if the format is valid.
00391     switch (nosh->dielfmt[i]) {
00392         // OpenDX (Data Explorer) format
00393         case VDF_DX:
00394             if (Vgrid_readDX(dielYMap[i], "FILE", "ASC", VNULL,
00395                             nosh->dielYpath[i]) != 1) {
00396                 Vnm_tprint( 2, "Fatal error while reading from %s\n",
00397                             nosh->dielYpath[i]);
00398                 return 0;
00399             }
00400
00401             // Read grid
00402             nx = dielYMap[i]->nx;
00403             ny = dielYMap[i]->ny;
00404             nz = dielYMap[i]->nz;
00405
00406             // Read spacings
00407             hx = dielYMap[i]->hx;
00408             hy = dielYMap[i]->hy;
00409             hzed = dielYMap[i]->hzed;
00410
00411             // Read minimum lower corner
00412             xmin = dielYMap[i]->xmin;
00413             ymin = dielYMap[i]->ymin;
00414             zmin = dielYMap[i]->zmin;
00415             Vnm_tprint(1, "  %d x %d x %d grid\n", nx, ny, nz);
00416             Vnm_tprint(1, "  (%g, %g, %g) A spacings\n", hx, hy, hzed);
00417             Vnm_tprint(1, "  (%g, %g, %g) A lower corner\n",
00418                         xmin, ymin, zmin);
00419             sum = 0;
00420             for (ii=0; ii<(nx*ny*nz); ii++)
00421                 sum += (dielYMap[i]->data[ii]);
00422             sum = sum*hx*hy*hzed;
00423             Vnm_tprint(1, "  Volume integral = %3.2e A^3\n", sum);
00424             break;
00425         //DX Binary file (.dxbin)
00426         case VDF_DXBIN:
00427             //TODO: add this funct/method and maybe change the if stmt.
00428             if (Vgrid_readDXBIN(dielYMap[i], "FILE", "ASC", VNULL,
00429                                nosh->dielYpath[i]) != 1) {
00430                 Vnm_tprint( 2, "Fatal error while reading from %s\n",
00431                             nosh->dielYpath[i]);
00432                 return 0;
00433             }
00434
00435             // Read grid
00436             nx = dielYMap[i]->nx;
00437             ny = dielYMap[i]->ny;
00438             nz = dielYMap[i]->nz;
00439
00440             // Read spacings
00441             hx = dielYMap[i]->hx;
00442             hy = dielYMap[i]->hy;
00443             hzed = dielYMap[i]->hzed;
00444
00445             // Read minimum lower corner
00446             xmin = dielYMap[i]->xmin;
00447             ymin = dielYMap[i]->ymin;
00448             zmin = dielYMap[i]->zmin;
00449             Vnm_tprint(1, "  %d x %d x %d grid\n", nx, ny, nz);
00450             Vnm_tprint(1, "  (%g, %g, %g) A spacings\n", hx, hy, hzed);
00451             Vnm_tprint(1, "  (%g, %g, %g) A lower corner\n",
00452                         xmin, ymin, zmin);
00453             sum = 0;
00454             for (ii=0; ii<(nx*ny*nz); ii++)
00455                 sum += (dielYMap[i]->data[ii]);
00456             sum = sum*hx*hy*hzed;
00457             Vnm_tprint(1, "  Volume integral = %3.2e A^3\n", sum);
00458             break;
00459         // Binary file (GZip) format

```

```

00460     case VDF_GZ:
00461         if (Vgrid_readGZ(dielYMap[i], nosh->dielYpath[i]) != 1) {
00462             Vnm_tprint( 2, "Fatal error while reading from %s\n",
00463                 nosh->dielYpath[i]);
00464             return 0;
00465         }
00466
00467         // Read grid
00468         nx = dielYMap[i]->nx;
00469         ny = dielYMap[i]->ny;
00470         nz = dielYMap[i]->nz;
00471
00472         // Read spacings
00473         hx = dielYMap[i]->hx;
00474         hy = dielYMap[i]->hy;
00475         hzed = dielYMap[i]->hzed;
00476
00477         // Read minimum lower corner
00478         xmin = dielYMap[i]->xmin;
00479         ymin = dielYMap[i]->ymin;
00480         zmin = dielYMap[i]->zmin;
00481         Vnm_tprint(1, "  %d x %d x %d grid\n", nx, ny, nz);
00482         Vnm_tprint(1, "  (%g, %g, %g) A spacings\n", hx, hy, hzed);
00483         Vnm_tprint(1, "  (%g, %g, %g) A lower corner\n",
00484             xmin, ymin, zmin);
00485         sum = 0;
00486         for (ii=0; ii<(nx*ny*nz); ii++)
00487             sum += (dielYMap[i]->data[ii]);
00488         sum = sum*hx*hy*hzed;
00489         Vnm_tprint(1, "  Volume integral = %3.2e A^3\n", sum);
00490         break;
00491     // UHBD format
00492     case VDF_UHBD:
00493         Vnm_tprint( 2, "UHBD input not supported yet!\n");
00494         return 0;
00495     // AVS UCD format
00496     case VDF_AVS:
00497         Vnm_tprint( 2, "AVS input not supported yet!\n");
00498         return 0;
00499     // FETk MC Simplex Format (MCSF)
00500     case VDF_MCSF:
00501         Vnm_tprint( 2, "MCSF input not supported yet!\n");
00502         return 0;
00503     default:
00504         Vnm_tprint( 2, "Invalid data format (%d)!\n",
00505             nosh->dielfmt[i]);
00506         return 0;
00507 }
00508
00509 Vnm_tprint( 1, "Reading z-shifted dielectric map data from \
00510 %s:\n", nosh->dielZpath[i]);
00511 dielZMap[i] = Vgrid_ctor(0, 0, 0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, VNULL);
00512
00513 // Determine the format and read data if the format is valid.
00514 switch (nosh->dielfmt[i]) {
00515     // OpenDX (Data Explorer) format
00516     case VDF_DX:
00517         if (Vgrid_readDX(dielZMap[i], "FILE", "ASC", VNULL,
00518             nosh->dielZpath[i]) != 1) {
00519             Vnm_tprint( 2, "Fatal error while reading from %s\n",
00520                 nosh->dielZpath[i]);
00521             return 0;
00522         }
00523
00524         // Read grid
00525         nx = dielZMap[i]->nx;
00526         ny = dielZMap[i]->ny;
00527         nz = dielZMap[i]->nz;
00528
00529         // Read spacings
00530         hx = dielZMap[i]->hx;
00531         hy = dielZMap[i]->hy;
00532         hzed = dielZMap[i]->hzed;
00533
00534         // Read minimum lower corner
00535         xmin = dielZMap[i]->xmin;
00536         ymin = dielZMap[i]->ymin;
00537         zmin = dielZMap[i]->zmin;
00538         Vnm_tprint(1, "  %d x %d x %d grid\n",
00539             nx, ny, nz);
00540         Vnm_tprint(1, "  (%g, %g, %g) A spacings\n",

```

```

00541             hx, hy, hzed);
00542     Vnm_tprint(1, " (%g, %g, %g) A lower corner\n",
00543             xmin, ymin, zmin);
00544     sum = 0;
00545     for (ii=0; ii<(nx*ny*nz); ii++) sum += (dielZMap[i]->data[ii]);
00546     sum = sum*hx*hy*hzed;
00547     Vnm_tprint(1, " Volume integral = %3.2e A^3\n", sum);
00548     break;
00549     //OpenDX Binary format (.dxbin)
00550     case VDF_DXBIN:
00551         //TODO: add this funct/method and maybe change the if stmt.
00552     if (Vgrid_readDXBIN(dielZMap[i], "FILE", "ASC", VNULL,
00553             nosh->dielZpath[i]) != 1) {
00554         Vnm_tprint( 2, "Fatal error while reading from %s\n",
00555             nosh->dielZpath[i]);
00556         return 0;
00557     }
00558
00559     // Read grid
00560     nx = dielZMap[i]->nx;
00561     ny = dielZMap[i]->ny;
00562     nz = dielZMap[i]->nz;
00563
00564     // Read spacings
00565     hx = dielZMap[i]->hx;
00566     hy = dielZMap[i]->hy;
00567     hzed = dielZMap[i]->hzed;
00568
00569     // Read minimum lower corner
00570     xmin = dielZMap[i]->xmin;
00571     ymin = dielZMap[i]->ymin;
00572     zmin = dielZMap[i]->zmin;
00573     Vnm_tprint(1, " %d x %d x %d grid\n",
00574             nx, ny, nz);
00575     Vnm_tprint(1, " (%g, %g, %g) A spacings\n",
00576             hx, hy, hzed);
00577     Vnm_tprint(1, " (%g, %g, %g) A lower corner\n",
00578             xmin, ymin, zmin);
00579     sum = 0;
00580     for (ii=0; ii<(nx*ny*nz); ii++) sum += (dielZMap[i]->data[ii]);
00581     sum = sum*hx*hy*hzed;
00582     Vnm_tprint(1, " Volume integral = %3.2e A^3\n", sum);
00583     break;
00584     // Binary file (GZip) format
00585     case VDF_GZ:
00586     if (Vgrid_readGZ(dielZMap[i], nosh->dielZpath[i]) != 1) {
00587         Vnm_tprint( 2, "Fatal error while reading from %s\n",
00588             nosh->dielZpath[i]);
00589         return 0;
00590     }
00591
00592     // Read grid
00593     nx = dielZMap[i]->nx;
00594     ny = dielZMap[i]->ny;
00595     nz = dielZMap[i]->nz;
00596
00597     // Read spacings
00598     hx = dielZMap[i]->hx;
00599     hy = dielZMap[i]->hy;
00600     hzed = dielZMap[i]->hzed;
00601
00602     // Read minimum lower corner
00603     xmin = dielZMap[i]->xmin;
00604     ymin = dielZMap[i]->ymin;
00605     zmin = dielZMap[i]->zmin;
00606     Vnm_tprint(1, " %d x %d x %d grid\n",
00607             nx, ny, nz);
00608     Vnm_tprint(1, " (%g, %g, %g) A spacings\n",
00609             hx, hy, hzed);
00610     Vnm_tprint(1, " (%g, %g, %g) A lower corner\n",
00611             xmin, ymin, zmin);
00612     sum = 0;
00613     for (ii=0; ii<(nx*ny*nz); ii++) sum += (dielZMap[i]->data[ii]);
00614     sum = sum*hx*hy*hzed;
00615     Vnm_tprint(1, " Volume integral = %3.2e A^3\n", sum);
00616     break;
00617     // UHBD format
00618     case VDF_UHBD:
00619         Vnm_tprint( 2, "UHBD input not supported yet!\n");
00620         return 0;
00621     // AVS UCD format

```

```

00622         case VDF_AVS:
00623             Vnm_tprint( 2, "AVS input not supported yet!\n");
00624             return 0;
00625         // FETk MC Simplex Format (MCSF)
00626         case VDF_MCSF:
00627             Vnm_tprint( 2, "MCSF input not supported yet!\n");
00628             return 0;
00629         default:
00630             Vnm_tprint( 2, "Invalid data format (%d)!\n",
00631                 nosh->dielfmt[i]);
00632             return 0;
00633     }
00634 }
00635
00636 return 1;
00637 }
00638
00639 VPUBLIC void killDielMaps(NOSH *nosh,
00640     Vgrid *dielXMap[NOSH_MAXMOL],
00641     Vgrid *dielYMap[NOSH_MAXMOL],
00642     Vgrid *dielZMap[NOSH_MAXMOL]) {
00643
00644     int i;
00645
00646     if (nosh->ndiel > 0) {
00647 #ifndef VAPBSQUIET
00648         Vnm_tprint( 1, "Destroying %d dielectric map sets\n",
00649             nosh->ndiel);
00650 #endif
00651         for (i=0; i<nosh->ndiel; i++) {
00652             Vgrid_dtor(&(dielXMap[i]));
00653             Vgrid_dtor(&(dielYMap[i]));
00654             Vgrid_dtor(&(dielZMap[i]));
00655         }
00656     }
00657     else return;
00658 }
00659 }
00660
00661 VPUBLIC int loadKappaMaps(NOSH *nosh,
00662     Vgrid *map[NOSH_MAXMOL]
00663 ) {
00664
00665     int i,
00666     ii,
00667     len;
00668     double sum;
00669
00670     if (nosh->nkappa > 0)
00671         Vnm_tprint( 1, "Got paths for %d kappa maps\n", nosh->nkappa);
00672     else return 1;
00673
00674     for (i=0; i<nosh->nkappa; i++) {
00675         Vnm_tprint( 1, "Reading kappa map data from %s:\n",
00676             nosh->kappapath[i]);
00677         map[i] = Vgrid_ctor(0, 0, 0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, VNULL);
00678
00679         // Determine the format and read data if the format is valid.
00680         switch (nosh->kappafmt[i]) {
00681             // OpenDX (Data Explorer) format
00682             case VDF_DX:
00683                 if (Vgrid_readDX(map[i], "FILE", "ASC", VNULL,
00684                     nosh->kappapath[i]) != 1) {
00685                     Vnm_tprint( 2, "Fatal error while reading from %s\n",
00686                         nosh->kappapath[i]);
00687                     return 0;
00688                 }
00689                 Vnm_tprint(1, "  %d x %d x %d grid\n",
00690                     map[i]->nx, map[i]->ny, map[i]->nz);
00691                 Vnm_tprint(1, "  (%g, %g, %g) A spacings\n",
00692                     map[i]->hx, map[i]->hy, map[i]->hz);
00693                 Vnm_tprint(1, "  (%g, %g, %g) A lower corner\n",
00694                     map[i]->xmin, map[i]->ymin, map[i]->zmin);
00695                 sum = 0;
00696                 for (ii = 0, len = map[i]->nx * map[i]->ny * map[i]->nz;
00697                     ii < len;
00698                     ii++)
00699                 ) {
00700                     sum += (map[i]->data[ii]);
00701                 }
00702                 sum = sum*map[i]->hx*map[i]->hy*map[i]->hz;
00703

```



```

00706         Vnm_tprint(1, " Volume integral = %3.2e A^3\n", sum);
00707         break;
00708         // OpenDX Binary (.dxbin) format
00709     case VDF_DXBIN:
00710         //TODO: write method and possible change if stmt.
00711         if (Vgrid_readDXBIN(map[i], "FILE", "ASC", VNULL,
00712             nosh->kappapath[i]) != 1) {
00713             Vnm_tprint( 2, "Fatal error while reading from %s\n",
00714                 nosh->kappapath[i]);
00715             return 0;
00716         }
00717         Vnm_tprint(1, " %d x %d x %d grid\n",
00718             map[i]->nx, map[i]->ny, map[i]->nz);
00719         Vnm_tprint(1, " (%g, %g, %g) A spacings\n",
00720             map[i]->hx, map[i]->hy, map[i]->hz);
00721         Vnm_tprint(1, " (%g, %g, %g) A lower corner\n",
00722             map[i]->xmin, map[i]->ymin, map[i]->zmin);
00723         sum = 0;
00724         for (ii = 0, len = map[i]->nx * map[i]->ny * map[i]->nz;
00725             ii < len;
00726             ii++)
00727         ) {
00728             sum += (map[i]->data[ii]);
00729         }
00730         sum = sum*map[i]->hx*map[i]->hy*map[i]->hz;
00731         Vnm_tprint(1, " Volume integral = %3.2e A^3\n", sum);
00732         break;
00733         // UHBD format
00734     case VDF_UHBD:
00735         Vnm_tprint( 2, "UHBD input not supported yet!\n");
00736         return 0;
00737         // FEtk MC Simplex Format (MCSF)
00738     case VDF_MCSF:
00739         Vnm_tprint( 2, "MCSF input not supported yet!\n");
00740         return 0;
00741         // AVS UCD format
00742     case VDF_AVS:
00743         Vnm_tprint( 2, "AVS input not supported yet!\n");
00744         return 0;
00745         // Binary file (GZip) format
00746     case VDF_GZ:
00747         if (Vgrid_readGZ(map[i], nosh->kappapath[i]) != 1) {
00748             Vnm_tprint( 2, "Fatal error while reading from %s\n",
00749                 nosh->kappapath[i]);
00750             return 0;
00751         }
00752         Vnm_tprint(1, " %d x %d x %d grid\n",
00753             map[i]->nx, map[i]->ny, map[i]->nz);
00754         Vnm_tprint(1, " (%g, %g, %g) A spacings\n",
00755             map[i]->hx, map[i]->hy, map[i]->hz);
00756         Vnm_tprint(1, " (%g, %g, %g) A lower corner\n",
00757             map[i]->xmin, map[i]->ymin, map[i]->zmin);
00758         sum = 0;
00759         for (ii=0, len=map[i]->nx*map[i]->ny*map[i]->nz; ii<len; ii++) {
00760             sum += (map[i]->data[ii]);
00761         }
00762         sum = sum*map[i]->hx*map[i]->hy*map[i]->hz;
00763         Vnm_tprint(1, " Volume integral = %3.2e A^3\n", sum);
00764         break;
00765     default:
00766         Vnm_tprint( 2, "Invalid data format (%d)!\n",
00767             nosh->kappafmt[i]);
00768         return 0;
00769     }
00770 }
00771
00772 return 1;
00773 }
00774 }
00775
00776 VPUBLIC void killKappaMaps(NOsh *nosh, Vgrid *map[NOSH_MAXMOL]) {
00777
00778     int i;
00779
00780     if (nosh->nkappa > 0) {
00781 #ifndef VAPBSQUIET
00782         Vnm_tprint( 1, "Destroying %d kappa maps\n", nosh->nkappa);
00783 #endif
00784         for (i=0; i<nosh->nkappa; i++) Vgrid_dtor(&(map[i]));
00785     }
00786     else return;

```

```

00787
00788 }
00789
00793 VPUBLIC int loadPotMaps(NOsh *nosh,
00794                        Vgrid *map[NOSH_MAXMOL]
00795                        ) {
00796
00797     int i,
00798         ii,
00799         len;
00800     double sum;
00801
00802     if (nosh->npot > 0)
00803         Vnm_tprint( 1, "Got paths for %d potential maps\n", nosh->npot);
00804     else return 1;
00805
00806     for (i=0; i<nosh->npot; i++) {
00807         Vnm_tprint( 1, "Reading potential map data from %s:\n",
00808                 nosh->potpath[i]);
00809         map[i] = Vgrid_ctor(0, 0, 0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, VNULL);
00810         switch (nosh->potfmt[i]) {
00811             // OpenDX (Data Explorer) format
00812             case VDF_DX:
00813                 // Binary file (GZip) format
00814             case VDF_GZ:
00815                 if (nosh->potfmt[i] == VDF_DX) {
00816                     if (Vgrid_readDX(map[i], "FILE", "ASC", VNULL,
00817                                     nosh->potpath[i]) != 1) {
00818                         Vnm_tprint( 2, "Fatal error while reading from %s\n",
00819                                     nosh->potpath[i]);
00820                         return 0;
00821                     }
00822                 } else {
00823                     if (Vgrid_readGZ(map[i], nosh->potpath[i]) != 1) {
00824                         Vnm_tprint( 2, "Fatal error while reading from %s\n",
00825                                     nosh->potpath[i]);
00826                         return 0;
00827                     }
00828                 }
00829                 Vnm_tprint(1, "  %d x %d x %d grid\n",
00830                         map[i]->nx, map[i]->ny, map[i]->nz);
00831                 Vnm_tprint(1, "    (%g, %g, %g) A spacings\n",
00832                         map[i]->hx, map[i]->hy, map[i]->hz);
00833                 Vnm_tprint(1, "    (%g, %g, %g) A lower corner\n",
00834                         map[i]->xmin, map[i]->ymin, map[i]->zmin);
00835                 sum = 0;
00836                 for (ii=0, len=map[i]->nx*map[i]->ny*map[i]->nz; ii<len; ii++) {
00837                     sum += (map[i]->data[ii]);
00838                 }
00839                 sum = sum*map[i]->hx*map[i]->hy*map[i]->hz;
00840                 Vnm_tprint(1, "  Volume integral = %3.2e A^3\n", sum);
00841                 break;
00842             // UHBD format
00843             case VDF_UHBD:
00844                 Vnm_tprint( 2, "UHBD input not supported yet!\n");
00845                 return 0;
00846             // FETk MC Simplex Format (MCSF)
00847             case VDF_MCSF:
00848                 Vnm_tprint( 2, "MCSF input not supported yet!\n");
00849                 return 0;
00850             // AVS UCD format
00851             case VDF_AVS:
00852                 Vnm_tprint( 2, "AVS input not supported yet!\n");
00853                 return 0;
00854             default:
00855                 Vnm_tprint( 2, "Invalid data format (%d)!\n",
00856                         nosh->potfmt[i]);
00857                 return 0;
00858         }
00859     }
00860
00861     return 1;
00862 }
00863
00865 VPUBLIC void killPotMaps(NOsh *nosh,
00866                        Vgrid *map[NOSH_MAXMOL]
00867                        ) {
00868
00869     int i;
00870

```

```

00871     if (nosh->npot > 0) {
00872 #ifndef VAPBSQUIET
00873         Vnm_tprint( 1, "Destroying %d potential maps\n", nosh->npot);
00874 #endif
00875         for (i=0; i<nosh->npot; i++) Vgrid_dtor(&(map[i]));
00876     }
00877     else return;
00878 }
00879 }
00880
00884 VPUBLIC int loadChargeMaps(NOsh *nosh,
00885                             Vgrid *map[NOSH_MAXMOL]
00886                             ) {
00887
00888     int i,
00889         ii,
00890         len;
00891     double sum;
00892
00893     if (nosh->ncharge > 0)
00894         Vnm_tprint( 1, "Got paths for %d charge maps\n", nosh->ncharge);
00895     else return 1;
00896
00897     for (i=0; i<nosh->ncharge; i++) {
00898         Vnm_tprint( 1, "Reading charge map data from %s:\n",
00899                     nosh->chargepath[i]);
00900         map[i] = Vgrid_ctor(0, 0, 0, 0.0, 0.0, 0.0, 0.0, 0.0, VNULL);
00901
00902         // Determine data format and read data
00903         switch (nosh->chargefmt[i]) {
00904             case VDF_DX:
00905                 if (Vgrid_readDX(map[i], "FILE", "ASC", VNULL,
00906                                 nosh->chargepath[i] != 1) {
00907                     Vnm_tprint( 2, "Fatal error while reading from %s\n",
00908                                 nosh->chargepath[i]);
00909                     return 0;
00910                 }
00911                 Vnm_tprint(1, " %d x %d x %d grid\n",
00912                             map[i]->nx, map[i]->ny, map[i]->nz);
00913                 Vnm_tprint(1, " (%g, %g, %g) A spacings\n",
00914                             map[i]->hx, map[i]->hy, map[i]->hz);
00915                 Vnm_tprint(1, " (%g, %g, %g) A lower corner\n",
00916                             map[i]->xmin, map[i]->ymin, map[i]->zmin);
00917                 sum = 0;
00918                 for (ii=0, len=map[i]->nx*map[i]->ny*map[i]->nz; ii<len; ii++) {
00919                     sum += (map[i]->data[ii]);
00920                 }
00921                 sum = sum*map[i]->hx*map[i]->hy*map[i]->hz;
00922                 Vnm_tprint(1, " Charge map integral = %3.2e e\n", sum);
00923                 break;
00924             case VDF_DXBIN:
00925                 //TODO: write Vgrid_readDXBIN and possibly change if stmt.
00926                 if (Vgrid_readDXBIN(map[i], "FILE", "ASC", VNULL,
00927                                     nosh->chargepath[i] != 1) {
00928                     Vnm_tprint( 2, "Fatal error while reading from %s\n",
00929                                 nosh->chargepath[i]);
00930                     return 0;
00931                 }
00932                 Vnm_tprint(1, " %d x %d x %d grid\n",
00933                             map[i]->nx, map[i]->ny, map[i]->nz);
00934                 Vnm_tprint(1, " (%g, %g, %g) A spacings\n",
00935                             map[i]->hx, map[i]->hy, map[i]->hz);
00936                 Vnm_tprint(1, " (%g, %g, %g) A lower corner\n",
00937                             map[i]->xmin, map[i]->ymin, map[i]->zmin);
00938                 sum = 0;
00939                 for (ii=0, len=map[i]->nx*map[i]->ny*map[i]->nz; ii<len; ii++) {
00940                     sum += (map[i]->data[ii]);
00941                 }
00942                 sum = sum*map[i]->hx*map[i]->hy*map[i]->hz;
00943                 Vnm_tprint(1, " Charge map integral = %3.2e e\n", sum);
00944                 break;
00945             case VDF_UHBD:
00946                 Vnm_tprint( 2, "UHBD input not supported yet!\n");
00947                 return 0;
00948             case VDF_AVS:
00949                 Vnm_tprint( 2, "AVS input not supported yet!\n");
00950                 return 0;
00951             case VDF_MCSF:
00952                 Vnm_tprint(2, "MCSF input not supported yet!\n");
00953                 return 0;
00954             case VDF_GZ:

```

```

00955         if (Vgrid_readGZ(map[i], nosh->chargepath[i]) != 1) {
00956             Vnm_tprint( 2, "Fatal error while reading from %s\n",
00957                 nosh->chargepath[i]);
00958             return 0;
00959         }
00960         Vnm_tprint(1, "  %d x %d x %d grid\n",
00961             map[i]->nx, map[i]->ny, map[i]->nz);
00962         Vnm_tprint(1, "    (%g, %g, %g) A spacings\n",
00963             map[i]->hx, map[i]->hy, map[i]->hz);
00964         Vnm_tprint(1, "    (%g, %g, %g) A lower corner\n",
00965             map[i]->xmin, map[i]->ymin, map[i]->zmin);
00966         sum = 0;
00967         for (ii=0, len=map[i]->nx*map[i]->ny*map[i]->nz; ii<len; ii++) {
00968             sum += (map[i]->data[ii]);
00969         }
00970         sum = sum*map[i]->hx*map[i]->hy*map[i]->hz;
00971         Vnm_tprint(1, "  Charge map integral = %3.2e e\n", sum);
00972         break;
00973     default:
00974         Vnm_tprint( 2, "Invalid data format (%d)!\n",
00975             nosh->kappafmt[i]);
00976         return 0;
00977     }
00978 }
00979
00980 return 1;
00981
00982 }
00983
00984 VPUBLIC void killChargeMaps(Nosh *nosh,
00985     Vgrid *map[NOSH_MAXMOL]
00986 ) {
00987
00988     int i;
00989
00990     if (nosh->ncharge > 0) {
00991 #ifndef VAPBSQUIET
00992         Vnm_tprint( 1, "Destroying %d charge maps\n", nosh->ncharge);
00993 #endif
00994         for (i=0; i<nosh->ncharge; i++) Vgrid_dtor(&(map[i]));
00995     }
00996
00997     else return;
00998
00999 }
01000
01001
01002 VPUBLIC void printPBEPARM(PBEParm *pbeparm) {
01003
01004     int i;
01005     double ionstr = 0.0;
01006
01007     for (i=0; i<pbeparm->nion; i++)
01008         ionstr += 0.5*(VSQR(pbeparm->ionq[i])*pbeparm->ionc[i]);
01009
01010     Vnm_tprint( 1, "  Molecule ID: %d\n", pbeparm->molid);
01011     switch (pbeparm->pbetype) {
01012     case PBE_NPBE:
01013         Vnm_tprint( 1, "  Nonlinear traditional PBE\n");
01014         break;
01015     case PBE_LPBE:
01016         Vnm_tprint( 1, "  Linearized traditional PBE\n");
01017         break;
01018     case PBE_NRPBE:
01019         Vnm_tprint( 1, "  Nonlinear regularized PBE\n");
01020         Vnm_tprint( 2, "  ** Sorry, but Nathan broke the nonlinear regularized PBE implementation.
01021         **\n");
01022         Vnm_tprint( 2, "  ** Please let us know if you are interested in using it. **\n");
01023         VASSERT(0);
01024         break;
01025     case PBE_LRPBE:
01026         Vnm_tprint( 1, "  Linearized regularized PBE\n");
01027         break;
01028     case PBE_SMPBE: /* SMPBE Added */
01029         Vnm_tprint( 1, "  Nonlinear Size-Modified PBE\n");
01030         break;
01031     default:
01032         Vnm_tprint(2, "  Unknown PBE type (%d)!\n", pbeparm->pbetype);
01033         break;
01034     }
01035     if (pbeparm->bconf == BCFL_ZERO) {

```

```

01035     Vnm_tprint( 1, " Zero boundary conditions\n");
01036 } else if (pbeparm->bcfl == BCFL_SDH) {
01037     Vnm_tprint( 1, " Single Debye-Huckel sphere boundary \
01038 conditions\n");
01039 } else if (pbeparm->bcfl == BCFL_MDH) {
01040     Vnm_tprint( 1, " Multiple Debye-Huckel sphere boundary \
01041 conditions\n");
01042 } else if (pbeparm->bcfl == BCFL_FOCUS) {
01043     Vnm_tprint( 1, " Boundary conditions from focusing\n");
01044 } else if (pbeparm->bcfl == BCFL_MAP) {
01045     Vnm_tprint( 1, " Boundary conditions from potential map\n");
01046 } else if (pbeparm->bcfl == BCFL_MEM) {
01047     Vnm_tprint( 1, " Membrane potential boundary conditions.\n");
01048 }
01049 Vnm_tprint( 1, " %d ion species (%4.3f M ionic strength):\n",
01050     pbeparm->nion, ionstr);
01051 for (i=0; i<pbeparm->nion; i++) {
01052     Vnm_tprint( 1, " %4.3f A-radius, %4.3f e-charge, \
01053 %4.3f M concentration\n",
01054         pbeparm->ionr[i], pbeparm->ionq[i], pbeparm->ionc[i]);
01055 }
01056
01057 if (pbeparm->pbetype == PBE_SMPBE) { /* SMPBE Added */
01058     Vnm_tprint( 1, " Lattice spacing: %4.3f A (SMPBE) \n", pbeparm->smvolume);
01059     Vnm_tprint( 1, " Relative size parameter: %4.3f (SMPBE) \n", pbeparm->smsize);
01060 }
01061
01062 Vnm_tprint( 1, " Solute dielectric: %4.3f\n", pbeparm->pdie);
01063 Vnm_tprint( 1, " Solvent dielectric: %4.3f\n", pbeparm->sdie);
01064 switch (pbeparm->srfm) {
01065     case 0:
01066         Vnm_tprint( 1, " Using \"molecular\" surface \
01067 definition; no smoothing\n");
01068         Vnm_tprint( 1, " Solvent probe radius: %4.3f A\n",
01069             pbeparm->srad);
01070         break;
01071     case 1:
01072         Vnm_tprint( 1, " Using \"molecular\" surface definition;\
01073 harmonic average smoothing\n");
01074         Vnm_tprint( 1, " Solvent probe radius: %4.3f A\n",
01075             pbeparm->srad);
01076         break;
01077     case 2:
01078         Vnm_tprint( 1, " Using spline-based surface definition;\
01079 window = %4.3f\n", pbeparm->swin);
01080         break;
01081     default:
01082         break;
01083 }
01084 Vnm_tprint( 1, " Temperature: %4.3f K\n", pbeparm->temp);
01085 if (pbeparm->calcenergy != PCE_NO) Vnm_tprint( 1, " Electrostatic \
01086 energies will be calculated\n");
01087 if (pbeparm->calcforce == PCF_TOTAL) Vnm_tprint( 1, " Net solvent \
01088 forces will be calculated\n");
01089 if (pbeparm->calcforce == PCF_COMPS) Vnm_tprint( 1, " All-atom \
01090 solvent forces will be calculated\n");
01091 for (i=0; i<pbeparm->numwrite; i++) {
01092     switch (pbeparm->writetype[i]) {
01093         case VDT_CHARGE:
01094             Vnm_tprint(1, " Charge distribution to be written to ");
01095             break;
01096         case VDT_POT:
01097             Vnm_tprint(1, " Potential to be written to ");
01098             break;
01099         case VDT_SMOL:
01100             Vnm_tprint(1, " Molecular solvent accessibility \
01101 to be written to ");
01102             break;
01103         case VDT_SSPL:
01104             Vnm_tprint(1, " Spline-based solvent accessibility \
01105 to be written to ");
01106             break;
01107         case VDT_VDW:
01108             Vnm_tprint(1, " van der Waals solvent accessibility \
01109 to be written to ");
01110             break;
01111         case VDT_IVDW:
01112             Vnm_tprint(1, " Ion accessibility to be written to ");
01113             break;
01114         case VDT_LAP:
01115             Vnm_tprint(1, " Potential Laplacian to be written to ");

```

```

01116         break;
01117     case VDT_EDENS:
01118         Vnm_tprint(1, " Energy density to be written to ");
01119         break;
01120     case VDT_NDENS:
01121         Vnm_tprint(1, " Ion number density to be written to ");
01122         break;
01123     case VDT_QDENS:
01124         Vnm_tprint(1, " Ion charge density to be written to ");
01125         break;
01126     case VDT_DIELX:
01127         Vnm_tprint(1, " X-shifted dielectric map to be written \
01128 to ");
01129         break;
01130     case VDT_DIELY:
01131         Vnm_tprint(1, " Y-shifted dielectric map to be written \
01132 to ");
01133         break;
01134     case VDT_DIELZ:
01135         Vnm_tprint(1, " Z-shifted dielectric map to be written \
01136 to ");
01137         break;
01138     case VDT_KAPPA:
01139         Vnm_tprint(1, " Kappa map to be written to ");
01140         break;
01141     case VDT_ATOMPOT:
01142         Vnm_tprint(1, " Atom potentials to be written to ");
01143         break;
01144     default:
01145         Vnm_tprint(2, " Invalid data type for writing!\n");
01146         break;
01147 }
01148 switch (pbeparm->writefmt[i]) {
01149     case VDF_DX:
01150         Vnm_tprint(1, "%s.%s\n", pbeparm->writestem[i], "dx");
01151         break;
01152     case VDF_DXBIN:
01153         Vnm_tprint(1, "%s.%s\n", pbeparm->writestem[i], "dxbin");
01154         break;
01155     case VDF_GZ:
01156         Vnm_tprint(1, "%s.%s\n", pbeparm->writestem[i], "dx.gz");
01157         break;
01158     case VDF_UHBD:
01159         Vnm_tprint(1, "%s.%s\n", pbeparm->writestem[i], "grd");
01160         break;
01161     case VDF_AVS:
01162         Vnm_tprint(1, "%s.%s\n", pbeparm->writestem[i], "ucd");
01163         break;
01164     case VDF_MCSF:
01165         Vnm_tprint(1, "%s.%s\n", pbeparm->writestem[i], "mcsf");
01166         break;
01167     case VDF_FLAT:
01168         Vnm_tprint(1, "%s.%s\n", pbeparm->writestem[i], "txt");
01169         break;
01170     default:
01171         Vnm_tprint(2, " Invalid format for writing!\n");
01172         break;
01173 }
01174 }
01175 }
01176 }
01177 }
01178
01179 VPUBLIC void printMGPARM(MGparm *mgparm, double realCenter[3]) {
01180
01181     switch (mgparm->chgm) {
01182     case 0:
01183         Vnm_tprint(1, " Using linear spline charge discretization.\n");
01184         break;
01185     case 1:
01186         Vnm_tprint(1, " Using cubic spline charge discretization.\n");
01187         break;
01188     default:
01189         break;
01190     }
01191     if (mgparm->type == MCT_PARALLEL) {
01192         Vnm_tprint(1, " Partition overlap fraction = %g\n",
01193             mgparm->ofrac);
01194         Vnm_tprint(1, " Processor array = %d x %d x %d\n",
01195             mgparm->pdime[0], mgparm->pdime[1], mgparm->pdime[2]);
01196     }

```

```

01197     Vnm_tprint( 1, "  Grid dimensions: %d x %d x %d\n",
01198                 mgparm->dime[0], mgparm->dime[1], mgparm->dime[2]);
01199     Vnm_tprint( 1, "  Grid spacings: %4.3f x %4.3f x %4.3f\n",
01200                 mgparm->grid[0], mgparm->grid[1], mgparm->grid[2]);
01201     Vnm_tprint( 1, "  Grid lengths: %4.3f x %4.3f x %4.3f\n",
01202                 mgparm->glen[0], mgparm->glen[1], mgparm->glen[2]);
01203     Vnm_tprint( 1, "  Grid center: (%4.3f, %4.3f, %4.3f)\n",
01204                 realCenter[0], realCenter[1], realCenter[2]);
01205     Vnm_tprint( 1, "  Multigrid levels: %d\n", mgparm->nlev);
01206
01207 }
01208
01212 VPUBLIC int initMG(int icalc,
01213                   Nosh *nosh, MGparm *mgparm,
01214                   PBEParm *pbeparm,
01215                   double realCenter[3],
01216                   Vpbe *pbe[NOSH_MAXCALC],
01217                   Valist *alist[NOSH_MAXMOL],
01218                   Vgrid *dielXMap[NOSH_MAXMOL],
01219                   Vgrid *dielYMap[NOSH_MAXMOL],
01220                   Vgrid *dielZMap[NOSH_MAXMOL],
01221                   Vgrid *kappaMap[NOSH_MAXMOL],
01222                   Vgrid *chargeMap[NOSH_MAXMOL],
01223                   Vpmgp *pmgp[NOSH_MAXCALC],
01224                   Vpmg *pmg[NOSH_MAXCALC],
01225                   Vgrid *potMap[NOSH_MAXMOL]
01226                 ) {
01227
01228     int j,
01229         focusFlag,
01230         iatom;
01231     size_t bytesTotal,
01232           highWater;
01233     double sparm,
01234           iparm,
01235           q;
01236     Vatom *atom = VNULL;
01237     Vgrid *theDielXMap = VNULL,
01238           *theDielYMap = VNULL,
01239           *theDielZMap = VNULL;
01240     Vgrid *theKappaMap = VNULL,
01241           *thePotMap = VNULL,
01242           *theChargeMap = VNULL;
01243     Valist *myalist = VNULL;
01244
01245     Vnm_tstart(APBS_TIMER_SETUP, "Setup timer");
01246
01247     /* Update the grid center */
01248     for (j=0; j<3; j++) realCenter[j] = mgparm->center[j];
01249
01250     /* Check for completely-neutral molecule */
01251     q = 0;
01252     myalist = alist[pbeparm->molid-1];
01253     for (iatom=0; iatom<Valist_getNumberAtoms(myalist); iatom++) {
01254         atom = Valist_getAtom(myalist, iatom);
01255         q += VSQR(Vatom_getCharge(atom));
01256     }
01257     /* D. Gohara 10/22/09 - disabled
01258     if (q < (1e-6)) {
01259         Vnm_tprint(2, "Molecule #%d is uncharged!\n", pbeparm->molid);
01260         Vnm_tprint(2, "Sum square charge = %g!\n", q);
01261         return 0;
01262     }
01263     */
01264
01265     /* Set up PBE object */
01266     Vnm_tprint(0, "Setting up PBE object...\n");
01267     if (pbeparm->srff == VSM_SPLINE) {
01268         sparm = pbeparm->swin;
01269     } else {
01270         sparm = pbeparm->srad;
01271     }
01272     if (pbeparm->nion > 0) {
01273         iparm = pbeparm->ionr[0];
01274     } else {
01275         iparm = 0.0;
01276     }
01277     if (pbeparm->bconf == BCFL_FOCUS) {
01278         if (icalc == 0) {
01279             Vnm_tprint( 2, "Can't focus first calculation!\n");
01280             return 0;

```

```

01281     }
01282     focusFlag = 1;
01283 } else {
01284     focusFlag = 0;
01285 }
01286
01287 // Construct Vpbe object
01288 pbe[icalc] = Vpbe_ctor(myalist, pbeparm->nion,
01289     pbeparm->ionc, pbeparm->ionr, pbeparm->ionq,
01290     pbeparm->temp, pbeparm->pdie,
01291     pbeparm->sdie, sparm, focusFlag, pbeparm->sdens,
01292     pbeparm->zmemo, pbeparm->Lmem, pbeparm->mdie,
01293     pbeparm->memv);
01294
01295 /* Set up PDE object */
01296 Vnm_tprint(0, "Setting up PDE object...\n");
01297 switch (pbeparm->pbetype) {
01298     case PBE_NPBE:
01299         /* TEMPORARY USEAQUA */
01300         mgparm->nonlintype = NONLIN_NPBE;
01301         mgparm->method = (mgparm->useAqua == 1) ? VSOL_NewtonAqua : VSOL_Newton;
01302         pmgp[icalc] = Vpmgp_ctor(mgparm);
01303         break;
01304     case PBE_LPBE:
01305         /* TEMPORARY USEAQUA */
01306         mgparm->nonlintype = NONLIN_LPBE;
01307         mgparm->method = (mgparm->useAqua == 1) ? VSOL_CMGMAqua : VSOL_MG;
01308         pmgp[icalc] = Vpmgp_ctor(mgparm);
01309         break;
01310     case PBE_LRPBE:
01311         Vnm_tprint(2, "Sorry, LRPBE isn't supported with the MG solver!\n");
01312         return 0;
01313     case PBE_NRPBE:
01314         Vnm_tprint(2, "Sorry, NRPBE isn't supported with the MG solver!\n");
01315         return 0;
01316     case PBE_SMPBE: /* SMPBE Added */
01317         /* Due to numerical issues the SMPBE is currently disabled. (JMB)*/
01318         Vnm_tprint(2, " ** Sorry, due to numerical stability issues SMPBE is currently disabled. We
01319 apologize for the inconvenience.\n");
01320         Vnm_tprint(2, " ** Please let us know if you would like to use it in the future.\n");
01321         return 0;
01322     /*
01323         mgparm->nonlintype = NONLIN_SMPBE;
01324         pmgp[icalc] = Vpmgp_ctor(mgparm);
01325     */
01326     /* Copy Code */
01327     /*
01328         pbe[icalc]->smsize = pbeparm->smsize;
01329         pbe[icalc]->smvolume = pbeparm->smvolume;
01330         pbe[icalc]->ipkey = pmgp[icalc]->ipkey;
01331     */
01332     break;
01333     /*
01334         default:
01335             Vnm_tprint(2, "Error! Unknown PBE type (%d)!\n", pbeparm->pbetype);
01336             return 0;
01337     */
01338     Vnm_tprint(0, "Setting PDE center to local center...\n");
01339     pmgp[icalc]->bcbf1 = pbeparm->bcbf1;
01340     pmgp[icalc]->xcent = realCenter[0];
01341     pmgp[icalc]->ycent = realCenter[1];
01342     pmgp[icalc]->zcent = realCenter[2];
01343
01344     if (pbeparm->bcbf1 == BCFL_FOCUS) {
01345         if (icalc == 0) {
01346             Vnm_tprint(2, "Can't focus first calculation!\n");
01347             return 0;
01348         }
01349         /* Focusing requires the previous calculation in order to setup the
01350         current run... */
01351         pmg[icalc] = Vpmg_ctor(pmgp[icalc], pbe[icalc], 1, pmg[icalc-1],
01352             mgparm, pbeparm->calcenergy);
01353         /* ...however, it should be done with the previous calculation now, so
01354         we should be able to destroy it here. */
01355         /* Vpmg_dtor(&(pmg[icalc-1])); */
01356     } else {
01357         if (icalc>0) Vpmg_dtor(&(pmg[icalc-1]));
01358         pmg[icalc] = Vpmg_ctor(pmgp[icalc], pbe[icalc], 0, VNULL, mgparm, PCE_NO);
01359     }
01360     if (icalc>0) {

```



```

01361         Vpmgp_dtor(&(pmgp[icalc-1]));
01362         Vpbe_dtor(&(pbe[icalc-1]));
01363     }
01364     if (pbeparm->useDielMap) {
01365         if ((pbeparm->dielMapID-1) < nosh->ndiel) {
01366             theDielXMap = dielXMap[pbeparm->dielMapID-1];
01367         } else {
01368             Vnm_print(2, "Error! %d is not a valid dielectric map ID!\n",
01369                 pbeparm->dielMapID);
01370             return 0;
01371         }
01372     }
01373     if (pbeparm->useDielMap) {
01374         if ((pbeparm->dielMapID-1) < nosh->ndiel) {
01375             theDielyMap = dielyMap[pbeparm->dielMapID-1];
01376         } else {
01377             Vnm_print(2, "Error! %d is not a valid dielectric map ID!\n",
01378                 pbeparm->dielMapID);
01379             return 0;
01380         }
01381     }
01382     if (pbeparm->useDielMap) {
01383         if ((pbeparm->dielMapID-1) < nosh->ndiel) {
01384             theDielZMap = dielZMap[pbeparm->dielMapID-1];
01385         } else {
01386             Vnm_print(2, "Error! %d is not a valid dielectric map ID!\n",
01387                 pbeparm->dielMapID);
01388             return 0;
01389         }
01390     }
01391     if (pbeparm->useKappaMap) {
01392         if ((pbeparm->kappaMapID-1) < nosh->nkappa) {
01393             theKappaMap = kappaMap[pbeparm->kappaMapID-1];
01394         } else {
01395             Vnm_print(2, "Error! %d is not a valid kappa map ID!\n",
01396                 pbeparm->kappaMapID);
01397             return 0;
01398         }
01399     }
01400     if (pbeparm->usePotMap) {
01401         if ((pbeparm->potMapID-1) < nosh->npot) {
01402             thePotMap = potMap[pbeparm->potMapID-1];
01403         } else {
01404             Vnm_print(2, "Error! %d is not a valid potential map ID!\n",
01405                 pbeparm->potMapID);
01406             return 0;
01407         }
01408     }
01409     if (pbeparm->useChargeMap) {
01410         if ((pbeparm->chargeMapID-1) < nosh->ncharge) {
01411             theChargeMap = chargeMap[pbeparm->chargeMapID-1];
01412         } else {
01413             Vnm_print(2, "Error! %d is not a valid charge map ID!\n",
01414                 pbeparm->chargeMapID);
01415             return 0;
01416         }
01417     }
01418     if (pbeparm->bcfl == BCFL_MAP && thePotMap == VNULL) {
01419         Vnm_print(2, "Warning: You specified 'bcfl map' in the input file, but no potential map was
01420 found.\n");
01421         Vnm_print(2, "          You must specify 'usemap pot' statement in the APBS input file!\n");
01422         Vnm_print(2, "Bailing out ...!\n");
01423         return 0;
01424     }
01425     // Initialize calculation coefficients
01426     if (!Vpmg_fillco(pmg[icalc],
01427         pbeparm->srfm, pbeparm->swin, mgparm->chgm,
01428         pbeparm->useDielMap, theDielXMap,
01429         pbeparm->useDielMap, theDielyMap,
01430         pbeparm->useDielMap, theDielZMap,
01431         pbeparm->useKappaMap, theKappaMap,
01432         pbeparm->usePotMap, thePotMap,
01433         pbeparm->useChargeMap, theChargeMap)) {
01434         Vnm_print(2, "initMG: problems setting up coefficients (fillco)!\n");
01435         return 0;
01436     }
01437 }
01438
01439 /* Print a few derived parameters */
01440 #ifndef VAPBSQUIET

```

```

01441     Vnm_tprint(1, " Debye length: %g A\n", Vpbe_getDeblen(pbe[icalc]));
01442 #endif
01443
01444     /* Setup time statistics */
01445     Vnm_tstop(APBS_TIMER_SETUP, "Setup timer");
01446
01447     /* Memory statistics */
01448     bytesTotal = Vmem_bytesTotal();
01449     highWater = Vmem_highWaterTotal();
01450
01451 #ifndef VAPBSQUIET
01452     Vnm_tprint( 1, " Current memory usage: %4.3f MB total, \
01453 %4.3f MB high water\n", (double) (bytesTotal)/(1024.*1024.),
01454                      (double) (highWater)/(1024.*1024.));
01455 #endif
01456     return 1;
01457 }
01458
01459 }
01460
01461 VPUBLIC void killMG(NOsh *nosh, Vpbe *pbe[NOSH_MAXCALC],
01462                   Vpmgp *pmgp[NOSH_MAXCALC], Vpmg *pmg[NOSH_MAXCALC]) {
01463
01464     int i;
01465
01466 #ifndef VAPBSQUIET
01467     Vnm_tprint(1, "Destroying multigrid structures.\n");
01468 #endif
01469
01470     /*
01471      There appears to be a relationship (or this is a bug in Linux, can't tell
01472      at the moment, since Linux is the only OS that seems to be affected)
01473      between one of the three object types: Vpbe, Vpmg or Vpmgp that requires
01474      deallocations to be performed in a specific order. This results in a
01475      bug some of the time when freeing Vpmg objects below. Therefore it
01476      appears to be important to release the Vpmg structs BEFORE the Vpmgp structs .
01477     */
01478     Vpmg_dtor(&(pmg[nosh->ncalc-1]));
01479
01480     for(i=0; i<nosh->ncalc; i++){
01481         Vpbe_dtor(&(pbe[i]));
01482         Vpmgp_dtor(&(pmgp[i]));
01483     }
01484 }
01485 }
01486
01487 VPUBLIC int solveMG(NOsh *nosh,
01488                   Vpmg *pmg,
01489                   MGparm_CalcType type
01490                   ) {
01491
01492     int nx,
01493         ny,
01494         nz,
01495         i;
01496
01497     if (nosh != VNULL) {
01498         if (nosh->bogus) return 1;
01499     }
01500
01501     Vnm_tstart(APBS_TIMER_SOLVER, "Solver timer");
01502
01503
01504     if (type != MCT_DUMMY) {
01505         if (!Vpmg_solve(pmg)) {
01506             Vnm_print(2, " Error during PDE solution!\n");
01507             return 0;
01508         }
01509     } else {
01510         Vnm_tprint( 1, " Skipping solve for mg-dummy run; zeroing \
01511 solution array\n");
01512         nx = pmg->pmgp->nx;
01513         ny = pmg->pmgp->ny;
01514         nz = pmg->pmgp->nz;
01515         for (i=0; i<nx*ny*nz; i++) pmg->u[i] = 0.0;
01516     }
01517     Vnm_tstop(APBS_TIMER_SOLVER, "Solver timer");
01518
01519     return 1;
01520 }
01521 }

```

```

01522
01523 VPUBLIC int setPartMG(NOsh *nosh,
01524                     MGparm *mgparm,
01525                     Vpmg *pmg
01526                     ) {
01527
01528     int j;
01529     double partMin[3],
01530            partMax[3];
01531
01532     if (nosh->bogus) return 1;
01533
01534     if (mgparm->type == MCT_PARALLEL) {
01535         for (j=0; j<3; j++) {
01536             partMin[j] = mgparm->partDisjCenter[j] - 0.5*mgparm->partDisjLength[j];
01537             partMax[j] = mgparm->partDisjCenter[j] + 0.5*mgparm->partDisjLength[j];
01538         }
01539     #if 0
01540         Vnm_tprint(1, "setPartMG (%s, %d): Disj part center = (%g, %g, %g)\n",
01541                  __FILE__, __LINE__,
01542                  mgparm->partDisjCenter[0],
01543                  mgparm->partDisjCenter[1],
01544                  mgparm->partDisjCenter[2]
01545                  );
01546         Vnm_tprint(1, "setPartMG (%s, %d): Disj part lower corner = (%g, %g, %g)\n",
01547                  __FILE__, __LINE__, partMin[0], partMin[1], partMin[2]);
01548         Vnm_tprint(1, "setPartMG (%s, %d): Disj part upper corner = (%g, %g, %g)\n",
01549                  __FILE__, __LINE__,
01550                  partMax[0], partMax[1], partMax[2]);
01551     #endif
01552     } else {
01553         for (j=0; j<3; j++) {
01554             partMin[j] = mgparm->center[j] - 0.5*mgparm->glen[j];
01555             partMax[j] = mgparm->center[j] + 0.5*mgparm->glen[j];
01556         }
01557     }
01558     /* Vnm_print(1, "DEBUG (%s, %d): setPartMG calling setPart with upper corner \
01559 %g %g %g and lower corner %g %g %g\n", __FILE__, __LINE__,
01560                partMin[0], partMin[1], partMin[2],
01561                partMax[0], partMax[1], partMax[2]); */
01562     Vpmg_setPart(pmg, partMin, partMax, mgparm->partDisjOwnSide);
01563
01564     return 1;
01565 }
01566
01567 }
01568
01569 VPUBLIC int energyMG(NOsh *nosh,
01570                    int icalc,
01571                    Vpmg *pmg,
01572                    int *nenergy,
01573                    double *totEnergy,
01574                    double *qfEnergy,
01575                    double *qmEnergy,
01576                    double *dielEnergy
01577                    ) {
01578
01579     Valist *alist;
01580     Vatom *atom;
01581     int i,
01582         extEnergy;
01583     double tenergy;
01584     MGparm *mgparm;
01585     PBeparm *pbeparm;
01586
01587     mgparm = nosh->calc[icalc]->mgparm;
01588     pbeparm = nosh->calc[icalc]->pbeparm;
01589
01590     Vnm_tstart(APBS_TIMER_ENERGY, "Energy timer");
01591     extEnergy = 1;
01592
01593     if (pbeparm->calcenergy == PCE_TOTAL) {
01594         *nenergy = 1;
01595         /* Some processors don't count */
01596         if (nosh->bogus == 0) {
01597             *totEnergy = Vpmg_energy(pmg, extEnergy);
01598         #ifndef VAPBS_QUIET
01599             Vnm_tprint( 1, " Total electrostatic energy = %1.12E kJ/mol\n",
01600                       Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(*totEnergy));
01601         #endif
01602     } else *totEnergy = 0;

```

```

01603     } else if (pbeparm->calcenergy == PCE_COMPS) {
01604         *nenergy = 1;
01605         *totEnergy = Vpmg_energy(pmg, extEnergy);
01606         *qfEnergy = Vpmg_qfEnergy(pmg, extEnergy);
01607         *qmEnergy = Vpmg_qmEnergy(pmg, extEnergy);
01608         *dielEnergy = Vpmg_dielEnergy(pmg, extEnergy);
01609 #ifndef VAPBSQUIET
01610         Vnm_tprint( 1, " Total electrostatic energy = %1.12E \
01611 kJ/mol\n", Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(totEnergy));
01612         Vnm_tprint( 1, " Fixed charge energy = %g kJ/mol\n",
01613             0.5*Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(qfEnergy));
01614         Vnm_tprint( 1, " Mobile charge energy = %g kJ/mol\n",
01615             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(qmEnergy));
01616         Vnm_tprint( 1, " Dielectric energy = %g kJ/mol\n",
01617             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(dielEnergy));
01618         Vnm_tprint( 1, " Per-atom energies:\n");
01619 #endif
01620         alist = pmg->pbe->alist;
01621         for (i=0; i<Valist_getNumberAtoms(alist); i++) {
01622             atom = Valist_getAtom(alist, i);
01623             tenergy = Vpmg_qfAtomEnergy(pmg, atom);
01624 #ifndef VAPBSQUIET
01625             Vnm_tprint( 1, " Atom %d: %1.12E kJ/mol\n", i,
01626                 0.5*Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*tenergy);
01627 #endif
01628         }
01629     } else *nenergy = 0;
01630
01631     Vnm_tstop(APBS_TIMER_ENERGY, "Energy timer");
01632
01633     return 1;
01634 }
01635
01636 VPUBLIC int forceMG(Vmem *mem,
01637     NOSH *nosh,
01638     PBeparm *pbeparm,
01639     MGparm *mgparm,
01640     Vpmg *pmg,
01641     int *nforce,
01642     AtomForce **atomForce,
01643     Valist *alist[NOSH_MAXMOL]
01644 ) {
01645
01646     int j,
01647         k;
01648     double qfForce[3],
01649         dbForce[3],
01650         ibForce[3];
01651
01652     Vnm_tstart(APBS_TIMER_FORCE, "Force timer");
01653
01654 #ifndef VAPBSQUIET
01655     Vnm_tprint( 1, " Calculating forces...\n");
01656 #endif
01657
01658     if (pbeparm->calcforce == PCF_TOTAL) {
01659         *nforce = 1;
01660         *atomForce = (AtomForce *)Vmem_malloc(mem, 1, sizeof(AtomForce));
01661         /* Clear out force arrays */
01662         for (j=0; j<3; j++) {
01663             (*atomForce)[0].qfForce[j] = 0;
01664             (*atomForce)[0].ibForce[j] = 0;
01665             (*atomForce)[0].dbForce[j] = 0;
01666         }
01667         for (j=0; j<Valist_getNumberAtoms(alist[pbeparm->molid-1]); j++) {
01668             if (nosh->bogus == 0) {
01669                 VASSERT(Vpmg_qfForce(pmg, qfForce, j, mgparm->chgm));
01670                 VASSERT(Vpmg_ibForce(pmg, ibForce, j, pbeparm->srfm));
01671                 VASSERT(Vpmg_dbForce(pmg, dbForce, j, pbeparm->srfm));
01672             } else {
01673                 for (k=0; k<3; k++) {
01674                     qfForce[k] = 0;
01675                     ibForce[k] = 0;
01676                     dbForce[k] = 0;
01677                 }
01678             }
01679             for (k=0; k<3; k++) {
01680                 (*atomForce)[0].qfForce[k] += qfForce[k];
01681                 (*atomForce)[0].ibForce[k] += ibForce[k];
01682                 (*atomForce)[0].dbForce[k] += dbForce[k];
01683             }
01684         }
01685     }

```

```

01684     }
01685 #ifndef VAPBSQUIET
01686     Vnm_tprint( 1, " Printing net forces for molecule %d (kJ/mol/A)\n",
01687         pbeparm->molid);
01688     Vnm_tprint( 1, " Legend:\n");
01689     Vnm_tprint( 1, "   qf -- fixed charge force\n");
01690     Vnm_tprint( 1, "   db -- dielectric boundary force\n");
01691     Vnm_tprint( 1, "   ib -- ionic boundary force\n");
01692     Vnm_tprint( 1, "   qf %4.3e %4.3e %4.3e\n",
01693         Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(atomForce)[0].qfForce[0],
01694         Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(atomForce)[0].qfForce[1],
01695         Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(atomForce)[0].qfForce[2]);
01696     Vnm_tprint( 1, "   ib %4.3e %4.3e %4.3e\n",
01697         Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(atomForce)[0].ibForce[0],
01698         Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(atomForce)[0].ibForce[1],
01699         Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(atomForce)[0].ibForce[2]);
01700     Vnm_tprint( 1, "   db %4.3e %4.3e %4.3e\n",
01701         Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(atomForce)[0].dbForce[0],
01702         Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(atomForce)[0].dbForce[1],
01703         Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(atomForce)[0].dbForce[2]);
01704 #endif
01705 } else if (pbeparm->calcforce == PCF_COMPS) {
01706     *nforce = Valist_getNumberAtoms(alist[pbeparm->molid-1]);
01707     *atomForce = (AtomForce *)Vmem_malloc(mem, *nforce,
01708         sizeof(AtomForce));
01709 #ifndef VAPBSQUIET
01710     Vnm_tprint( 1, " Printing per-atom forces for molecule %d (kJ/mol/A)\n",
01711         pbeparm->molid);
01712     Vnm_tprint( 1, " Legend:\n");
01713     Vnm_tprint( 1, "   tot n -- total force for atom n\n");
01714     Vnm_tprint( 1, "   qf n -- fixed charge force for atom n\n");
01715     Vnm_tprint( 1, "   db n -- dielectric boundary force for atom n\n");
01716     Vnm_tprint( 1, "   ib n -- ionic boundary force for atom n\n");
01717 #endif
01718     for (j=0; j<Valist_getNumberAtoms(alist[pbeparm->molid-1]); j++) {
01719         if (nosh->bogus == 0) {
01720             VASSERT(Vpmg_qfForce(pmg, (*atomForce)[j].qfForce, j,
01721                 mgparm->chgm));
01722             VASSERT(Vpmg_ibForce(pmg, (*atomForce)[j].ibForce, j,
01723                 pbeparm->srfm));
01724             VASSERT(Vpmg_dbForce(pmg, (*atomForce)[j].dbForce, j,
01725                 pbeparm->srfm));
01726         } else {
01727             for (k=0; k<3; k++) {
01728                 (*atomForce)[j].qfForce[k] = 0;
01729                 (*atomForce)[j].ibForce[k] = 0;
01730                 (*atomForce)[j].dbForce[k] = 0;
01731             }
01732         }
01733 #ifndef VAPBSQUIET
01734         Vnm_tprint( 1, "mgF tot %d %4.3e %4.3e %4.3e\n", j,
01735             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01736             *((atomForce)[j].qfForce[0]+(atomForce)[j].ibForce[0]+
01737             (atomForce)[j].dbForce[0]),
01738             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01739             *((atomForce)[j].qfForce[1]+(atomForce)[j].ibForce[1]+
01740             (atomForce)[j].dbForce[1]),
01741             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01742             *((atomForce)[j].qfForce[2]+(atomForce)[j].ibForce[2]+
01743             (atomForce)[j].dbForce[2]));
01744         Vnm_tprint( 1, "mgF qf %d %4.3e %4.3e %4.3e\n", j,
01745             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01746             *((atomForce)[j].qfForce[0],
01747             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01748             *((atomForce)[j].qfForce[1],
01749             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01750             *((atomForce)[j].qfForce[2]));
01751         Vnm_tprint( 1, "mgF ib %d %4.3e %4.3e %4.3e\n", j,
01752             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01753             *((atomForce)[j].ibForce[0],
01754             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01755             *((atomForce)[j].ibForce[1],
01756             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01757             *((atomForce)[j].ibForce[2]));
01758         Vnm_tprint( 1, "mgF db %d %4.3e %4.3e %4.3e\n", j,
01759             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01760             *((atomForce)[j].dbForce[0],
01761             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01762             *((atomForce)[j].dbForce[1],
01763             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01764             *((atomForce)[j].dbForce[2]));

```

```

01765 #endif
01766     }
01767     } else *nforce = 0;
01768
01769     Vnm_tstop(APBS_TIMER_FORCE, "Force timer");
01770
01771     return 1;
01772 }
01773
01774 VPUBLIC void killEnergy() {
01775
01776 #ifndef VAPBSQUIET
01777     Vnm_tprint(1, "No energy arrays to destroy.\n");
01778 #endif
01779 }
01780
01781
01782 VPUBLIC void killForce(Vmem *mem, NOsh *nosh, int nforce[NOSH_MAXCALC],
01783                      AtomForce *atomForce[NOSH_MAXCALC]) {
01784
01785     int i;
01786
01787 #ifndef VAPBSQUIET
01788     Vnm_tprint(1, "Destroying force arrays.\n");
01789 #endif
01790
01791     for (i=0; i<nosh->ncalc; i++) {
01792
01793         if (nforce[i] > 0) Vmem_free(mem, nforce[i], sizeof(AtomForce),
01794                                     (void **)&(atomForce[i]));
01795     }
01796 }
01797
01798
01799 VPUBLIC int writematMG(int rank, NOsh *nosh, PBEParm *pbeparm, Vpmg *pmg) {
01800
01801     char writematstem[VMAX_ARGLEN];
01802     char outpath[VMAX_ARGLEN];
01803     char mxtype[3];
01804     int strlenmax;
01805
01806     if (nosh->bogus) return 1;
01807
01808 #ifdef HAVE_MPI_H
01809     strlenmax = VMAX_ARGLEN-14;
01810     if (strlen(pbeparm->writematstem) > strlenmax) {
01811         Vnm_tprint(2, " Matrix name (%s) too long (%d char max)!\n",
01812                   pbeparm->writematstem, strlenmax);
01813         Vnm_tprint(2, " Not writing matrix!\n");
01814         return 0;
01815     }
01816     sprintf(writematstem, "%s-PE%d", pbeparm->writematstem, rank);
01817 #else
01818     strlenmax = (int)(VMAX_ARGLEN)-1;
01819     if ((int)strlen(pbeparm->writematstem) > strlenmax) {
01820         Vnm_tprint(2, " Matrix name (%s) too long (%d char max)!\n",
01821                   pbeparm->writematstem, strlenmax);
01822         Vnm_tprint(2, " Not writing matrix!\n");
01823         return 0;
01824     }
01825     if (nosh->ispara == 1){
01826         sprintf(writematstem, "%s-PE%d", pbeparm->writematstem, nosh->proc_rank);
01827     }else{
01828         sprintf(writematstem, "%s", pbeparm->writematstem);
01829     }
01830 #endif
01831
01832     if (pbeparm->writemat == 1) {
01833         strlenmax = VMAX_ARGLEN-5;
01834         if ((int)strlen(pbeparm->writematstem) > strlenmax) {
01835             Vnm_tprint(2, " Matrix name (%s) too long (%d char max)!\n",
01836                       pbeparm->writematstem, strlenmax);
01837             Vnm_tprint(2, " Not writing matrix!\n");
01838             return 0;
01839         }
01840         sprintf(outpath, "%s.%s", writematstem, "mat");
01841         mxtype[0] = 'R';
01842         mxtype[1] = 'S';
01843         mxtype[2] = 'A';
01844         /* Poisson operator only */
01845         if (pbeparm->writematflag == 0) {

```

```

01846         Vnm_tprint( 1, " Writing Poisson operator matrix \
01847 to %s...\n", outpath);
01848
01849         /* Linearization of Poisson-Boltzmann operator around solution */
01850     } else if (pbeparm->writematflag == 1) {
01851         Vnm_tprint( 1, " Writing linearization of full \
01852 Poisson-Boltzmann operator matrix to %s...\n", outpath);
01853
01854     } else {
01855         Vnm_tprint( 2, " Bogus matrix specification\
01856 (%d)!\n", pbeparm->writematflag);
01857         return 0;
01858     }
01859
01860     Vnm_tprint(0, " Printing operator...\n");
01861     //Vpmg_printColComp(pmg, outpath, outpath, mxtype,
01862 // pbeparm->writematflag);
01863     return 0;
01864 }
01865 }
01866
01867 return 1;
01868 }
01869
01870 VPUBLIC void storeAtomEnergy(Vpmg *pmg, int icalc, double **atomEnergy,
01871 int *nenergy){
01872
01873     Vatom *atom;
01874     Valist *alist;
01875     int i;
01876
01877     alist = pmg->pbe->alist;
01878     *nenergy = Valist_getNumberAtoms(alist);
01879     *atomEnergy = (double *)Vmem_malloc(pmg->vmem, *nenergy, sizeof(double));
01880
01881     for (i=0; i<*nenergy; i++) {
01882         atom = Valist_getAtom(alist, i);
01883         (*atomEnergy)[i] = Vpmg_qfAtomEnergy(pmg, atom);
01884     }
01885 }
01886
01887 VPUBLIC int writedataFlat(
01888     Nosh *nosh,
01889     Vcom *com,
01890     const char *fname,
01891     double totEnergy[NOSH_MAXCALC],
01892     double qfEnergy[NOSH_MAXCALC],
01893     double qmEnergy[NOSH_MAXCALC],
01894     double dielEnergy[NOSH_MAXCALC],
01895     int nenergy[NOSH_MAXCALC],
01896     double *atomEnergy[NOSH_MAXCALC],
01897     int nforce[NOSH_MAXCALC],
01898     AtomForce *atomForce[NOSH_MAXCALC]) {
01899
01900     FILE *file;
01901     time_t now;
01902     int ielec, icalc, i, j;
01903     char *timestring = VNULL;
01904     PBeparm *pbeparm = VNULL;
01905     MGparm *mgparm = VNULL;
01906     double conversion, ltenergy, gtenergy, scalar;
01907
01908     if (nosh->bogus) return 1;
01909
01910     /* Initialize some variables */
01911
01912     icalc = 0;
01913
01914     file = fopen(fname, "w");
01915     if (file == VNULL) {
01916         Vnm_print(2, "writedataFlat: Problem opening virtual socket %s\n",
01917 fname);
01918         return 0;
01919     }
01920
01921     /* Strip the newline character from the date */
01922
01923     now = time(VNULL);
01924     timestring = ctime(&now);
01925     fprintf(file,"%s\n", timestring);
01926

```

```

01927     for (ielec=0; ielec<nosh->nelec;ielec++) { /* elec loop */
01928
01929         /* Initialize per-elec pointers */
01930
01931         mgparm = nosh->calc[icalc]->mgparm;
01932         pbeparm = nosh->calc[icalc]->pbeparm;
01933
01934         /* Convert from kT/e to kJ/mol */
01935         conversion = Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na;
01936
01937         fprintf(file,"elec");
01938         if (Vstring_strcasecmp(nosh->elecname[ielec], "") != 0) {
01939             fprintf(file," name %s\n", nosh->elecname[ielec]);
01940         } else fprintf(file, "\n");
01941
01942         switch (mgparm->type) {
01943             case MCT_DUMMY:
01944                 fprintf(file,"      mg-dummy\n");
01945                 break;
01946             case MCT_MANUAL:
01947                 fprintf(file,"      mg-manual\n");
01948                 break;
01949             case MCT_AUTO:
01950                 fprintf(file,"      mg-auto\n");
01951                 break;
01952             case MCT_PARALLEL:
01953                 fprintf(file,"      mg-para\n");
01954                 break;
01955             default:
01956                 break;
01957         }
01958
01959         fprintf(file,"      mol %d\n", pbeparm->molid);
01960         fprintf(file,"      dime %d %d %d\n", mgparm->dime[0], mgparm->dime[1],\
01961             mgparm->dime[2]);
01962
01963         switch (pbeparm->pbetype) {
01964             case PBE_NPBE:
01965                 fprintf(file,"      npbe\n");
01966                 break;
01967             case PBE_LPBE:
01968                 fprintf(file,"      lpbe\n");
01969                 break;
01970             default:
01971                 break;
01972         }
01973
01974         if (pbeparm->nion > 0) {
01975             for (i=0; i<pbeparm->nion; i++) {
01976                 fprintf(file,"      ion %4.3f %4.3f %4.3f\n",
01977                     pbeparm->ionr[i], pbeparm->ionq[i], pbeparm->ionc[i]);
01978             }
01979         }
01980
01981         fprintf(file,"      pdie %4.3f\n", pbeparm->pdie);
01982         fprintf(file,"      sdie %4.3f\n", pbeparm->sdie);
01983
01984         switch (pbeparm->srfm) {
01985             case 0:
01986                 fprintf(file,"      srfm mol\n");
01987                 fprintf(file,"      srad %4.3f\n", pbeparm->srad);
01988                 break;
01989             case 1:
01990                 fprintf(file,"      srfm smol\n");
01991                 fprintf(file,"      srad %4.3f\n", pbeparm->srad);
01992                 break;
01993             case 2:
01994                 fprintf(file,"      srfm spl2\n");
01995                 fprintf(file,"      srad %4.3f\n", pbeparm->srad);
01996                 break;
01997             default:
01998                 break;
01999         }
02000
02001         switch (pbeparm->bcbfl) {
02002             case BCFL_ZERO:
02003                 fprintf(file,"      bcbfl zero\n");
02004                 break;
02005             case BCFL_SDH:
02006                 fprintf(file,"      bcbfl sdh\n");
02007                 break;

```



```

02008         case BCFL_MDH:
02009             fprintf(file, "    bcfl mdh\n");
02010             break;
02011         case BCFL_FOCUS:
02012             fprintf(file, "    bcfl focus\n");
02013             break;
02014         case BCFL_MAP:
02015             fprintf(file, "    bcfl map\n");
02016             break;
02017         case BCFL_MEM:
02018             fprintf(file, "    bcfl mem\n");
02019             break;
02020         default:
02021             break;
02022     }
02023
02024     fprintf(file, "    temp %4.3f\n", pbeparm->temp);
02025
02026     for (; icalc<=nosh->elec2calc[ielec]; icalc++){ /* calc loop */
02027
02028         /* Reinitialize per-calc pointers */
02029         mgparm = nosh->calc[icalc]->mgparm;
02030         pbeparm = nosh->calc[icalc]->pbeparm;
02031
02032         fprintf(file, "    calc\n");
02033         fprintf(file, "        id %i\n", (icalc+1));
02034         fprintf(file, "        grid %4.3f %4.3f %4.3f\n",
02035             mgparm->grid[0], mgparm->grid[1], mgparm->grid[2]);
02036         fprintf(file, "        glen %4.3f %4.3f %4.3f\n",
02037             mgparm->glen[0], mgparm->glen[1], mgparm->glen[2]);
02038
02039         if (pbeparm->calcenergy == PCE_TOTAL) {
02040             fprintf(file, "            totEnergy %1.12E kJ/mol\n",
02041                 (totEnergy[icalc]*conversion));
02042         } if (pbeparm->calcenergy == PCE_COMPS) {
02043             fprintf(file, "            totEnergy %1.12E kJ/mol\n",
02044                 (totEnergy[icalc]*conversion));
02045             fprintf(file, "            qfEnergy %1.12E kJ/mol\n",
02046                 (0.5*qfEnergy[icalc]*conversion));
02047             fprintf(file, "            qmEnergy %1.12E kJ/mol\n",
02048                 (qmEnergy[icalc]*conversion));
02049             fprintf(file, "            dielEnergy %1.12E kJ/mol\n",
02050                 (dielEnergy[icalc]*conversion));
02051             for (i=0; i<nenergy[icalc]; i++){
02052                 fprintf(file, "                atom %i %1.12E kJ/mol\n", i,
02053                     (0.5*atomEnergy[icalc][i]*conversion));
02054             }
02055         }
02056     }
02057
02058     if (pbeparm->calcforce == PCF_TOTAL) {
02059         fprintf(file, "        qfForce %1.12E %1.12E %1.12E kJ/mol/A\n",
02060             (atomForce[icalc][0].qfForce[0]*conversion),
02061             (atomForce[icalc][0].qfForce[1]*conversion),
02062             (atomForce[icalc][0].qfForce[2]*conversion));
02063         fprintf(file, "        ibForce %1.12E %1.12E %1.12E kJ/mol/A\n",
02064             (atomForce[icalc][0].ibForce[0]*conversion),
02065             (atomForce[icalc][0].ibForce[1]*conversion),
02066             (atomForce[icalc][0].ibForce[2]*conversion));
02067         fprintf(file, "        dbForce %1.12E %1.12E %1.12E kJ/mol/A\n",
02068             (atomForce[icalc][0].dbForce[0]*conversion),
02069             (atomForce[icalc][0].dbForce[1]*conversion),
02070             (atomForce[icalc][0].dbForce[2]*conversion));
02071     }
02072     fprintf(file, "    end\n");
02073 }
02074
02075     fprintf(file, "end\n");
02076 }
02077
02078 /* Handle print energy statements */
02079
02080 for (i=0; i<nosh->nprint; i++) {
02081     if (nosh->printwhat[i] == NPT_ENERGY) {
02082         fprintf(file, "print energy");
02083         fprintf(file, " %d", nosh->printcalc[i][0]+1);
02084
02085         for (j=1; j<nosh->printnarg[i]; j++) {
02086             if (nosh->printop[i][j-1] == 0) fprintf(file, " +");

```

```

02089         else if (nosh->printop[i][j-1] == 1) fprintf(file, " -");
02090         fprintf(file, " %d", nosh->printcalc[i][j]+1);
02091     }
02092
02093     fprintf(file, "\n");
02094     icalc = nosh->elec2calc[nosh->printcalc[i][0]];
02095
02096     ltenergy = Vunit_kb * (1e-3) * Vunit_Na * \
02097         nosh->calc[icalc]->pbeparm->temp * totEnergy[icalc];
02098
02099     for (j=1; j<nosh->printnarg[i]; j++) {
02100         icalc = nosh->elec2calc[nosh->printcalc[i][j]];
02101         /* Add or subtract? */
02102         if (nosh->printop[i][j-1] == 0) scalar = 1.0;
02103         else if (nosh->printop[i][j-1] == 1) scalar = -1.0;
02104         /* Accumulate */
02105         ltenergy += (scalar * Vunit_kb * (1e-3) * Vunit_Na *
02106             nosh->calc[icalc]->pbeparm->temp * totEnergy[icalc]);
02107
02108         Vcom_reduce(com, &ltenergy, &gtenergy, 1, 2, 0);
02109     }
02110     fprintf(file, "    localEnergy %1.12E kJ/mol\n", \
02111         ltenergy);
02112     fprintf(file, "    globalEnergy %1.12E kJ/mol\nend\n", \
02113         gtenergy);
02114 }
02115 }
02116 }
02117
02118 fclose(file);
02119
02120 return 1;
02121 }
02122
02123 VPUBLIC int writedataXML(Nosh *nosh, Vcom *com, const char *fname,
02124     double totEnergy[NOSH_MAXCALC],
02125     double qfEnergy[NOSH_MAXCALC],
02126     double qmEnergy[NOSH_MAXCALC],
02127     double dielEnergy[NOSH_MAXCALC],
02128     int nenergy[NOSH_MAXCALC],
02129     double *atomEnergy[NOSH_MAXCALC],
02130     int nforce[NOSH_MAXCALC],
02131     AtomForce *atomForce[NOSH_MAXCALC]) {
02132
02133     FILE *file;
02134     time_t now;
02135     int ielec, icalc, i, j;
02136     char *timestring = VNULL;
02137     char *c = VNULL;
02138     PBeparm *pbeparm = VNULL;
02139     MGparm *mgparm = VNULL;
02140     double conversion, ltenergy, gtenergy, scalar;
02141
02142     if (nosh->bogus) return 1;
02143
02144     /* Initialize some variables */
02145
02146     icalc = 0;
02147
02148     file = fopen(fname, "w");
02149     if (file == VNULL) {
02150         Vnm_print(2, "writedataXML: Problem opening virtual socket %s\n",
02151             fname);
02152         return 0;
02153     }
02154
02155     fprintf(file, "<?xml version=\"1.0\" encoding=\"UTF-8\"?>\n");
02156     fprintf(file, "<APBS>\n");
02157
02158     /* Strip the newline character from the date */
02159
02160     now = time(VNULL);
02161     timestring = ctime(&now);
02162     for(c = timestring; *c != '\n'; c++);
02163     *c = '\0';
02164     fprintf(file, "    <date>%s</date>\n", timestring);
02165
02166     for (ielec=0; ielec<nosh->nelec; ielec++){ /* elec loop */
02167
02168         /* Initialize per-elec pointers */
02169

```

```

02170     mgparm = nosh->calc[icalc]->mgparm;
02171     pbeparm = nosh->calc[icalc]->pbeparm;
02172
02173     /* Convert from kT/e to kJ/mol */
02174     conversion = Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na;
02175
02176     fprintf(file, "      <elec>\n");
02177     if (Vstring_strcasecmp(nosh->elecname[ielec], "") != 0) {
02178         fprintf(file, "      <name>%s</name>\n", nosh->elecname[ielec]);
02179     }
02180
02181     switch (mgparm->type) {
02182     case MCT_DUMMY:
02183         fprintf(file, "      <type>mg-dummy</type>\n");
02184         break;
02185     case MCT_MANUAL:
02186         fprintf(file, "      <type>mg-manual</type>\n");
02187         break;
02188     case MCT_AUTO:
02189         fprintf(file, "      <type>mg-auto</type>\n");
02190         break;
02191     case MCT_PARALLEL:
02192         fprintf(file, "      <type>mg-para</type>\n");
02193         break;
02194     default:
02195         break;
02196     }
02197
02198     fprintf(file, "      <molid>%d</molid>\n", pbeparm->molid);
02199     fprintf(file, "      <nx>%d</nx>\n", mgparm->dime[0]);
02200     fprintf(file, "      <ny>%d</ny>\n", mgparm->dime[1]);
02201     fprintf(file, "      <nz>%d</nz>\n", mgparm->dime[2]);
02202
02203     switch (pbeparm->pbetype) {
02204     case PBE_NPBE:
02205         fprintf(file, "      <pbe>npbe</pbe>\n");
02206         break;
02207     case PBE_LPBE:
02208         fprintf(file, "      <pbe>lpbe</pbe>\n");
02209         break;
02210     default:
02211         break;
02212     }
02213
02214     if (pbeparm->nion > 0) {
02215         for (i=0; i<pbeparm->nion; i++) {
02216             fprintf(file, "      <ion>\n");
02217             fprintf(file, "      <radius>%4.3f A</radius>\n",
02218                 pbeparm->ionr[i]);
02219             fprintf(file, "      <charge>%4.3f A</charge>\n",
02220                 pbeparm->ionq[i]);
02221             fprintf(file, "      <concentration>%4.3f M</concentration>\n",
02222                 pbeparm->ionc[i]);
02223             fprintf(file, "      </ion>\n");
02224         }
02225     }
02226
02227
02228     fprintf(file, "      <pdie>%4.3f</pdie>\n", pbeparm->pdie);
02229     fprintf(file, "      <sdie>%4.3f</sdie>\n", pbeparm->sdie);
02230
02231     switch (pbeparm->srfrm) {
02232     case 0:
02233         fprintf(file, "      <srfrm>mol</srfrm>\n");
02234         fprintf(file, "      <srad>%4.3f</srad>\n", pbeparm->srad);
02235         break;
02236     case 1:
02237         fprintf(file, "      <srfrm>smol</srfrm>\n");
02238         fprintf(file, "      <srad>%4.3f</srad>\n", pbeparm->srad);
02239         break;
02240     case 2:
02241         fprintf(file, "      <srfrm>spl2</srfrm>\n");
02242         break;
02243     default:
02244         break;
02245     }
02246
02247     switch (pbeparm->bcfl) {
02248     case BCFL_ZERO:
02249         fprintf(file, "      <bcfl>zero</bcfl>\n");
02250         break;

```

```

02251     case BCFL_SDH:
02252         fprintf(file, "        <bcfl>sdh</bcfl>\n");
02253         break;
02254     case BCFL_MDH:
02255         fprintf(file, "        <bcfl>mdh</bcfl>\n");
02256         break;
02257     case BCFL_FOCUS:
02258         fprintf(file, "        <bcfl>focus</bcfl>\n");
02259         break;
02260     case BCFL_MAP:
02261         fprintf(file, "        <bcfl>map</bcfl>\n");
02262         break;
02263     case BCFL_MEM:
02264         fprintf(file, "        <bcfl>mem</bcfl>\n");
02265         break;
02266     default:
02267         break;
02268 }
02269
02270 fprintf(file, "        <temp>%4.3f K</temp>\n", pbeparm->temp);
02271
02272 for (; icalc<=nosh->elec2calc[ielec]; icalc++){ /* calc loop */
02273
02274     /* Reinitialize per-calc pointers */
02275     mgparm = nosh->calc[icalc]->mgparm;
02276     pbeparm = nosh->calc[icalc]->pbeparm;
02277
02278     fprintf(file, "        <calc>\n");
02279     fprintf(file, "        <id>%i</id>\n", (icalc+1));
02280     fprintf(file, "        <hx>%4.3f A</hx>\n", mgparm->grid[0]);
02281     fprintf(file, "        <hy>%4.3f A</hy>\n", mgparm->grid[1]);
02282     fprintf(file, "        <hz>%4.3f A</hz>\n", mgparm->grid[2]);
02283     fprintf(file, "        <xlen>%4.3f A</xlen>\n", mgparm->glen[0]);
02284     fprintf(file, "        <ylen>%4.3f A</ylen>\n", mgparm->glen[1]);
02285     fprintf(file, "        <zlen>%4.3f A</zlen>\n", mgparm->glen[2]);
02286
02287     if (pbeparm->calcenergy == PCE_TOTAL) {
02288         fprintf(file, "        <totEnergy>%1.12E kJ/mol</totEnergy>\n",
02289             (totEnergy[icalc]*conversion));
02290     } else if (pbeparm->calcenergy == PCE_COMPS) {
02291         fprintf(file, "        <totEnergy>%1.12E kJ/mol</totEnergy>\n",
02292             (totEnergy[icalc]*conversion));
02293         fprintf(file, "        <qfEnergy>%1.12E kJ/mol</qfEnergy>\n",
02294             (0.5*qfEnergy[icalc]*conversion));
02295         fprintf(file, "        <qmEnergy>%1.12E kJ/mol</qmEnergy>\n",
02296             (qmEnergy[icalc]*conversion));
02297         fprintf(file, "        <dielEnergy>%1.12E kJ/mol</dielEnergy>\n",
02298             (dielEnergy[icalc]*conversion));
02299         for (i=0; i<nenergy[icalc]; i++){
02300             fprintf(file, "        <atom>\n");
02301             fprintf(file, "            <id>%i</id>\n", i+1);
02302             fprintf(file, "            <energy>%1.12E kJ/mol</energy>\n",
02303                 (0.5*atomEnergy[icalc][i]*conversion));
02304             fprintf(file, "            </atom>\n");
02305         }
02306     }
02307
02308     if (pbeparm->calcforce == PCF_TOTAL) {
02309         fprintf(file, "        <qfforce_x>%1.12E</qfforce_x>\n",
02310             atomForce[icalc][0].qfForce[0]*conversion);
02311         fprintf(file, "        <qfforce_y>%1.12E</qfforce_y>\n",
02312             atomForce[icalc][0].qfForce[1]*conversion);
02313         fprintf(file, "        <qfforce_z>%1.12E</qfforce_z>\n",
02314             atomForce[icalc][0].qfForce[2]*conversion);
02315         fprintf(file, "        <ibforce_x>%1.12E</ibforce_x>\n",
02316             atomForce[icalc][0].ibForce[0]*conversion);
02317         fprintf(file, "        <ibforce_y>%1.12E</ibforce_y>\n",
02318             atomForce[icalc][0].ibForce[1]*conversion);
02319         fprintf(file, "        <ibforce_z>%1.12E</ibforce_z>\n",
02320             atomForce[icalc][0].ibForce[2]*conversion);
02321         fprintf(file, "        <dbforce_x>%1.12E</dbforce_x>\n",
02322             atomForce[icalc][0].dbForce[0]*conversion);
02323         fprintf(file, "        <dbforce_y>%1.12E</dbforce_y>\n",
02324             atomForce[icalc][0].dbForce[1]*conversion);
02325         fprintf(file, "        <dbforce_z>%1.12E</dbforce_z>\n",
02326             atomForce[icalc][0].dbForce[2]*conversion);
02327     }
02328
02329     fprintf(file, "        </calc>\n");
02330 }
02331

```

```

02332
02333     fprintf(file, "    </elec>\n");
02334 }
02335
02336 /* Handle print energy statements */
02337
02338 for (i=0; i<nosh->nprint; i++) {
02339
02340     if (nosh->printwhat[i] == NPT_ENERGY) {
02341
02342         fprintf(file, "    <printEnergy>\n");
02343         fprintf(file, "        <equation>%d", nosh->printcalc[i][0]+1);
02344
02345         for (j=1; j<nosh->printnarg[i]; j++) {
02346             if (nosh->printop[i][j-1] == 0) fprintf(file, " +");
02347             else if (nosh->printop[i][j-1] == 1) fprintf(file, " -");
02348             fprintf(file, " %d", nosh->printcalc[i][j] +1);
02349         }
02350
02351         fprintf(file, " </equation>\n");
02352         icalc = nosh->elec2calc[nosh->printcalc[i][0]];
02353
02354         ltenergy = Vunit_kb * (1e-3) * Vunit_Na * \
02355             nosh->calc[icalc]->pbeparm->temp * totEnergy[icalc];
02356
02357         for (j=1; j<nosh->printnarg[i]; j++) {
02358             icalc = nosh->elec2calc[nosh->printcalc[i][j]];
02359             /* Add or subtract? */
02360             if (nosh->printop[i][j-1] == 0) scalar = 1.0;
02361             else if (nosh->printop[i][j-1] == 1) scalar = -1.0;
02362             /* Accumulate */
02363             ltenergy += (scalar * Vunit_kb * (1e-3) * Vunit_Na * \
02364                 nosh->calc[icalc]->pbeparm->temp * totEnergy[icalc]);
02365         }
02366         Vcom_reduce(com, &ltenergy, &gtenergy, 1, 2, 0);
02367         fprintf(file, "        <localEnergy>%1.12E kJ/mol</localEnergy>\n", \
02368             ltenergy);
02369         fprintf(file, "        <globalEnergy>%1.12E kJ/mol</globalEnergy>\n", \
02370             gtenergy);
02371
02372         fprintf(file, "    </printEnergy>\n");
02373     }
02374 }
02375
02376 /* Add ending tags and close the file */
02377 fprintf(file, "</APBS>\n");
02378 fclose(file);
02379
02380 return 1;
02381 }
02382
02383 VPUBLIC int writedataMG(int rank,
02384                       Nosh *nosh,
02385                       PBeparm *pbeparm,
02386                       Vpmg *pmg)
02387 {
02388
02389     char writestem[VMAX_ARGLEN];
02390     char outpath[VMAX_ARGLEN];
02391     char title[72];
02392     int i,
02393         nx,
02394         ny,
02395         nz,
02396         natoms;
02397     double hx,
02398         hy,
02399         hzed,
02400         xcent,
02401         ycent,
02402         zcent,
02403         xmin,
02404         ymin,
02405         zmin;
02406
02407     Vgrid *grid;
02408     Vio *sock;
02409
02410     if (nosh->bogus) return 1;
02411
02412     for (i=0; i<pbeparm->numwrite; i++) {

```

```

02413
02414     nx = pmg->pmgp->nx;
02415     ny = pmg->pmgp->ny;
02416     nz = pmg->pmgp->nz;
02417     hx = pmg->pmgp->hx;
02418     hy = pmg->pmgp->hy;
02419     hzed = pmg->pmgp->hzed;
02420
02421     switch (pbeparm->writetype[i]) {
02422
02423     case VDT_CHARGE:
02424
02425         Vnm_tprint(1, " Writing charge distribution to ");
02426         xcent = pmg->pmgp->xcent;
02427         ycent = pmg->pmgp->ycent;
02428         zcent = pmg->pmgp->zcent;
02429         xmin = xcent - 0.5*(nx-1)*hx;
02430         ymin = ycent - 0.5*(ny-1)*hy;
02431         zmin = zcent - 0.5*(nz-1)*hzed;
02432         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_CHARGE, 0.0,
02433                               pbeparm->pbetype, pbeparm));
02434         sprintf(title, "CHARGE DISTRIBUTION (e)");
02435         break;
02436
02437     case VDT_POT:
02438
02439         Vnm_tprint(1, " Writing potential to ");
02440         xcent = pmg->pmgp->xcent;
02441         ycent = pmg->pmgp->ycent;
02442         zcent = pmg->pmgp->zcent;
02443         xmin = xcent - 0.5*(nx-1)*hx;
02444         ymin = ycent - 0.5*(ny-1)*hy;
02445         zmin = zcent - 0.5*(nz-1)*hzed;
02446         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_POT, 0.0,
02447                               pbeparm->pbetype, pbeparm));
02448         sprintf(title, "POTENTIAL (kT/e)");
02449         break;
02450
02451     case VDT_SMOL:
02452
02453         Vnm_tprint(1, " Writing molecular accessibility to ");
02454         xcent = pmg->pmgp->xcent;
02455         ycent = pmg->pmgp->ycent;
02456         zcent = pmg->pmgp->zcent;
02457         xmin = xcent - 0.5*(nx-1)*hx;
02458         ymin = ycent - 0.5*(ny-1)*hy;
02459         zmin = zcent - 0.5*(nz-1)*hzed;
02460         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_SMOL,
02461                               pbeparm->srad, pbeparm->pbetype, pbeparm));
02462         sprintf(title,
02463                 "SOLVENT ACCESSIBILITY -- MOLECULAR (%4.3f PROBE)",
02464                 pbeparm->srad);
02465         break;
02466
02467     case VDT_SSPL:
02468
02469         Vnm_tprint(1, " Writing spline-based accessibility to ");
02470         xcent = pmg->pmgp->xcent;
02471         ycent = pmg->pmgp->ycent;
02472         zcent = pmg->pmgp->zcent;
02473         xmin = xcent - 0.5*(nx-1)*hx;
02474         ymin = ycent - 0.5*(ny-1)*hy;
02475         zmin = zcent - 0.5*(nz-1)*hzed;
02476         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_SSPL,
02477                               pbeparm->swin, pbeparm->pbetype, pbeparm));
02478         sprintf(title,
02479                 "SOLVENT ACCESSIBILITY -- SPLINE (%4.3f WINDOW)",
02480                 pbeparm->swin);
02481         break;
02482
02483     case VDT_VDW:
02484
02485         Vnm_tprint(1, " Writing van der Waals accessibility to ");
02486         xcent = pmg->pmgp->xcent;
02487         ycent = pmg->pmgp->ycent;
02488         zcent = pmg->pmgp->zcent;
02489         xmin = xcent - 0.5*(nx-1)*hx;
02490         ymin = ycent - 0.5*(ny-1)*hy;
02491         zmin = zcent - 0.5*(nz-1)*hzed;
02492         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_VDW, 0.0,
02493                               pbeparm->pbetype, pbeparm));

```

```
02494         sprintf(title, "SOLVENT ACCESSIBILITY -- VAN DER WAALS");
02495         break;
02496
02497     case VDT_IVDW:
02498
02499         Vnm_tprint(1, " Writing ion accessibility to ");
02500         xcent = pmg->pmgp->xcent;
02501         ycent = pmg->pmgp->ycent;
02502         zcent = pmg->pmgp->zcent;
02503         xmin = xcent - 0.5*(nx-1)*hx;
02504         ymin = ycent - 0.5*(ny-1)*hy;
02505         zmin = zcent - 0.5*(nz-1)*hzed;
02506         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_IVDW,
02507                                pmg->pbe->maxIonRadius, pbeparm->pbetype, pbeparm));
02508         sprintf(title,
02509                 "ION ACCESSIBILITY -- SPLINE (%4.3f RADIUS)",
02510                 pmg->pbe->maxIonRadius);
02511         break;
02512
02513     case VDT_LAP:
02514
02515         Vnm_tprint(1, " Writing potential Laplacian to ");
02516         xcent = pmg->pmgp->xcent;
02517         ycent = pmg->pmgp->ycent;
02518         zcent = pmg->pmgp->zcent;
02519         xmin = xcent - 0.5*(nx-1)*hx;
02520         ymin = ycent - 0.5*(ny-1)*hy;
02521         zmin = zcent - 0.5*(nz-1)*hzed;
02522         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_LAP, 0.0,
02523                                pbeparm->pbetype, pbeparm));
02524         sprintf(title,
02525                 "POTENTIAL LAPLACIAN (kT/e/A^2)");
02526         break;
02527
02528     case VDT_EDENS:
02529
02530         Vnm_tprint(1, " Writing energy density to ");
02531         xcent = pmg->pmgp->xcent;
02532         ycent = pmg->pmgp->ycent;
02533         zcent = pmg->pmgp->zcent;
02534         xmin = xcent - 0.5*(nx-1)*hx;
02535         ymin = ycent - 0.5*(ny-1)*hy;
02536         zmin = zcent - 0.5*(nz-1)*hzed;
02537         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_EDENS, 0.0,
02538                                pbeparm->pbetype, pbeparm));
02539         sprintf(title, "ENERGY DENSITY (kT/e/A)^2");
02540         break;
02541
02542     case VDT_NDENS:
02543
02544         Vnm_tprint(1, " Writing number density to ");
02545         xcent = pmg->pmgp->xcent;
02546         ycent = pmg->pmgp->ycent;
02547         zcent = pmg->pmgp->zcent;
02548         xmin = xcent - 0.5*(nx-1)*hx;
02549         ymin = ycent - 0.5*(ny-1)*hy;
02550         zmin = zcent - 0.5*(nz-1)*hzed;
02551         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_NDENS, 0.0,
02552                                pbeparm->pbetype, pbeparm));
02553         sprintf(title,
02554                 "ION NUMBER DENSITY (M)");
02555         break;
02556
02557     case VDT_QDENS:
02558
02559         Vnm_tprint(1, " Writing charge density to ");
02560         xcent = pmg->pmgp->xcent;
02561         ycent = pmg->pmgp->ycent;
02562         zcent = pmg->pmgp->zcent;
02563         xmin = xcent - 0.5*(nx-1)*hx;
02564         ymin = ycent - 0.5*(ny-1)*hy;
02565         zmin = zcent - 0.5*(nz-1)*hzed;
02566         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_QDENS, 0.0,
02567                                pbeparm->pbetype, pbeparm));
02568         sprintf(title,
02569                 "ION CHARGE DENSITY (e_c * M)");
02570         break;
02571
02572     case VDT_DIELX:
02573
02574         Vnm_tprint(1, " Writing x-shifted dielectric map to ");
```

```

02575         xcent = pmg->pmgp->xcent + 0.5*hx;
02576         ycent = pmg->pmgp->ycent;
02577         zcent = pmg->pmgp->zcent;
02578         xmin = xcent - 0.5*(nx-1)*hx;
02579         ymin = ycent - 0.5*(ny-1)*hy;
02580         zmin = zcent - 0.5*(nz-1)*hzed;
02581         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_DIELX, 0.0,
02582                                pbeparm->pbetype, pbeparm));
02583         sprintf(title,
02584                  "X-SHIFTED DIELECTRIC MAP");
02585         break;
02586
02587     case VDT_DIELY:
02588
02589         Vnm_tprint(1, " Writing y-shifted dielectric map to ");
02590         xcent = pmg->pmgp->xcent;
02591         ycent = pmg->pmgp->ycent + 0.5*hy;
02592         zcent = pmg->pmgp->zcent;
02593         xmin = xcent - 0.5*(nx-1)*hx;
02594         ymin = ycent - 0.5*(ny-1)*hy;
02595         zmin = zcent - 0.5*(nz-1)*hzed;
02596         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_DIELY, 0.0,
02597                                pbeparm->pbetype, pbeparm));
02598         sprintf(title,
02599                  "Y-SHIFTED DIELECTRIC MAP");
02600         break;
02601
02602     case VDT_DIELZ:
02603
02604         Vnm_tprint(1, " Writing z-shifted dielectric map to ");
02605         xcent = pmg->pmgp->xcent;
02606         ycent = pmg->pmgp->ycent;
02607         zcent = pmg->pmgp->zcent + 0.5*hzed;
02608         xmin = xcent - 0.5*(nx-1)*hx;
02609         ymin = ycent - 0.5*(ny-1)*hy;
02610         zmin = zcent - 0.5*(nz-1)*hzed;
02611         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_DIELZ, 0.0,
02612                                pbeparm->pbetype, pbeparm));
02613         sprintf(title,
02614                  "Z-SHIFTED DIELECTRIC MAP");
02615         break;
02616
02617     case VDT_KAPPA:
02618
02619         Vnm_tprint(1, " Writing kappa map to ");
02620         xcent = pmg->pmgp->xcent;
02621         ycent = pmg->pmgp->ycent;
02622         zcent = pmg->pmgp->zcent;
02623         xmin = xcent - 0.5*(nx-1)*hx;
02624         ymin = ycent - 0.5*(ny-1)*hy;
02625         zmin = zcent - 0.5*(nz-1)*hzed;
02626         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_KAPPA, 0.0,
02627                                pbeparm->pbetype, pbeparm));
02628         sprintf(title,
02629                  "KAPPA MAP");
02630         break;
02631
02632     case VDT_ATOMPOT:
02633
02634         Vnm_tprint(1, " Writing atom potentials to ");
02635         xcent = pmg->pmgp->xcent;
02636         ycent = pmg->pmgp->ycent;
02637         zcent = pmg->pmgp->zcent;
02638         xmin = xcent - 0.5*(nx-1)*hx;
02639         ymin = ycent - 0.5*(ny-1)*hy;
02640         zmin = zcent - 0.5*(nz-1)*hzed;
02641         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_ATOMPOT, 0.0,
02642                                pbeparm->pbetype, pbeparm));
02643         sprintf(title,
02644                  "ATOM POTENTIALS");
02645         break;
02646     default:
02647
02648         Vnm_tprint(2, "Invalid data type for writing!\n");
02649         return 0;
02650     }
02651
02652
02653 #ifdef HAVE_MPI_H
02654     sprintf(writestem, "%s-PE%d", pbeparm->writestem[i], rank);
02655 #else

```



```

02656     if(nosh->ispara){
02657         sprintf(writestem, "%s-PE%d", pbeparm->writestem[i], nosh->proc_rank);
02658     }else{
02659         sprintf(writestem, "%s", pbeparm->writestem[i]);
02660     }
02661 #endif
02662
02663     switch (pbeparm->writefmt[i]) {
02664
02665         case VDF_DX:
02666             sprintf(outpath, "%s.%s", writestem, "dx");
02667             Vnm_tprint(1, "%s\n", outpath);
02668             grid = Vgrid_ctor(nx, ny, nz, hx, hy, hzed, xmin, ymin, zmin,
02669                             pmg->rwork);
02670             Vgrid_writeDX(grid, "FILE", "ASC", VNULL, outpath, title,
02671                          pmg->pvec);
02672             Vgrid_dtor(&grid);
02673             break;
02674
02675         case VDF_DXBIN:
02676             sprintf(outpath, "%s.%s", writestem, "dxbin");
02677             Vnm_tprint(1, "%s\n", outpath);
02678             grid = Vgrid_ctor(nx, ny, nz, hx, hy, hzed, xmin, ymin, zmin,
02679                             pmg->rwork);
02680             //TODO: write Vgrid_writeDXBIN method
02681             Vgrid_writeDXBIN(grid, "FILE", "ASC", VNULL, outpath, title,
02682                             pmg->pvec);
02683             Vgrid_dtor(&grid);
02684             break;
02685
02686         case VDF_AVS:
02687             sprintf(outpath, "%s.%s", writestem, "ucd");
02688             Vnm_tprint(1, "%s\n", outpath);
02689             Vnm_tprint(2, "Sorry, AVS format isn't supported for \
02690 uniform meshes yet!\n");
02691             break;
02692
02693         case VDF_MCSF:
02694             sprintf(outpath, "%s.%s", writestem, "mcsf");
02695             Vnm_tprint(1, "%s\n", outpath);
02696             Vnm_tprint(2, "Sorry, MCSF format isn't supported for \
02697 uniform meshes yet!\n");
02698             break;
02699
02700         case VDF_UHBD:
02701             sprintf(outpath, "%s.%s", writestem, "grd");
02702             Vnm_tprint(1, "%s\n", outpath);
02703             grid = Vgrid_ctor(nx, ny, nz, hx, hy, hzed, xmin, ymin, zmin,
02704                             pmg->rwork);
02705             Vgrid_writeUHBD(grid, "FILE", "ASC", VNULL, outpath, title,
02706                             pmg->pvec);
02707             Vgrid_dtor(&grid);
02708             break;
02709
02710         case VDF_GZ:
02711             sprintf(outpath, "%s.%s", writestem, "dx.gz");
02712             Vnm_tprint(1, "%s\n", outpath);
02713             grid = Vgrid_ctor(nx, ny, nz, hx, hy, hzed, xmin, ymin, zmin,
02714                             pmg->rwork);
02715             Vgrid_writeGZ(grid, "FILE", "ASC", VNULL, outpath, title,
02716                           pmg->pvec);
02717             Vgrid_dtor(&grid);
02718             break;
02719         case VDF_FLAT:
02720             sprintf(outpath, "%s.%s", writestem, "txt");
02721             Vnm_tprint(1, "%s\n", outpath);
02722             Vnm_print(0, "routines: Opening virtual socket...\n");
02723             sock = Vio_ctor("FILE", "ASC", VNULL, outpath, "w");
02724             if (sock == VNULL) {
02725                 Vnm_print(2, "routines: Problem opening virtual socket %s\n",
02726                           outpath);
02727                 return 0;
02728             }
02729             if (Vio_connect(sock, 0) < 0) {
02730                 Vnm_print(2, "routines: Problem connecting virtual socket %s\n",
02731                           outpath);
02732                 return 0;
02733             }
02734             Vio_printf(sock, "# Data from %s\n", PACKAGE_STRING);
02735             Vio_printf(sock, "# \n");
02736             Vio_printf(sock, "# %s\n", title);

```

```

02737         Vio_printf(sock, "# \n");
02738         natoms = pmg->pbe->alist[pbeparm->molid-1].number;
02739         for(i=0;i<natoms;i++)
02740             Vio_printf(sock, "%12.6e\n", pmg->rwork[i]);
02741         break;
02742     default:
02743         Vnm_tprint(2, "Bogus data format (%d)!\n",
02744                 pbeparm->writefmt[i]);
02745         break;
02746     }
02747 }
02748 }
02749
02750 return 1;
02751 }
02752
02753 VPUBLIC double returnEnergy(Vcom *com,
02754                             Nosh *nosh,
02755                             double totEnergy[NOSH_MAXCALC],
02756                             int iprint
02757                             ){
02758
02759     int iarg,
02760         calcid;
02761     double ltenergy,
02762         scalar;
02763
02764     calcid = nosh->elec2calc[nosh->printcalc[iprint][0]];
02765     if (nosh->calc[calcid]->pbeparm->calcenergy != PCE_NO) {
02766         ltenergy = Vunit_kb * (1e-3) * Vunit_Na *
02767             nosh->calc[calcid]->pbeparm->temp * totEnergy[calcid];
02768     } else {
02769         Vnm_tprint( 2, " No energy available in Calculation %d\n", calcid+1);
02770         return 0.0;
02771     }
02772     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++){
02773         calcid = nosh->elec2calc[nosh->printcalc[iprint][iarg]];
02774         /* Add or subtract */
02775         if (nosh->printop[iprint][iarg-1] == 0) scalar = 1.0;
02776         else if (nosh->printop[iprint][iarg-1] == 1) scalar = -1.0;
02777         /* Accumulate */
02778         ltenergy += (scalar * Vunit_kb * (1e-3) * Vunit_Na *
02779                     nosh->calc[calcid]->pbeparm->temp * totEnergy[calcid]);
02780     }
02781
02782     return ltenergy;
02783 }
02784
02785 VPUBLIC int printEnergy(Vcom *com,
02786                       Nosh *nosh,
02787                       double totEnergy[NOSH_MAXCALC],
02788                       int iprint
02789                       ){
02790
02791     int iarg,
02792         calcid;
02793     double ltenergy,
02794         gtenergy,
02795         scalar;
02796
02797     Vnm_tprint( 2, "Warning: The 'energy' print keyword is deprecated.\n" \
02798               "      Use eilecEnergy for electrostatics energy calcs.\n\n");
02799
02800     if (Vstring_strcasecmp(nosh->elecname[nosh->printcalc[iprint][0]], "") == 0){
02801         Vnm_tprint( 1, "print energy %d ", nosh->printcalc[iprint][0]+1);
02802     } else {
02803         Vnm_tprint( 1, "print energy %d (%s) ", nosh->printcalc[iprint][0]+1,
02804                   nosh->elecname[nosh->printcalc[iprint][0]]);
02805     }
02806     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
02807         if (nosh->printop[iprint][iarg-1] == 0)
02808             Vnm_tprint(1, "+ ");
02809         else if (nosh->printop[iprint][iarg-1] == 1)
02810             Vnm_tprint(1, "- ");
02811         else {
02812             Vnm_tprint( 2, "Undefined PRINT operation!\n");
02813             return 0;
02814         }
02815         if (Vstring_strcasecmp(nosh->elecname[nosh->printcalc[iprint][iarg]],
02816                               "") == 0) {
02817             Vnm_tprint( 1, "%d ", nosh->printcalc[iprint][iarg]+1);

```

```

02818         } else {
02819             Vnm_tprint( 1, "%d (%s) ", nosh->printcalc[iprint][iarg]+1,
02820                 nosh->elecname[nosh->printcalc[iprint][iarg]]);
02821         }
02822     }
02823     Vnm_tprint(1, "end\n");
02824     calcid = nosh->elec2calc[nosh->printcalc[iprint][0]];
02825     if (nosh->calc[calcid]->pbeparm->calcenergy != PCE_NO) {
02826         ltenergy = Vunit_kb * (1e-3) * Vunit_Na *
02827             nosh->calc[calcid]->pbeparm->temp * totEnergy[calcid];
02828     } else {
02829         Vnm_tprint( 2, " Didn't calculate energy in Calculation \
02830 #d\n", calcid+1);
02831         return 0;
02832     }
02833     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
02834         calcid = nosh->elec2calc[nosh->printcalc[iprint][iarg]];
02835         /* Add or subtract? */
02836         if (nosh->printop[iprint][iarg-1] == 0) scalar = 1.0;
02837         else if (nosh->printop[iprint][iarg-1] == 1) scalar = -1.0;
02838         /* Accumulate */
02839         ltenergy += (scalar * Vunit_kb * (1e-3) * Vunit_Na *
02840             nosh->calc[calcid]->pbeparm->temp * totEnergy[calcid]);
02841     }
02842
02843     Vnm_tprint( 1, " Local net energy (PE %d) = %1.12E kJ/mol\n",
02844         Vcom_rank(com), ltenergy);
02845     Vnm_tprint( 0, "printEnergy: Performing global reduction (sum)\n");
02846     Vcom_reduce(com, &ltenergy, &gtenergy, 1, 2, 0);
02847     Vnm_tprint( 1, " Global net ELEC energy = %1.12E kJ/mol\n", gtenery);
02848
02849     return 1;
02850 }
02851
02852
02853 VPUBLIC int printElecEnergy(Vcom *com,
02854     Nosh *nosh,
02855     double totEnergy[NOSH_MAXCALC],
02856     int iprint
02857 ) {
02858
02859     int iarg,
02860         calcid;
02861     double ltenergy,
02862         gtenergy,
02863         scalar;
02864
02865     if (Vstring_strcasecmp(nosh->elecname[nosh->printcalc[iprint][0]], "") == 0) {
02866         Vnm_tprint( 1, "\nprint energy %d ", nosh->printcalc[iprint][0]+1);
02867     } else {
02868         Vnm_tprint( 1, "\nprint energy %d (%s) ", nosh->printcalc[iprint][0]+1,
02869             nosh->elecname[nosh->printcalc[iprint][0]]);
02870     }
02871     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
02872         if (nosh->printop[iprint][iarg-1] == 0)
02873             Vnm_tprint(1, "+ ");
02874         else if (nosh->printop[iprint][iarg-1] == 1)
02875             Vnm_tprint(1, "- ");
02876         else {
02877             Vnm_tprint( 2, "Undefined PRINT operation!\n");
02878             return 0;
02879         }
02880         if (Vstring_strcasecmp(nosh->elecname[nosh->printcalc[iprint][iarg]],
02881             "") == 0) {
02882             Vnm_tprint( 1, "%d ", nosh->printcalc[iprint][iarg]+1);
02883         } else {
02884             Vnm_tprint( 1, "%d (%s) ", nosh->printcalc[iprint][iarg]+1,
02885                 nosh->elecname[nosh->printcalc[iprint][iarg]]);
02886         }
02887     }
02888     Vnm_tprint(1, "end\n");
02889     calcid = nosh->elec2calc[nosh->printcalc[iprint][0]];
02890     if (nosh->calc[calcid]->pbeparm->calcenergy != PCE_NO) {
02891         ltenergy = Vunit_kb * (1e-3) * Vunit_Na *
02892             nosh->calc[calcid]->pbeparm->temp * totEnergy[calcid];
02893     } else {
02894         Vnm_tprint( 2, " Didn't calculate energy in Calculation \
02895 #d\n", calcid+1);
02896         return 0;
02897     }
02898     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {

```

```

02899         calcid = nosh->elec2calc[nosh->printcalc[iprint][iarg]];
02900         /* Add or subtract? */
02901         if (nosh->printop[iprint][iarg-1] == 0) scalar = 1.0;
02902         else if (nosh->printop[iprint][iarg-1] == 1) scalar = -1.0;
02903         /* Accumulate */
02904         ltenergy += (scalar * Vunit_kb * (1e-3) * Vunit_Na *
02905                     nosh->calc[calcid]->pbeparm->temp * totEnergy[calcid]);
02906     }
02907
02908     Vnm_tprint( 1, " Local net energy (PE %d) = %1.12E kJ/mol\n",
02909                Vcom_rank(com), ltenergy);
02910     Vnm_tprint( 0, "printEnergy: Performing global reduction (sum)\n");
02911     Vcom_reduce(com, &ltenergy, &gtenergy, 1, 2, 0);
02912     Vnm_tprint( 1, " Global net ELEC energy = %1.12E kJ/mol\n", gtenery);
02913
02914     return 1;
02915 }
02916
02917
02918 VPUBLIC int printApolEnergy(NOsh *nosh,
02919                            int iprint
02920                            ) {
02921
02922     int iarg,
02923         calcid;
02924     double gtenergy,
02925         scalar;
02926     APOLparm *apolparm = VNULL;
02927
02928     if (Vstring_strcasecmp(nosh->apolname[nosh->printcalc[iprint][0]], "") == 0){
02929         Vnm_tprint( 1, "\nprint APOL energy %d ", nosh->printcalc[iprint][0]+1);
02930     } else {
02931         Vnm_tprint( 1, "\nprint APOL energy %d (%s) ", nosh->printcalc[iprint][0]+1,
02932                    nosh->apolname[nosh->printcalc[iprint][0]]);
02933     }
02934     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
02935         if (nosh->printop[iprint][iarg-1] == 0)
02936             Vnm_tprint(1, "+ ");
02937         else if (nosh->printop[iprint][iarg-1] == 1)
02938             Vnm_tprint(1, "- ");
02939         else {
02940             Vnm_tprint( 2, "Undefined PRINT operation!\n");
02941             return 0;
02942         }
02943         if (Vstring_strcasecmp(nosh->apolname[nosh->printcalc[iprint][iarg]],
02944                               "") == 0) {
02945             Vnm_tprint( 1, "%d ", nosh->printcalc[iprint][iarg]+1);
02946         } else {
02947             Vnm_tprint( 1, "%d (%s) ", nosh->printcalc[iprint][iarg]+1,
02948                        nosh->apolname[nosh->printcalc[iprint][iarg]]);
02949         }
02950     }
02951     Vnm_tprint(1, "end\n");
02952
02953     calcid = nosh->apol2calc[nosh->printcalc[iprint][0]];
02954     apolparm = nosh->calc[calcid]->apolparm;
02955
02956     if (apolparm->calcenergy == ACE_TOTAL) {
02957         gtenergy = ((apolparm->gamma*apolparm->sasa) + (apolparm->press*apolparm->sav) +
02958                    (apolparm->wcaEnergy));
02959     } else {
02960         Vnm_tprint( 2, " Didn't calculate energy in Calculation #%d\n", calcid+1);
02961         return 0;
02962     }
02963     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
02964         calcid = nosh->apol2calc[nosh->printcalc[iprint][iarg]];
02965         apolparm = nosh->calc[calcid]->apolparm;
02966
02967         /* Add or subtract? */
02968         if (nosh->printop[iprint][iarg-1] == 0) scalar = 1.0;
02969         else if (nosh->printop[iprint][iarg-1] == 1) scalar = -1.0;
02970         /* Accumulate */
02971         gtenergy += (scalar * ((apolparm->gamma*apolparm->sasa) +
02972                                (apolparm->press*apolparm->sav) +
02973                                (apolparm->wcaEnergy)));
02974     }
02975
02976     Vnm_tprint( 1, " Global net APOL energy = %1.12E kJ/mol\n", gtenergy);
02977     return 1;
02978 }

```

```

02979
02980 VPUBLIC int printForce(Vcom *com,
02981                       Nosh *nosh,
02982                       int nforce[NOSH_MAXCALC],
02983                       AtomForce *atomForce[NOSH_MAXCALC],
02984                       int iprint
02985                       ) {
02986
02987     int iarg,
02988         ifr,
02989         ivc,
02990         calcid,
02991         refnforce,
02992         refcalcforce;
02993     double temp,
02994         scalar,
02995         totforce[3];
02996     AtomForce *lforce,
02997         *gforce,
02998         *aforce;
02999
03000     Vnm_tprint( 2, "Warning: The 'force' print keyword is deprecated.\n" \
03001               "           Use elecForce for electrostatics force calcs.\n\n");
03002
03003     if (Vstring_strcasecmp(nosh->elecname[nosh->printcalc[iprint][0]], "") == 0){
03004         Vnm_tprint( 1, "print force %d ", nosh->printcalc[iprint][0]+1);
03005     } else {
03006         Vnm_tprint( 1, "print force %d (%s) ", nosh->printcalc[iprint][0]+1,
03007                   nosh->elecname[nosh->printcalc[iprint][0]]);
03008     }
03009     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
03010         if (nosh->printtop[iprint][iarg-1] == 0)
03011             Vnm_tprint(1, "+ ");
03012         else if (nosh->printtop[iprint][iarg-1] == 1)
03013             Vnm_tprint(1, "- ");
03014         else {
03015             Vnm_tprint( 2, "Undefined PRINT operation!\n");
03016             return 0;
03017         }
03018         if (Vstring_strcasecmp(nosh->elecname[nosh->printcalc[iprint][iarg]],
03019                               "") == 0) {
03020             Vnm_tprint( 1, "%d ", nosh->printcalc[iprint][iarg]+1);
03021         } else {
03022             Vnm_tprint( 1, "%d (%s) ", nosh->printcalc[iprint][iarg]+1,
03023                       nosh->elecname[nosh->printcalc[iprint][iarg]]);
03024         }
03025     }
03026     Vnm_tprint(1, "end\n");
03027
03028     /* First, go through and make sure we did the same type of force
03029      * evaluation in each of the requested calculations */
03030     calcid = nosh->elec2calc[nosh->printcalc[iprint][0]];
03031     refnforce = nforce[calcid];
03032     refcalcforce = nosh->calc[calcid]->pbeparm->calcforce;
03033     if (refcalcforce == PCF_NO) {
03034         Vnm_tprint( 2, " Didn't calculate force in calculation \
03035 #d\n", calcid+1);
03036         return 0;
03037     }
03038     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
03039         calcid = nosh->elec2calc[nosh->printcalc[iprint][iarg]-1];
03040         if (nosh->calc[calcid]->pbeparm->calcforce != refcalcforce) {
03041             Vnm_tprint(2, " Inconsistent calcforce declarations in \
03042 calculations %d and %d\n", nosh->elec2calc[nosh->printcalc[iprint][0]]+1,
03043                       calcid+1);
03044             return 0;
03045         }
03046         if (nforce[calcid] != refnforce) {
03047             Vnm_tprint(2, " Inconsistent number of forces evaluated in \
03048 calculations %d and %d\n", nosh->elec2calc[nosh->printcalc[iprint][0]]+1,
03049                       calcid+1);
03050             return 0;
03051         }
03052     }
03053
03054     /* Now, allocate space to accumulate the forces */
03055     lforce = (AtomForce *)Vmem_malloc(VNULL, refnforce, sizeof(AtomForce));
03056     gforce = (AtomForce *)Vmem_malloc(VNULL, refnforce, sizeof(AtomForce));
03057
03058     /* Now, accumulate the forces */
03059     calcid = nosh->elec2calc[nosh->printcalc[iprint][0]];

```

```

03060     aforce = atomForce[calcid];
03061     temp = nosh->calc[calcid]->pbeparm->temp;
03062
03063     /* Load up the first calculation */
03064     if (refcalcforce == PCF_TOTAL) {
03065         /* Set to total force */
03066         for (ivc=0; ivc<3; ivc++) {
03067             lforce[0].qfForce[ivc] =
03068                 Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].qfForce[ivc];
03069             lforce[0].ibForce[ivc] =
03070                 Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].ibForce[ivc];
03071             lforce[0].dbForce[ivc] =
03072                 Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].dbForce[ivc];
03073         }
03074     } else if (refcalcforce == PCF_COMPS) {
03075         for (ifr=0; ifr<refnforce; ifr++) {
03076             for (ivc=0; ivc<3; ivc++) {
03077                 lforce[ifr].qfForce[ivc] =
03078                     Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].qfForce[ivc];
03079                 lforce[ifr].ibForce[ivc] =
03080                     Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].ibForce[ivc];
03081                 lforce[ifr].dbForce[ivc] =
03082                     Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].dbForce[ivc];
03083             }
03084         }
03085     }
03086
03087     /* Load up the rest of the calculations */
03088     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
03089         calcid = nosh->elec2calc[nosh->printcalc[iprint][iarg]];
03090         temp = nosh->calc[calcid]->pbeparm->temp;
03091         aforce = atomForce[calcid];
03092         /* Get operation */
03093         if (nosh->printop[iprint][iarg-1] == 0) scalar = +1.0;
03094         else if (nosh->printop[iprint][iarg-1] == 1) scalar = -1.0;
03095         else scalar = 0.0;
03096         /* Accumulate */
03097         if (refcalcforce == PCF_TOTAL) {
03098             /* Set to total force */
03099             for (ivc=0; ivc<3; ivc++) {
03100                 lforce[0].qfForce[ivc] +=
03101                     (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].qfForce[ivc]);
03102                 lforce[0].ibForce[ivc] +=
03103                     (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].ibForce[ivc]);
03104                 lforce[0].dbForce[ivc] +=
03105                     (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].dbForce[ivc]);
03106             }
03107         } else if (refcalcforce == PCF_COMPS) {
03108             for (ifr=0; ifr<refnforce; ifr++) {
03109                 for (ivc=0; ivc<3; ivc++) {
03110                     lforce[ifr].qfForce[ivc] +=
03111                         (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].qfForce[ivc]);
03112                     lforce[ifr].ibForce[ivc] +=
03113                         (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].ibForce[ivc]);
03114                     lforce[ifr].dbForce[ivc] +=
03115                         (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].dbForce[ivc]);
03116                 }
03117             }
03118         }
03119     }
03120
03121     Vnm_tprint( 0, "printEnergy: Performing global reduction (sum)\n");
03122     for (ifr=0; ifr<refnforce; ifr++) {
03123         Vcom_reduce(com, lforce[ifr].qfForce, gforce[ifr].qfForce, 3, 2, 0);
03124         Vcom_reduce(com, lforce[ifr].ibForce, gforce[ifr].ibForce, 3, 2, 0);
03125         Vcom_reduce(com, lforce[ifr].dbForce, gforce[ifr].dbForce, 3, 2, 0);
03126     }
03127
03128     #if 0
03129     if (refcalcforce == PCF_TOTAL) {
03130         Vnm_tprint( 1, " Local net fixed charge force = \
03131 (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", lforce[0].qfForce[0],
03132 lforce[0].qfForce[1], lforce[0].qfForce[2]);
03133         Vnm_tprint( 1, " Local net ionic boundary force = \
03134 (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", lforce[0].ibForce[0],
03135 lforce[0].ibForce[1], lforce[0].ibForce[2]);
03136         Vnm_tprint( 1, " Local net dielectric boundary force = \
03137 (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", lforce[0].dbForce[0],
03138 lforce[0].dbForce[1], lforce[0].dbForce[2]);
03139     } else if (refcalcforce == PCF_COMPS) {
03140         for (ifr=0; ifr<refnforce; ifr++) {

```

```

03141         Vnm_tprint( 1, " Local fixed charge force \
03142 (atom %d) = (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", ifr, lforce[ifr].qfForce[0],
03143                 lforce[ifr].qfForce[1], lforce[ifr].qfForce[2]);
03144         Vnm_tprint( 1, " Local ionic boundary force \
03145 (atom %d) = (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", ifr, lforce[ifr].ibForce[0],
03146                 lforce[ifr].ibForce[1], lforce[ifr].ibForce[2]);
03147         Vnm_tprint( 1, " Local dielectric boundary force \
03148 (atom %d) = (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", ifr, lforce[ifr].dbForce[0],
03149                 lforce[ifr].dbForce[1], lforce[ifr].dbForce[2]);
03150     }
03151 }
03152 #endif
03153
03154 if (refcalcfrc == PCF_TOTAL) {
03155     Vnm_tprint( 1, " Printing net forces (kJ/mol/A).\n");
03156     Vnm_tprint( 1, " Legend:\n");
03157     Vnm_tprint( 1, " tot -- Total force\n");
03158     Vnm_tprint( 1, " qf -- Fixed charge force\n");
03159     Vnm_tprint( 1, " db -- Dielectric boundary force\n");
03160     Vnm_tprint( 1, " ib -- Ionic boundary force\n");
03161
03162     for (ivc=0; ivc<3; ivc++) {
03163         totforce[ivc] =
03164             gforce[0].qfForce[ivc] + gforce[0].ibForce[ivc] \
03165             + gforce[0].dbForce[ivc];
03166     }
03167
03168     Vnm_tprint( 1, " tot %1.12E %1.12E %1.12E\n", totforce[0],
03169                 totforce[1], totforce[2]);
03170     Vnm_tprint( 1, " qf %1.12E %1.12E %1.12E\n", gforce[0].qfForce[0],
03171                 gforce[0].qfForce[1], gforce[0].qfForce[2]);
03172     Vnm_tprint( 1, " ib %1.12E %1.12E %1.12E\n", gforce[0].ibForce[0],
03173                 gforce[0].ibForce[1], gforce[0].ibForce[2]);
03174     Vnm_tprint( 1, " db %1.12E %1.12E %1.12E\n", gforce[0].dbForce[0],
03175                 gforce[0].dbForce[1], gforce[0].dbForce[2]);
03176
03177 } else if (refcalcfrc == PCF_COMPS) {
03178
03179     Vnm_tprint( 1, " Printing per-atom forces (kJ/mol/A).\n");
03180     Vnm_tprint( 1, " Legend:\n");
03181     Vnm_tprint( 1, " tot n -- Total force for atom n\n");
03182     Vnm_tprint( 1, " qf n -- Fixed charge force for atom n\n");
03183     Vnm_tprint( 1, " db n -- Dielectric boundary force for atom n\n");
03184     Vnm_tprint( 1, " ib n -- Ionic boundary force for atom n\n");
03185     Vnm_tprint( 1, " tot all -- Total force for system\n");
03186
03187     totforce[0] = 0.0;
03188     totforce[1] = 0.0;
03189     totforce[2] = 0.0;
03190
03191     for (ifr=0; ifr<refnforce; ifr++) {
03192         Vnm_tprint( 1, " qf %d %1.12E %1.12E %1.12E\n", ifr,
03193                 gforce[ifr].qfForce[0], gforce[ifr].qfForce[1],
03194                 gforce[ifr].qfForce[2]);
03195         Vnm_tprint( 1, " ib %d %1.12E %1.12E %1.12E\n", ifr,
03196                 gforce[ifr].ibForce[0], gforce[ifr].ibForce[1],
03197                 gforce[ifr].ibForce[2]);
03198         Vnm_tprint( 1, " db %d %1.12E %1.12E %1.12E\n", ifr,
03199                 gforce[ifr].dbForce[0], gforce[ifr].dbForce[1],
03200                 gforce[ifr].dbForce[2]);
03201         Vnm_tprint( 1, " tot %d %1.12E %1.12E %1.12E\n", ifr,
03202                 (gforce[ifr].dbForce[0] \
03203                  + gforce[ifr].ibForce[0] +
03204                  gforce[ifr].qfForce[0]),
03205                 (gforce[ifr].dbForce[1] \
03206                  + gforce[ifr].ibForce[1] +
03207                  gforce[ifr].qfForce[1]),
03208                 (gforce[ifr].dbForce[2] \
03209                  + gforce[ifr].ibForce[2] +
03210                  gforce[ifr].qfForce[2]));
03211         for (ivc=0; ivc<3; ivc++) {
03212             totforce[ivc] += (gforce[ifr].dbForce[ivc] \
03213                             + gforce[ifr].ibForce[ivc] \
03214                             + gforce[ifr].qfForce[ivc]);
03215         }
03216     }
03217     Vnm_tprint( 1, " tot all %1.12E %1.12E %1.12E\n", totforce[0],
03218                 totforce[1], totforce[2]);
03219 }
03220
03221 Vmem_free(VNULL, refnforce, sizeof(AtomForce), (void **>(&lforce));

```

```

03222     Vmem_free(VNULL, refnforce, sizeof(AtomForce), (void **>(&gforce));
03223
03224     return 1;
03225 }
03226 }
03227
03228 VPUBLIC int printElecForce(Vcom *com,
03229                          Nosh *nosh,
03230                          int nforce[NOSH_MAXCALC],
03231                          AtomForce *atomForce[NOSH_MAXCALC],
03232                          int iprint
03233                          ) {
03234
03235     int iarg,
03236         ifr,
03237         ivc,
03238         calcid,
03239         refnforce,
03240         refcalcforce;
03241     double temp,
03242         scalar,
03243         totforce[3];
03244     AtomForce *lforce, *gforce, *aforce;
03245
03246     if (Vstring_strcasecmp(nosh->elecname[nosh->printcalc[iprint][0]], "") == 0){
03247         Vnm_tprint( 1, "print force %d ", nosh->printcalc[iprint][0]+1);
03248     } else {
03249         Vnm_tprint( 1, "print force %d (%s) ", nosh->printcalc[iprint][0]+1,
03250                     nosh->elecname[nosh->printcalc[iprint][0]]);
03251     }
03252     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
03253         if (nosh->printop[iprint][iarg-1] == 0)
03254             Vnm_tprint(1, "+ ");
03255         else if (nosh->printop[iprint][iarg-1] == 1)
03256             Vnm_tprint(1, "- ");
03257         else {
03258             Vnm_tprint( 2, "Undefined PRINT operation!\n");
03259             return 0;
03260         }
03261         if (Vstring_strcasecmp(nosh->elecname[nosh->printcalc[iprint][iarg]],
03262                               "") == 0) {
03263             Vnm_tprint( 1, "%d ", nosh->printcalc[iprint][iarg]+1);
03264         } else {
03265             Vnm_tprint( 1, "%d (%s) ", nosh->printcalc[iprint][iarg]+1,
03266                         nosh->elecname[nosh->printcalc[iprint][iarg]]);
03267         }
03268     }
03269     Vnm_tprint(1, "end\n");
03270
03271     /* First, go through and make sure we did the same type of force
03272      * evaluation in each of the requested calculations */
03273     calcid = nosh->elec2calc[nosh->printcalc[iprint][0]];
03274     refnforce = nforce[calcid];
03275     refcalcforce = nosh->calc[calcid]->pbeparm->calcforce;
03276     if (refcalcforce == PCF_NO) {
03277         Vnm_tprint( 2, " Didn't calculate force in calculation \
03278 #d\n", calcid+1);
03279         return 0;
03280     }
03281     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
03282         calcid = nosh->elec2calc[nosh->printcalc[iprint][iarg]-1];
03283         if (nosh->calc[calcid]->pbeparm->calcforce != refcalcforce) {
03284             Vnm_tprint(2, " Inconsistent calcforce declarations in \
03285 calculations %d and %d\n", nosh->elec2calc[nosh->printcalc[iprint][0]]+1,
03286                         calcid+1);
03287             return 0;
03288         }
03289         if (nforce[calcid] != refnforce) {
03290             Vnm_tprint(2, " Inconsistent number of forces evaluated in \
03291 calculations %d and %d\n", nosh->elec2calc[nosh->printcalc[iprint][0]]+1,
03292                         calcid+1);
03293             return 0;
03294         }
03295     }
03296
03297     /* Now, allocate space to accumulate the forces */
03298     lforce = (AtomForce *)Vmem_malloc(VNULL, refnforce, sizeof(AtomForce));
03299     gforce = (AtomForce *)Vmem_malloc(VNULL, refnforce, sizeof(AtomForce));
03300
03301     /* Now, accumulate the forces */
03302     calcid = nosh->elec2calc[nosh->printcalc[iprint][0]];

```



```

03303     aforce = atomForce[calcid];
03304     temp = nosh->calc[calcid]->pbeparm->temp;
03305
03306     /* Load up the first calculation */
03307     if (refcalcforce == PCF_TOTAL) {
03308         /* Set to total force */
03309         for (ivc=0; ivc<3; ivc++) {
03310             lforce[0].qfForce[ivc] =
03311                 Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].qfForce[ivc];
03312             lforce[0].ibForce[ivc] =
03313                 Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].ibForce[ivc];
03314             lforce[0].dbForce[ivc] =
03315                 Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].dbForce[ivc];
03316         }
03317     } else if (refcalcforce == PCF_COMPS) {
03318         for (ifr=0; ifr<refnforce; ifr++) {
03319             for (ivc=0; ivc<3; ivc++) {
03320                 lforce[ifr].qfForce[ivc] =
03321                     Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].qfForce[ivc];
03322                 lforce[ifr].ibForce[ivc] =
03323                     Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].ibForce[ivc];
03324                 lforce[ifr].dbForce[ivc] =
03325                     Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].dbForce[ivc];
03326             }
03327         }
03328     }
03329
03330     /* Load up the rest of the calculations */
03331     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
03332         calcid = nosh->elec2calc[nosh->printcalc[iprint][iarg]];
03333         temp = nosh->calc[calcid]->pbeparm->temp;
03334         aforce = atomForce[calcid];
03335         /* Get operation */
03336         if (nosh->printop[iprint][iarg-1] == 0) scalar = +1.0;
03337         else if (nosh->printop[iprint][iarg-1] == 1) scalar = -1.0;
03338         else scalar = 0.0;
03339         /* Accumulate */
03340         if (refcalcforce == PCF_TOTAL) {
03341             /* Set to total force */
03342             for (ivc=0; ivc<3; ivc++) {
03343                 lforce[0].qfForce[ivc] +=
03344                     (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].qfForce[ivc]);
03345                 lforce[0].ibForce[ivc] +=
03346                     (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].ibForce[ivc]);
03347                 lforce[0].dbForce[ivc] +=
03348                     (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].dbForce[ivc]);
03349             }
03350         } else if (refcalcforce == PCF_COMPS) {
03351             for (ifr=0; ifr<refnforce; ifr++) {
03352                 for (ivc=0; ivc<3; ivc++) {
03353                     lforce[ifr].qfForce[ivc] +=
03354                         (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].qfForce[ivc]);
03355                     lforce[ifr].ibForce[ivc] +=
03356                         (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].ibForce[ivc]);
03357                     lforce[ifr].dbForce[ivc] +=
03358                         (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].dbForce[ivc]);
03359                 }
03360             }
03361         }
03362     }
03363
03364     Vnm_tprint( 0, "printEnergy: Performing global reduction (sum)\n");
03365     for (ifr=0; ifr<refnforce; ifr++) {
03366         Vcom_reduce(com, lforce[ifr].qfForce, gforce[ifr].qfForce, 3, 2, 0);
03367         Vcom_reduce(com, lforce[ifr].ibForce, gforce[ifr].ibForce, 3, 2, 0);
03368         Vcom_reduce(com, lforce[ifr].dbForce, gforce[ifr].dbForce, 3, 2, 0);
03369     }
03370
03371     #if 0
03372     if (refcalcforce == PCF_TOTAL) {
03373         Vnm_tprint( 1, " Local net fixed charge force = \
03374 (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", lforce[0].qfForce[0],
03375             lforce[0].qfForce[1], lforce[0].qfForce[2]);
03376         Vnm_tprint( 1, " Local net ionic boundary force = \
03377 (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", lforce[0].ibForce[0],
03378             lforce[0].ibForce[1], lforce[0].ibForce[2]);
03379         Vnm_tprint( 1, " Local net dielectric boundary force = \
03380 (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", lforce[0].dbForce[0],
03381             lforce[0].dbForce[1], lforce[0].dbForce[2]);
03382     } else if (refcalcforce == PCF_COMPS) {
03383         for (ifr=0; ifr<refnforce; ifr++) {

```

```

03384         Vnm_tprint( 1, " Local fixed charge force \
03385 (atom %d) = (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", ifr, lforce[ifr].qfForce[0],
03386                 lforce[ifr].qfForce[1], lforce[ifr].qfForce[2]);
03387         Vnm_tprint( 1, " Local ionic boundary force \
03388 (atom %d) = (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", ifr, lforce[ifr].ibForce[0],
03389                 lforce[ifr].ibForce[1], lforce[ifr].ibForce[2]);
03390         Vnm_tprint( 1, " Local dielectric boundary force \
03391 (atom %d) = (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", ifr, lforce[ifr].dbForce[0],
03392                 lforce[ifr].dbForce[1], lforce[ifr].dbForce[2]);
03393     }
03394 }
03395 #endif
03396
03397 if (refcalcforce == PCF_TOTAL) {
03398     Vnm_tprint( 1, " Printing net forces (kJ/mol/A).\n");
03399     Vnm_tprint( 1, " Legend:\n");
03400     Vnm_tprint( 1, " tot -- Total force\n");
03401     Vnm_tprint( 1, " qf -- Fixed charge force\n");
03402     Vnm_tprint( 1, " db -- Dielectric boundary force\n");
03403     Vnm_tprint( 1, " ib -- Ionic boundary force\n");
03404
03405     for (ivc=0; ivc<3; ivc++) {
03406         totforce[ivc] =
03407             gforce[0].qfForce[ivc] + gforce[0].ibForce[ivc] \
03408             + gforce[0].dbForce[ivc];
03409     }
03410
03411     Vnm_tprint( 1, " tot %1.12E %1.12E %1.12E\n", totforce[0],
03412                 totforce[1], totforce[2]);
03413     Vnm_tprint( 1, " qf %1.12E %1.12E %1.12E\n", gforce[0].qfForce[0],
03414                 gforce[0].qfForce[1], gforce[0].qfForce[2]);
03415     Vnm_tprint( 1, " ib %1.12E %1.12E %1.12E\n", gforce[0].ibForce[0],
03416                 gforce[0].ibForce[1], gforce[0].ibForce[2]);
03417     Vnm_tprint( 1, " db %1.12E %1.12E %1.12E\n", gforce[0].dbForce[0],
03418                 gforce[0].dbForce[1], gforce[0].dbForce[2]);
03419
03420 } else if (refcalcforce == PCF_COMPS) {
03421
03422     Vnm_tprint( 1, " Printing per-atom forces (kJ/mol/A).\n");
03423     Vnm_tprint( 1, " Legend:\n");
03424     Vnm_tprint( 1, " tot n -- Total force for atom n\n");
03425     Vnm_tprint( 1, " qf n -- Fixed charge force for atom n\n");
03426     Vnm_tprint( 1, " db n -- Dielectric boundary force for atom n\n");
03427     Vnm_tprint( 1, " ib n -- Ionic boundary force for atom n\n");
03428     Vnm_tprint( 1, " tot all -- Total force for system\n");
03429
03430     totforce[0] = 0.0;
03431     totforce[1] = 0.0;
03432     totforce[2] = 0.0;
03433
03434     for (ifr=0; ifr<refnforce; ifr++) {
03435         Vnm_tprint( 1, " qf %d %1.12E %1.12E %1.12E\n", ifr,
03436                 gforce[ifr].qfForce[0], gforce[ifr].qfForce[1],
03437                 gforce[ifr].qfForce[2]);
03438         Vnm_tprint( 1, " ib %d %1.12E %1.12E %1.12E\n", ifr,
03439                 gforce[ifr].ibForce[0], gforce[ifr].ibForce[1],
03440                 gforce[ifr].ibForce[2]);
03441         Vnm_tprint( 1, " db %d %1.12E %1.12E %1.12E\n", ifr,
03442                 gforce[ifr].dbForce[0], gforce[ifr].dbForce[1],
03443                 gforce[ifr].dbForce[2]);
03444         Vnm_tprint( 1, " tot %d %1.12E %1.12E %1.12E\n", ifr,
03445                 (gforce[ifr].dbForce[0] \
03446                  + gforce[ifr].ibForce[0] +
03447                  gforce[ifr].qfForce[0]),
03448                 (gforce[ifr].dbForce[1] \
03449                  + gforce[ifr].ibForce[1] +
03450                  gforce[ifr].qfForce[1]),
03451                 (gforce[ifr].dbForce[2] \
03452                  + gforce[ifr].ibForce[2] +
03453                  gforce[ifr].qfForce[2]));
03454         for (ivc=0; ivc<3; ivc++) {
03455             totforce[ivc] += (gforce[ifr].dbForce[ivc] \
03456                             + gforce[ifr].ibForce[ivc] \
03457                             + gforce[ifr].qfForce[ivc]);
03458         }
03459     }
03460     Vnm_tprint( 1, " tot all %1.12E %1.12E %1.12E\n", totforce[0],
03461                 totforce[1], totforce[2]);
03462 }
03463
03464 Vmem_free(VNULL, refnforce, sizeof(AtomForce), (void **>(&lforce));

```

```

03465     Vmem_free(VNULL, refnforce, sizeof(AtomForce), (void **)(&gforce));
03466
03467     return 1;
03468 }
03469 }
03470
03471 VPUBLIC int printApolForce(Vcom *com,
03472                          Nosh *nosh,
03473                          int nforce[NOSH_MAXCALC],
03474                          AtomForce *atomForce[NOSH_MAXCALC],
03475                          int iprint
03476                          ) {
03477
03478     int iarg,
03479         ifr,
03480         ivc,
03481         calcid,
03482         refnforce,
03483         refcalcforce;
03484     double temp,
03485         scalar,
03486         totforce[3];
03487     AtomForce *lforce,
03488         *gforce,
03489         *aforce;
03490
03491     if (Vstring_strcasecmp(nosh->apolname[nosh->printcalc[iprint][0]], "") == 0){
03492         Vnm_tprint( 1, "\nprint APOL force %d ", nosh->printcalc[iprint][0]+1);
03493     } else {
03494         Vnm_tprint( 1, "\nprint APOL force %d (%s) ", nosh->printcalc[iprint][0]+1,
03495                   nosh->apolname[nosh->printcalc[iprint][0]]);
03496     }
03497     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
03498         if (nosh->printop[iprint][iarg-1] == 0)
03499             Vnm_tprint(1, "+ ");
03500         else if (nosh->printop[iprint][iarg-1] == 1)
03501             Vnm_tprint(1, "- ");
03502         else {
03503             Vnm_tprint( 2, "Undefined PRINT operation!\n");
03504             return 0;
03505         }
03506         if (Vstring_strcasecmp(nosh->apolname[nosh->printcalc[iprint][iarg]],
03507                               "") == 0) {
03508             Vnm_tprint( 1, "%d ", nosh->printcalc[iprint][iarg]+1);
03509         } else {
03510             Vnm_tprint( 1, "%d (%s) ", nosh->printcalc[iprint][iarg]+1,
03511                       nosh->apolname[nosh->printcalc[iprint][iarg]]);
03512         }
03513     }
03514     Vnm_tprint(1, "end\n");
03515
03516     /* First, go through and make sure we did the same type of force
03517      * evaluation in each of the requested calculations */
03518     calcid = nosh->apol2calc[nosh->printcalc[iprint][0]];
03519     refnforce = nforce[calcid];
03520     refcalcforce = nosh->calc[calcid]->apolparm->calcforce;
03521     if (refcalcforce == ACF_NO) {
03522         Vnm_tprint( 2, " Didn't calculate force in calculation \
03523         %#d\n", calcid+1);
03524         return 0;
03525     }
03526     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
03527         calcid = nosh->apol2calc[nosh->printcalc[iprint][iarg]-1];
03528         if (nosh->calc[calcid]->apolparm->calcforce != refcalcforce) {
03529             Vnm_tprint(2, " Inconsistent calcforce declarations in \
03530             calculations %d and %d\n", nosh->apol2calc[nosh->printcalc[iprint][0]]+1,
03531                       calcid+1);
03532             return 0;
03533         }
03534         if (nforce[calcid] != refnforce) {
03535             Vnm_tprint(2, " Inconsistent number of forces evaluated in \
03536             calculations %d and %d\n", nosh->apol2calc[nosh->printcalc[iprint][0]]+1,
03537                       calcid+1);
03538             return 0;
03539         }
03540     }
03541
03542     /* Now, allocate space to accumulate the forces */
03543     lforce = (AtomForce *)Vmem_malloc(VNULL, refnforce, sizeof(AtomForce));
03544     gforce = (AtomForce *)Vmem_malloc(VNULL, refnforce, sizeof(AtomForce));
03545

```

```

03546  /* Now, accumulate the forces */
03547  calcid = nosh->apol2calc[nosh->printcalc[iprint][0]];
03548  aforce = atomForce[calcid];
03549  temp = nosh->calc[calcid]->apolparm->temp;
03550
03551  /* Load up the first calculation */
03552  if (refcalcforce == ACF_TOTAL) {
03553      /* Set to total force */
03554      for (ivc=0; ivc<3; ivc++) {
03555          lforce[0].sasaForce[ivc] = aforce[0].sasaForce[ivc];
03556          lforce[0].savForce[ivc] = aforce[0].savForce[ivc];
03557          lforce[0].wcaForce[ivc] = aforce[0].wcaForce[ivc];
03558      }
03559  } else if (refcalcforce == ACF_COMPS) {
03560      for (ifr=0; ifr<refnforce; ifr++) {
03561          for (ivc=0; ivc<3; ivc++) {
03562              lforce[ifr].sasaForce[ivc] = aforce[ifr].sasaForce[ivc];
03563              lforce[ifr].savForce[ivc] = aforce[ifr].savForce[ivc];
03564              lforce[ifr].wcaForce[ivc] = aforce[ifr].wcaForce[ivc];
03565          }
03566      }
03567  }
03568
03569  /* Load up the rest of the calculations */
03570  for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
03571      calcid = nosh->apol2calc[nosh->printcalc[iprint][iarg]];
03572      temp = nosh->calc[calcid]->apolparm->temp;
03573      aforce = atomForce[calcid];
03574      /* Get operation */
03575      if (nosh->printop[iprint][iarg-1] == 0) scalar = +1.0;
03576      else if (nosh->printop[iprint][iarg-1] == 1) scalar = -1.0;
03577      else scalar = 0.0;
03578      /* Accumulate */
03579      if (refcalcforce == ACF_TOTAL) {
03580          /* Set to total force */
03581          for (ivc=0; ivc<3; ivc++) {
03582              lforce[0].sasaForce[ivc] += aforce[0].sasaForce[ivc];
03583              lforce[0].savForce[ivc] += aforce[0].savForce[ivc];
03584              lforce[0].wcaForce[ivc] += aforce[0].wcaForce[ivc];
03585          }
03586      } else if (refcalcforce == ACF_COMPS) {
03587          for (ifr=0; ifr<refnforce; ifr++) {
03588              for (ivc=0; ivc<3; ivc++) {
03589                  lforce[ifr].sasaForce[ivc] += aforce[ifr].sasaForce[ivc];
03590                  lforce[ifr].savForce[ivc] += aforce[ifr].savForce[ivc];
03591                  lforce[ifr].wcaForce[ivc] += aforce[ifr].wcaForce[ivc];
03592              }
03593          }
03594      }
03595  }
03596
03597  Vnm_tprint( 0, "printForce: Performing global reduction (sum)\n");
03598  for (ifr=0; ifr<refnforce; ifr++) {
03599      Vcom_reduce(com, lforce[ifr].sasaForce, gforce[ifr].sasaForce, 3, 2, 0);
03600      Vcom_reduce(com, lforce[ifr].savForce, gforce[ifr].savForce, 3, 2, 0);
03601      Vcom_reduce(com, lforce[ifr].wcaForce, gforce[ifr].wcaForce, 3, 2, 0);
03602  }
03603
03604  if (refcalcforce == ACF_TOTAL) {
03605      Vnm_tprint( 1, " Printing net forces (kJ/mol/A)\n");
03606      Vnm_tprint( 1, " Legend:\n");
03607      Vnm_tprint( 1, " tot -- Total force\n");
03608      Vnm_tprint( 1, " sasa -- SASA force\n");
03609      Vnm_tprint( 1, " sav -- SAV force\n");
03610      Vnm_tprint( 1, " wca -- WCA force\n");
03611
03612      for (ivc=0; ivc<3; ivc++) {
03613          totforce[ivc] =
03614              gforce[0].sasaForce[ivc] + gforce[0].savForce[ivc] \
03615              + gforce[0].wcaForce[ivc];
03616      }
03617
03618      Vnm_tprint( 1, " tot %1.12E %1.12E %1.12E\n", totforce[0],
03619                  totforce[1], totforce[2]);
03620      Vnm_tprint( 1, " sasa %1.12E %1.12E %1.12E\n", gforce[0].sasaForce[0],
03621                  gforce[0].sasaForce[1], gforce[0].sasaForce[2]);
03622      Vnm_tprint( 1, " sav %1.12E %1.12E %1.12E\n", gforce[0].savForce[0],
03623                  gforce[0].savForce[1], gforce[0].savForce[2]);
03624      Vnm_tprint( 1, " wca %1.12E %1.12E %1.12E\n", gforce[0].wcaForce[0],
03625                  gforce[0].wcaForce[1], gforce[0].wcaForce[2]);
03626  }

```

```

03627     } else if (refcalcforce == ACF_COMPS) {
03628
03629         Vnm_tprint( 1, "   Printing per atom forces (kJ/mol/A)\n");
03630         Vnm_tprint( 1, "   Legend:\n");
03631         Vnm_tprint( 1, "       tot   n -- Total force for atom n\n");
03632         Vnm_tprint( 1, "       sasa  n -- SASA force for atom n\n");
03633         Vnm_tprint( 1, "       sav   n -- SAV force for atom n\n");
03634         Vnm_tprint( 1, "       wca   n -- WCA force for atom n\n");
03635         Vnm_tprint( 1, "       tot all -- Total force for system\n");
03636
03637         //Vnm_tprint( 1, "       gamma, pressure, bconc are: %f %f %f\n",
03638         //           gamma,press,bconc);
03639
03640         totforce[0] = 0.0;
03641         totforce[1] = 0.0;
03642         totforce[2] = 0.0;
03643
03644         for (ifr=0; ifr<refnforce; ifr++) {
03645             Vnm_tprint( 1, "   sasa  %d %1.12E %1.12E %1.12E\n", ifr,
03646                 gforce[ifr].sasaForce[0], gforce[ifr].sasaForce[1],
03647                 gforce[ifr].sasaForce[2]);
03648             Vnm_tprint( 1, "   sav   %d %1.12E %1.12E %1.12E\n", ifr,
03649                 gforce[ifr].savForce[0], gforce[ifr].savForce[1],
03650                 gforce[ifr].savForce[2]);
03651             Vnm_tprint( 1, "   wca   %d %1.12E %1.12E %1.12E\n", ifr,
03652                 gforce[ifr].wcaForce[0], gforce[ifr].wcaForce[1],
03653                 gforce[ifr].wcaForce[2]);
03654             Vnm_tprint( 1, "   tot   %d %1.12E %1.12E %1.12E\n", ifr,
03655                 (gforce[ifr].wcaForce[0] \
03656                  + gforce[ifr].savForce[0] +
03657                  gforce[ifr].sasaForce[0]),
03658                 (gforce[ifr].wcaForce[1] \
03659                  + gforce[ifr].savForce[1] +
03660                  gforce[ifr].sasaForce[1]),
03661                 (gforce[ifr].wcaForce[2] \
03662                  + gforce[ifr].savForce[2] +
03663                  gforce[ifr].sasaForce[2]));
03664             for (ivc=0; ivc<3; ivc++) {
03665                 totforce[ivc] += (gforce[ifr].wcaForce[ivc] \
03666                     + gforce[ifr].savForce[ivc] \
03667                     + gforce[ifr].sasaForce[ivc]);
03668             }
03669         }
03670         Vnm_tprint( 1, "   tot all %1.12E %1.12E %1.12E\n", totforce[0],
03671             totforce[1], totforce[2]);
03672     }
03673
03674     Vmem_free(VNULL, refnforce, sizeof(AtomForce), (void **)(&lforce));
03675     Vmem_free(VNULL, refnforce, sizeof(AtomForce), (void **)(&gforce));
03676
03677     return 1;
03678 }
03679
03680 #ifdef HAVE_MC_H
03681
03682
03683 VPUBLIC void killFE(NOsh *nosh,
03684     Vpbe *pbe[NOSH_MAXCALC],
03685     Vfetk *fetk[NOSH_MAXCALC],
03686     Gem *gm[NOSH_MAXMOL]
03687 ) {
03688
03689     int i;
03690
03691 #ifndef VAPBSQUIET
03692     Vnm_tprint(1, "Destroying finite element structures.\n");
03693 #endif
03694
03695     for(i=0; i<nosh->ncalc; i++){
03696         Vpbe_dtor(&(pbe[i]));
03697         Vfetk_dtor(&(fetk[i]));
03698     }
03699     for (i=0; i<nosh->nmesh; i++) {
03700         Gem_dtor(&(gm[i]));
03701     }
03702 }
03703
03711 VPUBLIC Vrc_Codes initFE(int icalc,
03712     NOsh *nosh,
03713     FEMparm *feparm,
03714     PBEparm *pbeparm,

```

```

03715         Vpbe *pbe[NOSH_MAXCALC],
03716         Valist *alist[NOSH_MAXMOL],
03717         Vfetk *fetk[NOSH_MAXCALC]
03718     ) {
03719
03720     int iatom,
03721         imesh,
03722         i,
03723         j,
03724         theMol,
03725         focusFlag = 0;
03726     Vio *sock = VNULL;
03727     size_t bytesTotal,
03728         highWater;
03729     Vfetk_MeshLoad meshType;
03730     double length[3],
03731         center[3],
03732         sparm,
03733         q,
03734         iparm = 0.0;
03735     Vrc_Codes vrc;
03736     Valist *myalist;
03737     Vatom *atom = VNULL;
03739     Vnm_tstart(27, "Setup timer");
03740
03741     /* Print some warning messages */
03742     if (pbeparm->useDielMap) Vnm_tprint(2, "FEM ignoring dielectric map!\n");
03743     if (pbeparm->useKappaMap) Vnm_tprint(2, "FEM ignoring kappa map!\n");
03744     if (pbeparm->useChargeMap) Vnm_tprint(2, "FEM ignoring charge map!\n");
03745
03746     /* Fix mesh center for "GCENT MOL #" types of declarations. */
03747     Vnm_tprint(0, "Re-centering mesh...\n");
03748     theMol = pbeparm->molid-1;
03749     myalist = alist[theMol];
03750     for (j=0; j<3; j++) {
03751         if (theMol < nosh->nmol) {
03752             center[j] = (myalist)->center[j];
03753         } else {
03754             Vnm_tprint(2, "ERROR! Bogus molecule number (%d)!\n",
03755                 (theMol+1));
03756             return VRC_FAILURE;
03757         }
03758     }
03759
03760     /* Check for completely-neutral molecule */
03761     q = 0;
03762     for (iatom=0; iatom<Valist_getNumberAtoms(myalist); iatom++) {
03763         atom = Valist_getAtom(myalist, iatom);
03764         q += VSQR(Vatom_getCharge(atom));
03765     }
03766     /* D. Gohara 10/22/09 - disabled
03767     if (q < (1e-6)) {
03768         Vnm_tprint(2, "Molecule #%d is uncharged!\n", pbeparm->molid);
03769         Vnm_tprint(2, "Sum square charge = %g!\n", q);
03770         return VRC_FAILURE;
03771     }
03772     */
03773
03774     /* Set the feparm pkey value based on the presence of an HB solver */
03775     #ifdef USE_HB
03776     feparm->pkey = 1;
03777     #else
03778     feparm->pkey = 0;
03779     #endif
03780
03781     /* Set up PBE object */
03782     Vnm_tprint(0, "Setting up PBE object...\n");
03783     if (pbeparm->srfm == VSM_SPLINE) {
03784         sparm = pbeparm->swin;
03785     }
03786     else {
03787         sparm = pbeparm->srad;
03788     }
03789     if (pbeparm->nion > 0) {
03790         iparm = pbeparm->ionr[0];
03791     }
03792
03793     pbe[icalc] = Vpbe_ctor(myalist, pbeparm->nion,
03794         pbeparm->ionc, pbeparm->ionr, pbeparm->ionq,
03795         pbeparm->temp, pbeparm->pdie,
03796         pbeparm->sdie, sparm, focusFlag, pbeparm->sdens,

```

```

03797             pbeparm->zmem, pbeparm->Lmem, pbeparm->mdie,
03798             pbeparm->memv);
03799
03800     /* Print a few derived parameters */
03801     Vnm_tprint(1, " Debye length: %g A\n", Vpbe_getDeblen(pbe[icalc]));
03802
03803     /* Set up FEtk objects */
03804     Vnm_tprint(0, "Setting up FEtk object...\n");
03805     fetk[icalc] = Vfetk_ctor(pbe[icalc], pbeparm->pbetype);
03806     Vfetk_setParameters(fetk[icalc], pbeparm, feparm);
03807
03808     /* Build mesh - this merely loads an MCSF file from an external source if one is specified or uses the
03809     * current molecule and sets center/length values based on that molecule if no external source is
03810     * specified. */
03811     Vnm_tprint(0, "Setting up mesh...\n");
03812     sock = VNULL;
03813     if (feparm->useMesh) {
03814         imesh = feparm->meshID-1;
03815         meshType = VML_EXTERNAL;
03816         for (i=0; i<3; i++) {
03817             center[i] = 0.0;
03818             length[i] = 0.0;
03819         }
03820         Vnm_print(0, "Using mesh %d (%s) in calculation.\n", imesh+1,
03821             nosh->meshpath[imesh]);
03822         switch (nosh->meshfmt[imesh]) {
03823             case VDF_DX:
03824                 Vnm_tprint(2, "DX finite element mesh input not supported yet!\n");
03825                 return VRC_FAILURE;
03826             case VDF_DXBIN:
03827                 Vnm_tprint(2, "DXBIN finite element mesh input not supported yet!\n");
03828                 return VRC_FAILURE;
03829             case VDF_UHBD:
03830                 Vnm_tprint( 2, "UHBD finite element mesh input not supported!\n");
03831                 return VRC_FAILURE;
03832             case VDF_AVS:
03833                 Vnm_tprint( 2, "AVS finite element mesh input not supported!\n");
03834                 return VRC_FAILURE;
03835             case VDF_MCSF:
03836                 Vnm_tprint(1, "Reading MCSF-format input finite element mesh from %s.\n",
03837                     nosh->meshpath[imesh]);
03838                 sock = Vio_ctor("FILE", "ASC", VNULL, nosh->meshpath[imesh], "r");
03839                 if (sock == VNULL) {
03840                     Vnm_print(2, "Problem opening virtual socket %s!\n",
03841                         nosh->meshpath[imesh]);
03842                     return VRC_FAILURE;
03843                 }
03844                 if (Vio_accept(sock, 0) < 0) {
03845                     Vnm_print(2, "Problem accepting virtual socket %s!\n",
03846                         nosh->meshpath[imesh]);
03847                     return VRC_FAILURE;
03848                 }
03849                 break;
03850             default:
03851                 Vnm_tprint( 2, "Invalid data format (%d)!\n",
03852                     nosh->meshfmt[imesh]);
03853                 return VRC_FAILURE;
03854         }
03855     } else { /* if (feparm->useMesh) */
03856         meshType = VML_DIRICUBE;
03857         for (i=0; i<3; i++) {
03858             center[i] = alist[theMol]->center[i];
03859             length[i] = feparm->glen[i];
03860         }
03861     }
03862
03863     /* Load the mesh with a particular center and vertex length using the provided input socket */
03864     vrc = Vfetk_loadMesh(fetk[icalc], center, length, meshType, sock);
03865     if (vrc == VRC_FAILURE) {
03866         Vnm_print(2, "Error constructing finite element mesh!\n");
03867         return VRC_FAILURE;
03868     }
03869     //Vnm_redirect(0); // Redirect output to io.mc
03870     Gem_shapeChk(fetk[icalc]->gm); // Traverse simplices and check shapes using the geometry manager.
03871     //Vnm_redirect(1);
03872
03873     /* Uniformly refine the mesh a bit */
03874     for (j=0; j<2; j++) {
03875         /* AM_* calls below are from the MC package, mc/src/nam/am.c. Note that these calls actually are
03876         * wrappers around Aprx_* functions found in MC as well. */
03877     }

```

```

03878      /* Mark the mesh for needed refinements */
03879      AM_markRefine(fetk[icalc]->am, 0, -1, 0, 0.0);
03880      /* Do actual mesh refinement */
03881      AM_refine(fetk[icalc]->am, 2, 0, feparm->pkey);
03882      //Vnm_redirect(0); // Redirect output to io.mc
03883      Gem_shapeChk(fetk[icalc]->gm); // Traverse simplices and check shapes using the geometry manager.
03884      //Vnm_redirect(1);
03885  }
03886
03887  /* Setup time statistics */
03888  Vnm_tstop(27, "Setup timer");
03889
03890  /* Memory statistics */
03891  bytesTotal = Vmem_bytesTotal();
03892  highWater = Vmem_highWaterTotal();
03893
03894  #ifndef VAPBSQUIET
03895      Vnm_tprint( 1, " Current memory usage: %4.3f MB total, \
03896 %4.3f MB high water\n", (double) (bytesTotal)/(1024.*1024.),
03897                      (double) (highWater)/(1024.*1024.));
03898  #endif
03899
03900      return VRC_SUCCESS;
03901  }
03902
03903  VPUBLIC void printFEPARM(int icalc,
03904                          Nosh *nosh,
03905                          FEMParm *feparm,
03906                          Vfetk *fetk[NOSH_MAXCALC]
03907                          ) {
03908
03909      Vnm_tprint(1, " Domain size: %g A x %g A x %g A\n",
03910                feparm->glen[0], feparm->glen[1],
03911                feparm->glen[2]);
03912      switch(feparm->ekey) {
03913      case FET_SIMP:
03914          Vnm_tprint(1, " Per-simplex error tolerance: %g\n", feparm->etol);
03915          break;
03916      case FET_GLOB:
03917          Vnm_tprint(1, " Global error tolerance: %g\n", feparm->etol);
03918          break;
03919      case FET_FRAC:
03920          Vnm_tprint(1, " Fraction of simps to refine: %g\n", feparm->etol);
03921          break;
03922      default:
03923          Vnm_tprint(2, "Invalid ekey (%d)!\n", feparm->ekey);
03924          VASSERT(0);
03925          break;
03926      }
03927      switch(feparm->akeyPRE) {
03928      case FRT_UNIF:
03929          Vnm_tprint(1, " Uniform pre-solve refinement.\n");
03930          break;
03931      case FRT_GEOM:
03932          Vnm_tprint(1, " Geometry-based pre-solve refinement.\n");
03933          break;
03934      default:
03935          Vnm_tprint(2, "Invalid akeyPRE (%d)!\n", feparm->akeyPRE);
03936          VASSERT(0);
03937          break;
03938      }
03939      switch(feparm->akeySOLVE) {
03940      case FRT_RESI:
03941          Vnm_tprint(1, " Residual-based a posteriori refinement.\n");
03942          break;
03943      case FRT_DUAL:
03944          Vnm_tprint(1, " Dual-based a posteriori refinement.\n");
03945          break;
03946      case FRT_LOCA:
03947          Vnm_tprint(1, " Local-based a posteriori refinement.\n");
03948          break;
03949      default:
03950          Vnm_tprint(2, "Invalid akeySOLVE (%d)!\n", feparm->akeySOLVE);
03951          break;
03952      }
03953      Vnm_tprint(1, " Refinement of initial mesh to ~%d vertices\n",
03954                feparm->targetNum);
03955      Vnm_tprint(1, " Geometry-based refinement lower bound: %g A\n",
03956                feparm->targetRes);
03957      Vnm_tprint(1, " Maximum number of solve-estimate-refine cycles: %d\n",
03958                feparm->maxsolve);

```



```

03959     Vnm_tprint(1, "   Maximum number of vertices in mesh: %d\n",
03960                feparm->maxvert);
03961
03962     /* FOLLOWING IS SOLVER-RELATED; BAIL IF NOT SOLVING */
03963     if (nosh->bogus) return;
03964 #ifdef USE_HB
03965     Vnm_tprint(1, "   HB linear solver:  AM_hPcg\n");
03966 #else
03967     Vnm_tprint(1, "   Non-HB linear solver:  ");
03968     switch (fetk[icalc]->lkey) {
03969     case VLT_SLU:
03970         Vnm_print(1, "SLU direct\n");
03971         break;
03972     case VLT_MG:
03973         Vnm_print(1, "multigrid\n");
03974         break;
03975     case VLT_CG:
03976         Vnm_print(1, "conjugate gradient\n");
03977         break;
03978     case VLT_BCG:
03979         Vnm_print(1, "BiCGStab\n");
03980         break;
03981     default:
03982         Vnm_print(1, "???\n");
03983         break;
03984     }
03985 #endif
03986
03987     Vnm_tprint(1, "   Linear solver tol.: %g\n", fetk[icalc]->ltol);
03988     Vnm_tprint(1, "   Linear solver max. iters.: %d\n", fetk[icalc]->lmax);
03989     Vnm_tprint(1, "   Linear solver preconditioner:  ");
03990     switch (fetk[icalc]->lprec) {
03991     case VPT_IDEN:
03992         Vnm_print(1, "identity\n");
03993         break;
03994     case VPT_DIAG:
03995         Vnm_print(1, "diagonal\n");
03996         break;
03997     case VPT_MG:
03998         Vnm_print(1, "multigrid\n");
03999         break;
04000     default:
04001         Vnm_print(1, "???\n");
04002         break;
04003     }
04004     Vnm_tprint(1, "   Nonlinear solver:  ");
04005     switch (fetk[icalc]->nkey) {
04006     case VNT_NEW:
04007         Vnm_print(1, "newton\n");
04008         break;
04009     case VNT_INC:
04010         Vnm_print(1, "incremental\n");
04011         break;
04012     case VNT_ARC:
04013         Vnm_print(1, "pseudo-arclength\n");
04014         break;
04015     default:
04016         Vnm_print(1, "??? ");
04017         break;
04018     }
04019     Vnm_tprint(1, "   Nonlinear solver tol.: %g\n", fetk[icalc]->ntol);
04020     Vnm_tprint(1, "   Nonlinear solver max. iters.: %d\n", fetk[icalc]->nmax);
04021     Vnm_tprint(1, "   Initial guess:  ");
04022     switch (fetk[icalc]->gues) {
04023     case VGT_ZERO:
04024         Vnm_tprint(1, "zero\n");
04025         break;
04026     case VGT_DIRI:
04027         Vnm_tprint(1, "boundary function\n");
04028         break;
04029     case VGT_PREV:
04030         Vnm_tprint(1, "interpolated previous solution\n");
04031         break;
04032     default:
04033         Vnm_tprint(1, "???\n");
04034         break;
04035     }
04036 }
04037 }
04038
04039 VPUBLIC int partFE(int icalc, NOsh *nosh, FEMparm *feparm,

```

```

04040             Vfetk *fetk[NOSH_MAXCALC]) {
04041
04042     Vfetk_setAtomColors(fetk[icalc]);
04043     return 1;
04044 }
04045
04046 VPUBLIC int preRefineFE(int icalc, /* Calculation index */
04047                        FEMparm *feparm, /* FE-specific parameters */
04048                        Vfetk *fetk[NOSH_MAXCALC] /* Array of FE solver objects */
04049                        ) {
04050
04051     int nverts,
04052         marked;
04053     /* Based on the refinement type, alert the user to what we're trying to refine with. */
04054     switch(feparm->akeyPRE) {
04055     case FRT_UNIF:
04056         Vnm_tprint(1, " Commencing uniform refinement to %d verts.\n",
04057                   feparm->targetNum);
04058         break;
04059     case FRT_GEOM:
04060         Vnm_tprint(1, " Commencing geometry-based refinement to %d \
04061 verts or %g A resolution.\n", feparm->targetNum, feparm->targetRes);
04062         break;
04063     case FRT_DUAL:
04064         Vnm_tprint(2, "What? You can't do a posteriori error estimation \
04065 before you solve!\n");
04066         VASSERT(0);
04067         break;
04068     case FRT_RESI:
04069     case FRT_LOCA:
04070     default:
04071         VASSERT(0);
04072         break;
04073     }
04074
04075     Vnm_tprint(1, " Initial mesh has %d vertices\n",
04076               Gem_numVV(fetk[icalc]->gm));
04077
04078     /* As long as we have simplices marked that need to be refined, run MC's
04079      * AM_markRefine against our data until we hit the error or size tolerance
04080      * for the refinement. */
04081     while (1) {
04082         nverts = Gem_numVV(fetk[icalc]->gm);
04083         if (nverts > feparm->targetNum) {
04084             Vnm_tprint(1, " Hit vertex number limit.\n");
04085             break;
04086         }
04087         marked = AM_markRefine(fetk[icalc]->am, feparm->akeyPRE, -1,
04088                               feparm->ekey, feparm->etol);
04089         if (marked == 0) {
04090             Vnm_tprint(1, " Marked 0 simp; hit error/size tolerance.\n");
04091             break;
04092         }
04093         Vnm_tprint(1, " Have %d verts, marked %d. Refining...\n", nverts,
04094                   marked);
04095         AM_refine(fetk[icalc]->am, 0, 0, feparm->pkey);
04096     }
04097
04098     nverts = Gem_numVV(fetk[icalc]->gm);
04099     Vnm_tprint(1, " Done refining; have %d verts.\n", nverts);
04100
04101     return 1;
04102 }
04103
04104 VPUBLIC int solveFE(int icalc,
04105                   PBEparm *pbeparm,
04106                   FEMparm *feparm,
04107                   Vfetk *fetk[NOSH_MAXCALC]
04108                   ) {
04109
04110     int lkeyHB = 3,
04111         meth = 2,
04112         prob = 0,
04113         prec = 0;
04114     if ((pbeparm->pbetype==PBE_NPBE) ||
04115         (pbeparm->pbetype == PBE_NRPBE) ||
04116         (pbeparm->pbetype == PBE_SMPBE)) {
04117
04118         /* Call MC's nonlinear solver - mc/src/nam/nsolv.c */
04119         AM_nSolve(

```

```

04133         fetk[icalc]->am,
04134         fetk[icalc]->nkey,
04135         fetk[icalc]->nmax,
04136         fetk[icalc]->ntol,
04137         meth,
04138         fetk[icalc]->lmax,
04139         fetk[icalc]->ltol,
04140         prec,
04141         fetk[icalc]->gues,
04142         fetk[icalc]->pjac
04143     );
04144     } else if ((pbeparm->pbetype==PBE_LPBE) ||
04145         (pbeparm->pbetype==PBE_LRPBE)) {
04146         /* Note: USEHB is a compile time defined macro. The program flow
04147         is to always take the route using AM_hlSolve when the solver
04148         is linear. D. Gohara 6/29/06
04149         */
04150         #ifdef USE_HB
04151         Vnm_print(2, "SORRY! DON'T USE HB!!!\n");
04152         VASSERT(0);
04153
04154         /* Call MC's hierarchical linear solver - mc/src/nam/lsolv.c */
04155         AM_hlSolve(fetk[icalc]->am, meth, lkeyHB, fetk[icalc]->lmax,
04156             fetk[icalc]->ltol, fetk[icalc]->gues, fetk[icalc]->pjac);
04157     #else
04158
04159         /* Call MC's linear solver - mc/src/nam/lsolv.c */
04160         AM_lSolve(
04161             fetk[icalc]->am,
04162             prob,
04163             meth,
04164             fetk[icalc]->lmax,
04165             fetk[icalc]->ltol,
04166             prec,
04167             fetk[icalc]->gues,
04168             fetk[icalc]->pjac
04169         );
04170     #endif
04171     }
04172     return 1;
04173 }
04174
04175
04179 VPUBLIC int energyFE(Nosh *nosh,
04180     int icalc,
04181     Vfetk *fetk[NOSH_MAXCALC],
04182     int *nenergy,
04183     double *totEnergy,
04184     double *qfEnergy,
04185     double *qmEnergy,
04186     double *dielEnergy
04187 ) {
04188
04189     FEMparm *feparm = nosh->calc[icalc]->feparm;
04190     PBEParm *pbeparm = nosh->calc[icalc]->pbeparm;
04191     *nenergy = 1;
04192     *totEnergy = 0;
04193
04194     if (nosh->bogus == 0) {
04201         if ((pbeparm->pbetype==PBE_NPBE) ||
04202             (pbeparm->pbetype==PBE_NRPBE) ||
04203             (pbeparm->pbetype == PBE_SMPBE)) {
04204             *totEnergy = Vfetk_energy(fetk[icalc], -1, 1); /* Last parameter indicates NPBE */
04205         } else if ((pbeparm->pbetype==PBE_LPBE) ||
04206             (pbeparm->pbetype==PBE_LRPBE)) {
04207             *totEnergy = Vfetk_energy(fetk[icalc], -1, 0); /* Last parameter indicates LPBE */
04208         } else {
04209             VASSERT(0);
04210         }
04211     }
04212
04213     #ifndef VAPBSQUIET
04214     Vnm_tprint(1, "        Total electrostatic energy = %1.12E kJ/mol\n",
04215         Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(totEnergy));
04216     fflush(stdout);
04217     #endif
04218     }
04219
04220     if (pbeparm->calcenergy == PCE_COMPS) {
04221         Vnm_tprint(2, "Error! Verbose energy evaluation not available for FEM yet!\n");
04222         Vnm_tprint(2, "E-mail nathan.baker@pnl.gov if you want this.\n");
04223         *qfEnergy = 0;

```

```

04224         *qmEnergy = 0;
04225         *dielEnergy = 0;
04226     } else {
04227         *nenergy = 0;
04228     }
04229     return 1;
04230 }
04231
04239 VPUBLIC int postRefineFE(int icalc,
04240                         FEMparm *feparm,
04241                         Vfetk *fetk[NOSH_MAXCALC]
04242                         ) {
04243
04244     int nverts,
04245         marked;
04247     nverts = Gem_numVV(fetk[icalc]->gm);
04248     if (nverts > feparm->maxvert) {
04249         Vnm_tprint(1, "    Current number of vertices (%d) exceeds max (%d)!\n",
04250                 nverts, feparm->maxvert);
04251         return 0;
04252     }
04253     Vnm_tprint(1, "    Mesh currently has %d vertices\n", nverts);
04254
04255     switch(feparm->akeySOLVE) {
04256     case FRT_UNIF:
04257         Vnm_tprint(1, "    Commencing uniform refinement.\n");
04258         break;
04259     case FRT_GEOM:
04260         Vnm_tprint(1, "    Commencing geometry-based refinement.\n");
04261         break;
04262     case FRT_RESI:
04263         Vnm_tprint(1, "    Commencing residual-based refinement.\n");
04264         break;
04265     case FRT_DUAL:
04266         Vnm_tprint(1, "    Commencing dual problem-based refinement.\n");
04267         break;
04268     case FRT_LOCA:
04269         Vnm_tprint(1, "    Commencing local-based refinement.\n");
04270         break;
04271     default:
04272         Vnm_tprint(2, "    Error -- unknown refinement type (%d)!\n",
04273                 feparm->akeySOLVE);
04274         return 0;
04275         break;
04276     }
04277
04278     /* Run MC's refinement algorithm */
04279     marked = AM_markRefine(fetk[icalc]->am, feparm->akeySOLVE, -1,
04280                         feparm->ekey, feparm->etol);
04281     if (marked == 0) {
04282         Vnm_tprint(1, "    Marked 0 simpes; hit error/size tolerance.\n");
04283         return 0;
04284     }
04285     Vnm_tprint(1, "    Have %d verts, marked %d. Refining...\n", nverts,
04286             marked);
04287     AM_refine(fetk[icalc]->am, 0, 0, feparm->pkey);
04288     nverts = Gem_numVV(fetk[icalc]->gm);
04289     Vnm_tprint(1, "    Done refining; have %d verts.\n", nverts);
04290     //Vnm_redirect(0); // Redirect output to io.mc
04291     Gem_shapeChk(fetk[icalc]->gm); // Traverse simplices and check shapes using the geometry manager.
04292     //Vnm_redirect(1);
04293
04294     return 1;
04295 }
04296
04300 VPUBLIC int writedataFE(int rank,
04301                       NOSH *nosh,
04302                       PBEparm *pbeparm,
04303                       Vfetk *fetk
04304                       ) {
04305
04306     char writestem[VMAX_ARGLEN];
04307     char outpath[VMAX_ARGLEN];
04308     int i,
04309         writeit;
04310     AM *am;
04311     Bvec *vec;
04312     if (nosh->bogus) return 1;
04313
04314     am = fetk->am;
04315     vec = am->w0;

```

```
04317
04318     for (i=0; i<pbeparm->numwrite; i++) {
04319
04320         writeit = 1;
04321
04322         switch (pbeparm->writetype[i]) {
04323
04324             case VDT_CHARGE:
04325
04326                 Vnm_tprint(2, "    Sorry; can't write charge distribution for FEM!\n");
04327                 writeit = 0;
04328                 break;
04329
04330             case VDT_POT:
04331
04332                 Vnm_tprint(1, "    Writing potential to ");
04333                 Vfetk_fillArray(fetk, vec, VDT_POT);
04334                 break;
04335
04336             case VDT_SMOL:
04337
04338                 Vnm_tprint(1, "    Writing molecular accessibility to ");
04339                 Vfetk_fillArray(fetk, vec, VDT_SMOL);
04340                 break;
04341
04342             case VDT_SSPL:
04343
04344                 Vnm_tprint(1, "    Writing spline-based accessibility to ");
04345                 Vfetk_fillArray(fetk, vec, VDT_SSPL);
04346                 break;
04347
04348             case VDT_VDW:
04349
04350                 Vnm_tprint(1, "    Writing van der Waals accessibility to ");
04351                 Vfetk_fillArray(fetk, vec, VDT_VDW);
04352                 break;
04353
04354             case VDT_IVDW:
04355
04356                 Vnm_tprint(1, "    Writing ion accessibility to ");
04357                 Vfetk_fillArray(fetk, vec, VDT_IVDW);
04358                 break;
04359
04360             case VDT_LAP:
04361
04362                 Vnm_tprint(2, "    Sorry; can't write charge distribution for FEM!\n");
04363                 writeit = 0;
04364                 break;
04365
04366             case VDT_EDENS:
04367
04368                 Vnm_tprint(2, "    Sorry; can't write energy density for FEM!\n");
04369                 writeit = 0;
04370                 break;
04371
04372             case VDT_NDENS:
04373
04374                 Vnm_tprint(1, "    Writing number density to ");
04375                 Vfetk_fillArray(fetk, vec, VDT_NDENS);
04376                 break;
04377
04378             case VDT_QDENS:
04379
04380                 Vnm_tprint(1, "    Writing charge density to ");
04381                 Vfetk_fillArray(fetk, vec, VDT_QDENS);
04382                 break;
04383
04384             case VDT_DIELX:
04385
04386                 Vnm_tprint(2, "    Sorry; can't write x-shifted dielectric map for FEM!\n");
04387                 writeit = 0;
04388                 break;
04389
04390             case VDT_DIELY:
04391
04392                 Vnm_tprint(2, "    Sorry; can't write y-shifted dielectric map for FEM!\n");
04393                 writeit = 0;
04394                 break;
04395
04396             case VDT_DIELZ:
04397
```

```

04398         Vnm_tprint(2, "    Sorry; can't write z-shifted dielectric map for FEM!\n");
04399         writeit = 0;
04400         break;
04401
04402     case VDT_KAPPA:
04403
04404         Vnm_tprint(1, "    Sorry; can't write kappa map for FEM!\n");
04405         writeit = 0;
04406         break;
04407
04408     case VDT_ATOMPOT:
04409
04410         Vnm_tprint(1, "    Sorry; can't write atom potentials for FEM!\n");
04411         writeit = 0;
04412         break;
04413
04414     default:
04415
04416         Vnm_tprint(2, "Invalid data type for writing!\n");
04417         writeit = 0;
04418         return 0;
04419     }
04420
04421     if (!writeit) return 0;
04422
04423
04424 #ifdef HAVE_MPI_H
04425     sprintf(writestem, "%s-PE%d", pbeparm->writestem[i], rank);
04426 #else
04427     if (nosh->ispara) {
04428         sprintf(writestem, "%s-PE%d", pbeparm->writestem[i], nosh->proc_rank);
04429     } else {
04430         sprintf(writestem, "%s", pbeparm->writestem[i]);
04431     }
04432 #endif
04433
04434     switch (pbeparm->writefmt[i]) {
04435
04436     case VDF_DX:
04437         sprintf(outpath, "%s.%s", writestem, "dx");
04438         Vnm_tprint(1, "%s\n", outpath);
04439         Vfetc_write(fetc, "FILE", "ASC", VNULL, outpath, vec, VDF_DX);
04440         break;
04441
04442     case VDF_DXBIN:
04443         //TODO: probably change some or all of below.
04444         sprintf(outpath, "%s.%s", writestem, "dxbin");
04445         Vnm_tprint(1, "%s\n", outpath);
04446         Vfetc_write(fetc, "FILE", "ASC", VNULL, outpath, vec, VDF_DXBIN);
04447         break;
04448
04449     case VDF_AVS:
04450         sprintf(outpath, "%s.%s", writestem, "ucd");
04451         Vnm_tprint(1, "%s\n", outpath);
04452         Vfetc_write(fetc, "FILE", "ASC", VNULL, outpath, vec, VDF_AVS);
04453         break;
04454
04455     case VDF_UHBD:
04456         Vnm_tprint(2, "UHBD format not supported for FEM!\n");
04457         break;
04458
04459     case VDF_MCSF:
04460         Vnm_tprint(2, "MCSF format not supported yet!\n");
04461         break;
04462
04463     default:
04464         Vnm_tprint(2, "Bogus data format (%d)!\n",
04465                 pbeparm->writefmt[i]);
04466         break;
04467     }
04468 }
04469
04470
04471     return 1;
04472 }
04473 #endif /* ifdef HAVE_MCX_H */
04474
04475 VPUBLIC int initAPOL(Nosh *nosh,
04476                    Vmem *mem,
04477                    Vparam *param,
04478                    APOLparam *apolparam,

```

```

04479             int *nforce,
04480             AtomForce **atomForce,
04481             Valist *alist
04482         ) {
04483     int i,
04484         natoms,
04485         len,
04486         inhash[3],
04487         rc = 0;
04489     time_t ts;
04490     Vclist *clist = VNULL;
04491     Vacc *acc = VNULL;
04492     Vatom *atom = VNULL;
04493     Vparam_AtomData *atomData = VNULL;
04495     double sasa,
04496         sav,
04497         nhash[3],
04498         sradPad,
04499         x,
04500         y,
04501         z,
04502         atomRadius,
04503         srad,
04504         *atomsasa,
04505         *atomwcaEnergy,
04506         energy = 0.0,
04507         dist,
04508         charge,
04509         xmin,
04510         xmax,
04511         ymin,
04512         ymax,
04513         zmin,
04514         zmax,
04515         disp[3],
04516         center[3],
04517         soluteXlen,
04518         soluteYlen,
04519         soluteZlen;
04521     atomsasa = (double *)Vmem_malloc(VNULL, Valist_getNumberAtoms(alist), sizeof(double));
04522     atomwcaEnergy = (double *)Vmem_malloc(VNULL, Valist_getNumberAtoms(alist), sizeof(double));
04523
04524     /* Determine solute length and charge */
04525     atom = Valist_getAtom(alist, 0);
04526     xmin = Vatom_getPosition(atom)[0];
04527     xmax = Vatom_getPosition(atom)[0];
04528     ymin = Vatom_getPosition(atom)[1];
04529     ymax = Vatom_getPosition(atom)[1];
04530     zmin = Vatom_getPosition(atom)[2];
04531     zmax = Vatom_getPosition(atom)[2];
04532     charge = 0;
04533     natoms = Valist_getNumberAtoms(alist);
04534
04535     for (i=0; i < natoms; i++) {
04536         atom = Valist_getAtom(alist, i);
04537         atomRadius = Vatom_getRadius(atom);
04538         x = Vatom_getPosition(atom)[0];
04539         y = Vatom_getPosition(atom)[1];
04540         z = Vatom_getPosition(atom)[2];
04541         if ((x+atomRadius) > xmax) xmax = x + atomRadius;
04542         if ((x-atomRadius) < xmin) xmin = x - atomRadius;
04543         if ((y+atomRadius) > ymax) ymax = y + atomRadius;
04544         if ((y-atomRadius) < ymin) ymin = y - atomRadius;
04545         if ((z+atomRadius) > zmax) zmax = z + atomRadius;
04546         if ((z-atomRadius) < zmin) zmin = z - atomRadius;
04547         disp[0] = (x - center[0]);
04548         disp[1] = (y - center[1]);
04549         disp[2] = (z - center[2]);
04550         dist = (disp[0]*disp[0]) + (disp[1]*disp[1]) + (disp[2]*disp[2]);
04551         dist = VSQRT(dist) + atomRadius;
04552         charge += Vatom_getCharge(Valist_getAtom(alist, i));
04553     }
04554     soluteXlen = xmax - xmin;
04555     soluteYlen = ymax - ymin;
04556     soluteZlen = zmax - zmin;
04557
04558     /* Set up the hash table for the cell list */
04559     Vnm_print(0, "APOL: Setting up hash table and accessibility object...\n");
04560     nhash[0] = soluteXlen/0.5;
04561     nhash[1] = soluteYlen/0.5;
04562     nhash[2] = soluteZlen/0.5;

```

```

04563     for (i=0; i<3; i++) inhash[i] = (int)(nhash[i]);
04564
04565     for (i=0;i<3;i++){
04566         if (inhash[i] < 3) inhash[i] = 3;
04567         if (inhash[i] > MAX_HASH_DIM) inhash[i] = MAX_HASH_DIM;
04568     }
04569
04570     /* Pad the radius by 2x the maximum displacement value */
04571     srاد = apolparm->srاد;
04572     srادPad = srاد + (2*apolparm->dpos);
04573     clist = Vclist_ctor(alist, srادPad, inhash, CLIST_AUTO_DOMAIN,
04574                        VNULL, VNULL);
04575     acc = Vacc_ctor(alist, clist, apolparm->sdens);
04576
04577     /* Get WAT (water) LJ parameters from Vparam object */
04578     if (param == VNULL && (apolparm->bconc != 0.0)) {
04579         Vnm_tprint(2, "initAPOL: Got NULL Vparam object!\n");
04580         Vnm_tprint(2, "initAPOL: You are performing an apolar calculation with the van der Waals integral
term,\n");
04581         Vnm_tprint(2, "initAPOL: this term requires van der Waals parameters which are not available from
the \n");
04582         Vnm_tprint(2, "initAPOL: PQR file. Therefore, you need to supply a parameter file with the parm
keyword,\n");
04583         Vnm_tprint(2, "initAPOL: for example,\n");
04584         Vnm_tprint(2, "initAPOL: read parm flat amber94.dat end\n");
04585         Vnm_tprint(2, "initAPOL: where the relevant parameter files can be found in
apbs/tools/conversion/param/vparam.\n");
04586         return VRC_FAILURE;
04587     }
04588
04589     if (apolparm->bconc != 0.0){
04590         atomData = Vparam_getAtomData(param, "WAT", "OW");
04591         if (atomData == VNULL) atomData = Vparam_getAtomData(param, "WAT", "O");
04592         if (atomData == VNULL) {
04593             Vnm_tprint(2, "initAPOL: Couldn't find parameters for WAT OW or WAT O!\n");
04594             Vnm_tprint(2, "initAPOL: These parameters must be present in your file\n");
04595             Vnm_tprint(2, "initAPOL: for apolar calculations.\n");
04596             return VRC_FAILURE;
04597         }
04598         apolparm->watepsilon = atomData->epsilon;
04599         apolparm->watsigma = atomData->radius;
04600         apolparm->setwat = 1;
04601     }
04602
04603     /* Calculate Energy and Forces */
04604     if(apolparm->calcforce) {
04605         rc = forceAPOL(acc, mem, apolparm, nforce, atomForce, alist, clist);
04606         if(rc == VRC_FAILURE) {
04607             Vnm_print(2, "Error in apolar force calculation!\n");
04608             return VRC_FAILURE;
04609         }
04610     }
04611
04612     /* Get the SAV and SAS */
04613     sasa = 0.0;
04614     sav = 0.0;
04615
04616     if (apolparm->calcenergy) {
04617         len = Valist_getNumberAtoms(alist);
04618
04619         if (VABS(apolparm->gamma) > VSMALL) {
04620             /* Total Solvent Accessible Surface Area (SASA) */
04621             apolparm->sasa = Vacc_totalSASA(acc, srاد);
04622             /* SASA for each atom */
04623             for (i = 0; i < len; i++) {
04624                 atom = Valist_getAtom(alist, i);
04625                 atomsasa[i] = Vacc_atomSASA(acc, srاد, atom);
04626             }
04627         } else {
04628             /* Total Solvent Accessible Surface Area (SASA) set to zero */
04629             apolparm->sasa = 0.0;
04630             /* SASA for each atom set to zero*/
04631             for (i = 0; i < len; i++) {
04632                 atomsasa[i] = 0.0;
04633             }
04634         }
04635
04636         /* Inflated van der Waals accessibility */
04637         if (VABS(apolparm->press) > VSMALL){
04638             apolparm->sav = Vacc_totalSAV(acc, clist, apolparm, srاد);
04639         } else {

```



```

04640         apolparm->sav = 0.0;
04641     }
04642
04643     /* wcaEnergy integral code */
04644     if (VABS(apolparm->bconc) > VSMALL) {
04645         /* wcaEnergy for each atom */
04646         for (i = 0; i < len; i++) {
04647             rc = Vacc_wcaEnergyAtom(acc, apolparm, alist, clist, i, &energy);
04648             if (rc == 0) {
04649                 Vnm_print(2, "Error in apolar energy calculation!\n");
04650                 return 0;
04651             }
04652             atomwcaEnergy[i] = energy;
04653         }
04654         /* Total WCA Energy */
04655         rc = Vacc_wcaEnergy(acc, apolparm, alist, clist);
04656         if (rc == 0) {
04657             Vnm_print(2, "Error in apolar energy calculation!\n");
04658             return 0;
04659         }
04660     } else {
04661         apolparm->wcaEnergy = 0.0;
04662     }
04663     energyAPOL(apolparm, apolparm->sasa, apolparm->sav, atomsasa, atomwcaEnergy,
Valist_getNumberAtoms(alist));
04664 }
04665
04666 Vmem_free(VNULL, Valist_getNumberAtoms(alist), sizeof(double), (void **)&(atomsasa));
04667 Vmem_free(VNULL, Valist_getNumberAtoms(alist), sizeof(double), (void **)&(atomwcaEnergy));
04668 Vclist_dtor(&clist);
04669 Vacc_dtor(&acc);
04670
04671 return VRC_SUCCESS;
04672 }
04673
04674 VPUBLIC int energyAPOL(APOLparm *apolparm,
04675                     double sasa,
04676                     double sav,
04677                     double atomsasa[],
04678                     double atomwcaEnergy[],
04679                     int numatoms
04680                     ){
04681
04682     double energy = 0.0;
04683     int i = 0;
04684
04685     #ifndef VAPBSQUIET
04686         Vnm_print(1, "\nSolvent Accessible Surface Area (SASA) for each atom:\n");
04687         for (i = 0; i < numatoms; i++) {
04688             Vnm_print(1, "  SASA for atom %i: %1.12E\n", i, atomsasa[i]);
04689         }
04690
04691         Vnm_print(1, "\nTotal solvent accessible surface area: %g A^2\n", sasa);
04692     #endif
04693
04694     switch(apolparm->calcenergy){
04695     case ACE_NO:
04696         break;
04697     case ACE_COMPS:
04698         Vnm_print(1, "energyAPOL: Cannot calculate component energy, skipping.\n");
04699         break;
04700     case ACE_TOTAL:
04701         energy = (apolparm->gamma*sasa) + (apolparm->press*sav)
04702             + (apolparm->wcaEnergy);
04703     #ifndef VAPBSQUIET
04704         Vnm_print(1, "\nSurface tension*area energies (gamma * SASA) for each atom:\n");
04705         for (i = 0; i < numatoms; i++) {
04706             Vnm_print(1, "  Surface tension*area energy for atom %i: %1.12E\n", i,
apolparm->gamma*atomsasa[i]);
04707         }
04708
04709         Vnm_print(1, "\nTotal surface tension energy: %g kJ/mol\n", apolparm->gamma*sasa);
04710         Vnm_print(1, "\nTotal solvent accessible volume: %g A^3\n", sav);
04711         Vnm_print(1, "\nTotal pressure*volume energy: %g kJ/mol\n", apolparm->press*sav);
04712         Vnm_print(1, "\nWCA dispersion Energies for each atom:\n");
04713         for (i = 0; i < numatoms; i++) {
04714             Vnm_print(1, "  WCA energy for atom %i: %1.12E\n", i, atomwcaEnergy[i]);
04715         }
04716
04717         Vnm_print(1, "\nTotal WCA energy: %g kJ/mol\n", (apolparm->wcaEnergy));
04718         Vnm_print(1, "\nTotal non-polar energy = %1.12E kJ/mol\n", energy);

```

```

04719 #endif
04720         break;
04721     default:
04722         Vnm_print(2, "energyAPOL: Error in energyAPOL. Unknown option.\n");
04723         break;
04724     }
04725
04726     return VRC_SUCCESS;
04727 }
04728
04729 VPUBLIC int forceAPOL(Vacc *acc,
04730                     Vmem *mem,
04731                     APOLparm *apolparm,
04732                     int *nforce,
04733                     AtomForce **atomForce,
04734                     Valist *alist,
04735                     Vclist *clist
04736                 ) {
04737     time_t ts, ts_main, ts_sub;
04738
04739     int i,
04740         j,
04741         natom;
04742
04743     double srad, /* Probe radius */
04744            xF,
04745            yF,
04746            zF, /* Individual forces */
04747            press,
04748            gamma,
04749            offset,
04750            bconc,
04751            dSASA[3],
04752            dSAV[3],
04753            force[3],
04754            *apos;
04755
04756     Vatom *atom = VNULL;
04757     ts_main = clock();
04758
04759     srad = apolparm->srad;
04760     press = apolparm->press;
04761     gamma = apolparm->gamma;
04762     offset = apolparm->dpos;
04763     bconc = apolparm->bconc;
04764
04765     natom = Valist_getNumberAtoms(alist);
04766
04767     /* Check to see if we need to build the surface */
04768     Vnm_print(0, "forceAPOL: Trying atom surf...\n");
04769     ts = clock();
04770     if (acc->surf == VNULL) {
04771         acc->surf = (VaccSurf**)Vmem_malloc(acc->mem, natom, sizeof(VaccSurf *));
04772         for (i=0; i<natom; i++) {
04773             atom = Valist_getAtom(acc->alist, i);
04774             //apos = Vatom_getPosition(atom); // apos never referenced? - Peter
04775             /* NOTE: RIGHT NOW WE DO THIS FOR THE ENTIRE MOLECULE WHICH IS
04776              * INCREDIBLY INEFFICIENT, PARTICULARLY DURING FOCUSING!!! */
04777             acc->surf[i] = Vacc_atomSurf(acc, atom, acc->refSphere, srad);
04778         }
04779     }
04780     Vnm_print(0, "forceAPOL: atom surf: Time elapsed: %f\n", ((double)clock() - ts) / CLOCKS_PER_SEC);
04781
04782     if (apolparm->calcforce == ACF_TOTAL) {
04783         Vnm_print(0, "forceAPOL: calcforce == ACF_TOTAL\n");
04784         ts = clock();
04785
04786         *nforce = 1;
04787         if (*atomForce != VNULL) {
04788             Vmem_free(mem, *nforce, sizeof(AtomForce), (void **)atomForce);
04789         }
04790
04791         *atomForce = (AtomForce *)Vmem_malloc(mem, *nforce,
04792                                             sizeof(AtomForce));
04793
04794         /* Clear out force arrays */
04795         for (j=0; j<3; j++) {
04796             (*atomForce)[0].sasaForce[j] = 0.0;
04797             (*atomForce)[0].savForce[j] = 0.0;
04798             (*atomForce)[0].wcaForce[j] = 0.0;
04799         }
04800     }

```

```

04800         // problem block
04801         for (i=0; i<natom; i++) {
04802             atom = Valist_getAtom(alist, i);
04803
04804             for(j=0; j<3; j++){
04805                 dSASA[j] = 0.0;
04806                 dSAV[j] = 0.0;
04807                 force[j] = 0.0;
04808             }
04809
04810             if(VABS(gamma) > VSMALL) {
04811                 Vacc_atomdSASA(acc, offset, srاد, atom, dSASA);
04812             }
04813             if(VABS(press) > VSMALL) {
04814                 Vacc_atomdSAV(acc, srاد, atom, dSAV);
04815             }
04816             if(VABS(bconc) > VSMALL) {
04817                 Vacc_wcaForceAtom(acc, apolparm, clist, atom, force);
04818             }
04819
04820             for(j=0; j<3; j++){
04821                 (*atomForce)[0].sasaForce[j] += dSASA[j];
04822                 (*atomForce)[0].savForce[j] += dSAV[j];
04823                 (*atomForce)[0].wcaForce[j] += force[j];
04824             }
04825         }
04826         // end block
04827
04828         Vnm_tprint( 1, "   Printing net forces (kJ/mol/A)\n");
04829         Vnm_tprint( 1, "   Legend:\n");
04830         Vnm_tprint( 1, "       sasa -- SASA force\n");
04831         Vnm_tprint( 1, "       sav  -- SAV force\n");
04832         Vnm_tprint( 1, "       wca  -- WCA force\n");
04833
04834         Vnm_tprint( 1, "   sasa %4.3e %4.3e %4.3e\n",
04835             (*atomForce)[0].sasaForce[0],
04836             (*atomForce)[0].sasaForce[1],
04837             (*atomForce)[0].sasaForce[2]);
04838         Vnm_tprint( 1, "   sav  %4.3e %4.3e %4.3e\n",
04839             (*atomForce)[0].savForce[0],
04840             (*atomForce)[0].savForce[1],
04841             (*atomForce)[0].savForce[2]);
04842         Vnm_tprint( 1, "   wca  %4.3e %4.3e %4.3e\n",
04843             (*atomForce)[0].wcaForce[0],
04844             (*atomForce)[0].wcaForce[1],
04845             (*atomForce)[0].wcaForce[2]);
04846
04847         Vnm_print(0, "forceAPOL: calcforce == ACF_TOTAL: %f\n", ((double)clock() - ts) / CLOCKS_PER_SEC);
04848     } else if (apolparm->calcforce == ACF_COMPS ) {
04849         *nforce = Valist_getNumberAtoms(alist);
04850         if(*atomForce == VNULL){
04851             *atomForce = (AtomForce *)Vmem_malloc(mem, *nforce,
04852                 sizeof(AtomForce));
04853         } else {
04854             Vmem_free(mem, *nforce, sizeof(AtomForce), (void **)atomForce);
04855             *atomForce = (AtomForce *)Vmem_malloc(mem, *nforce,
04856                 sizeof(AtomForce));
04857         }
04858
04859 #ifndef VAPBSQUIET
04860         Vnm_tprint( 1, "   Printing per atom forces (kJ/mol/A)\n");
04861         Vnm_tprint( 1, "   Legend:\n");
04862         Vnm_tprint( 1, "       tot  n -- Total force for atom n\n");
04863         Vnm_tprint( 1, "       sasa n -- SASA force for atom n\n");
04864         Vnm_tprint( 1, "       sav  n -- SAV force for atom n\n");
04865         Vnm_tprint( 1, "       wca  n -- WCA force for atom n\n");
04866
04867         Vnm_tprint( 1, "       gamma %f\n" \
04868             "       pressure %f\n" \
04869             "       bconc %f\n",
04870             gamma, press, bconc);
04871 #endif
04872
04873         for (i=0; i<natom; i++) {
04874             atom = Valist_getAtom(alist, i);
04875
04876             for(j=0; j<3; j++){
04877                 dSASA[j] = 0.0;
04878                 dSAV[j] = 0.0;
04879                 force[j] = 0.0;
04880             }

```

```

04881
04882     /* Clear out force arrays */
04883     for (j=0; j<3; j++) {
04884         (*atomForce)[i].sasaForce[j] = 0.0;
04885         (*atomForce)[i].savForce[j] = 0.0;
04886         (*atomForce)[i].wcaForce[j] = 0.0;
04887     }
04888
04889     if (VABS(gamma) > VSMALL) Vacc_atomdSASA(acc, offset, srاد, atom, dSASA);
04890     if (VABS(press) > VSMALL) Vacc_atomdSAV(acc, srاد, atom, dSAV);
04891     if (VABS(bconc) > VSMALL) Vacc_wcaForceAtom(acc, apolparm, clist, atom, force);
04892
04893     xF = -((gamma*dSASA[0]) + (press*dSAV[0]) + (bconc*force[0]));
04894     yF = -((gamma*dSASA[1]) + (press*dSAV[1]) + (bconc*force[1]));
04895     zF = -((gamma*dSASA[2]) + (press*dSAV[2]) + (bconc*force[2]));
04896
04897     for (j=0; j<3; j++) {
04898         (*atomForce)[i].sasaForce[j] += dSASA[j];
04899         (*atomForce)[i].savForce[j] += dSAV[j];
04900         (*atomForce)[i].wcaForce[j] += force[j];
04901     }
04902
04903 #ifndef VAPBSQUIET
04904     Vnm_print( 1, " tot %i %4.3e %4.3e %4.3e\n",
04905               i,
04906               xF,
04907               yF,
04908               zF);
04909     Vnm_print( 1, " sasa %i %4.3e %4.3e %4.3e\n",
04910               i,
04911               (*atomForce)[i].sasaForce[0],
04912               (*atomForce)[i].sasaForce[1],
04913               (*atomForce)[i].sasaForce[2]);
04914     Vnm_print( 1, " sav %i %4.3e %4.3e %4.3e\n",
04915               i,
04916               (*atomForce)[i].savForce[0],
04917               (*atomForce)[i].savForce[1],
04918               (*atomForce)[i].savForce[2]);
04919     Vnm_print( 1, " wca %i %4.3e %4.3e %4.3e\n",
04920               i,
04921               (*atomForce)[i].wcaForce[0],
04922               (*atomForce)[i].wcaForce[1],
04923               (*atomForce)[i].wcaForce[2]);
04924 #endif
04925     }
04926 } else *nforce = 0;
04927
04928 #ifndef VAPBSQUIET
04929     Vnm_print(1, "\n");
04930 #endif
04931
04932     Vnm_print(0, "forceAPOL: Time elapsed: %f\n", ((double)clock() - ts_main) / CLOCKS_PER_SEC);
04933     return VRC_SUCCESS;
04934 }
04935
04936 #ifdef ENABLE_BEM
04937 VPUBLIC int initBEM(int icalc,
04938                   NOsh *nosh,
04939                   BEMparm *bemparm,
04940                   PBEparm *pbeparm,
04941                   Vpbe *pbe[NOSH_MAXCALC]
04942                   ) {
04943
04944     Vnm_tstart(APBS_TIMER_SETUP, "Setup timer");
04945
04946     /* Setup time statistics */
04947     Vnm_tstop(APBS_TIMER_SETUP, "Setup timer");
04948
04949     return 1;
04950 }
04951
04952 VPUBLIC void killBEM(NOsh *nosh, Vpbe *pbe[NOSH_MAXCALC]
04953                   ) {
04954     int i;
04955
04956 #ifndef VAPBSQUIET
04957     Vnm_tprint(1, "Destroying boundary element structures.\n");

```

```
04965 #endif
04966
04967
04968 }
04969
04970
04971 void apbs2tabipb_(TABIPBparm* tabiparm,
04972                  TABIPBvars* tabivars);
04973
04974 VPUBLIC int solveBEM(Valist* molecules[NOSH_MAXMOL],
04975                    Nosh *nosh,
04976                    PBEparm *pbeparm,
04977                    BEMparm *bemparm,
04978                    BEMparm_CalcType type) {
04979
04980     int nx,
04981         ny,
04982         nz,
04983         i;
04984
04985     if (nosh != VNULL) {
04986         if (nosh->bogus) return 1;
04987     }
04988
04989     Vnm_tstart(APBS_TIMER_SOLVER, "Solver timer");
04990
04991     TABIPBparm *tabiparm = (TABIPBparm*)calloc(1, sizeof(TABIPBparm));
04992
04993     sprintf(tabiparm->fpath, "");
04994     strncpy(tabiparm->fname, nosh->molpath[0], 4);
04995     tabiparm->fname[4] = '\0';
04996     tabiparm->density = pbeparm->sdens;
04997     tabiparm->probe_radius = pbeparm->srad;
04998
04999     tabiparm->epsp = pbeparm->pdie;
05000     tabiparm->epsw = pbeparm->sdie;
05001     tabiparm->bulk_strength = 0.0;
05002     for (i=0; i<pbeparm->nion; i++)
05003         tabiparm->bulk_strength += pbeparm->ionc[i]
05004             *pbeparm->ionq[i]*pbeparm->ionq[i];
05005     tabiparm->temp = pbeparm->temp;
05006
05007     tabiparm->order = bemparm->tree_order;
05008     tabiparm->maxparnode = bemparm->tree_n0;
05009     tabiparm->theta = bemparm->mac;
05010
05011     tabiparm->mesh_flag = bemparm->mesh;
05012
05013     tabiparm->number_of_lines = Valist_getNumberAtoms(molecules[0]);
05014
05015     tabiparm->output_datafile = bemparm->outdata;
05016
05017     TABIPBvars *tabivars = (TABIPBvars*)calloc(1, sizeof(TABIPBvars));
05018     if ((tabivars->chrpos = (double *) malloc(3 * tabiparm->number_of_lines * sizeof(double))) == NULL) {
05019         printf("Error in allocating t_chrpos!\n");
05020     }
05021     if ((tabivars->atmchr = (double *) malloc(tabiparm->number_of_lines * sizeof(double))) == NULL) {
05022         printf("Error in allocating t_atmchr!\n");
05023     }
05024     if ((tabivars->atmrad = (double *) malloc(tabiparm->number_of_lines * sizeof(double))) == NULL) {
05025         printf("Error in allocating t_atmrad!\n");
05026     }
05027
05028     Vatom *atom;
05029
05030     for (i = 0; i < tabiparm->number_of_lines; i++){
05031         atom = Valist_getAtom(molecules[0], i);
05032         tabivars->chrpos[3*i] = Vatom_getPosition(atom)[0];
05033         tabivars->chrpos[3*i + 1] = Vatom_getPosition(atom)[1];
05034         tabivars->chrpos[3*i + 2] = Vatom_getPosition(atom)[2];
05035         tabivars->atmchr[i] = Vatom_getCharge(atom);
05036         tabivars->atmrad[i] = Vatom_getRadius(atom);
05037     }
05038
05039     //apbs2tabipb(TABIPBparm* tabiparm, Valist* molecules[NOSH_MAXMOL]);
05040     apbs2tabipb_(tabiparm, tabivars);
05041
05042     free(tabiparm);
05043     free(tabivars->chrpos);
05044     free(tabivars->atmchr);
05045     free(tabivars->atmrad);
```

```

05046     free(tabivars->vert_ptl); // allocate in output_potential()
05047     free(tabivars->xvct); // allocate in output_potential()
05048     free_matrix(tabivars->vert); // allocate in output_potential()
05049     free_matrix(tabivars->snrm); // allocate in output_potential()
05050     free_matrix(tabivars->face); // allocate in output_potential()
05051
05052     Vnm_tprint(1, "\n\nReturning to APBS caller...\n\n");
05053     Vnm_tprint(1, "Solvation energy and Coulombic energy in kJ/mol...\n\n");
05054     Vnm_tprint(1, "  Global net ELEC energy = %1.12E\n", tabivars->soleng);
05055     Vnm_tprint(1, "  Global net COULOMBIC energy = %1.12E\n\n", tabivars->couleng);
05056
05057     free(tabivars);
05058
05059     Vnm_tstop(APBS_TIMER_SOLVER, "Solver timer");
05060
05061     return 1;
05062 }
05063
05064 VPUBLIC int setPartBEM(NOsh *nosh,
05065                      BEMparm *BEMparm
05066                      ) {
05067
05068     int j;
05069     double partMin[3],
05070            partMax[3];
05071
05072     if (nosh->bogus) return 1;
05073
05074     return 1;
05075 }
05076
05077 VPUBLIC int energyBEM(NOsh *nosh,
05078                     int icalc,
05079                     int *nenergy,
05080                     double *totEnergy,
05081                     double *qfEnergy,
05082                     double *qmEnergy,
05083                     double *dielEnergy
05084                     ) {
05085
05086     Valist *alist;
05087     Vatom *atom;
05088     int i,
05089         extEnergy;
05090     double tenergy;
05091     BEMparm *bemparm;
05092     PBEParm *pbeparm;
05093
05094     bemparm = nosh->calc[icalc]->bemparm;
05095     pbeparm = nosh->calc[icalc]->pbeparm;
05096
05097     Vnm_tstart(APBS_TIMER_ENERGY, "Energy timer");
05098     Vnm_tstop(APBS_TIMER_ENERGY, "Energy timer");
05099
05100     return 1;
05101 }
05102
05103 VPUBLIC int forceBEM(
05104     NOsh *nosh,
05105     PBEParm *pbeparm,
05106     BEMparm *bemparm,
05107     int *nforce,
05108     AtomForce **atomForce,
05109     Valist *alist[NOSH_MAXMOL]
05110     ) {
05111
05112     int j,
05113         k;
05114     double qfForce[3],
05115            dbForce[3],
05116            ibForce[3];
05117
05118     Vnm_tstart(APBS_TIMER_FORCE, "Force timer");
05119
05120     #ifndef VAPBSQUIET
05121         Vnm_tprint(1, "  Calculating forces...\n");
05122     #endif
05123
05124     Vnm_tstop(APBS_TIMER_FORCE, "Force timer");

```

```
05127
05128     return 1;
05129 }
05130
05131 VPUBLIC void printBEMParm(BEMParm *bemparm) {
05132
05133 }
05134
05135
05136 VPUBLIC int writedataBEM(int rank,
05137                         Nosh *nosh,
05138                         PBEparm *pbeparm
05139                     ) {
05140
05141     return 1;
05142 }
05143
05144
05145 VPUBLIC int writematBEM(int rank, Nosh *nosh, PBEparm *pbeparm) {
05146
05147
05148     if (nosh->bogus) return 1;
05149     return 1;
05150 }
05151
05152 #endif
05153
05154
05155 #ifdef ENABLE_GEOFLOW
05156
05160 VPUBLIC int solveGeometricFlow( Valist* molecules[NOSH_MAXMOL],
05161                                Nosh *nosh,
05162                                PBEparm *pbeparm,
05163                                APOLparm *apolparm,
05164                                GEOFLOWparm *parm )
05165 {
05166     //printf("solveGeometricFlow!!!\n");
05167     if (nosh != VNULL) {
05168         if (nosh->bogus) return 1;
05169     }
05170
05171     Vnm_tstart(APBS_TIMER_SOLVER, "Solver timer");
05172
05173     struct GeometricFlowInput geoflowIn = getGeometricFlowParams();
05174
05175     // change any of the parameters you want...
05176     geoflowIn.m_boundaryCondition = (int) pbeparm->bcbf ;
05177     geoflowIn.m_grid[0] = apolparm->grid[0];
05178     geoflowIn.m_grid[1] = apolparm->grid[1];
05179     geoflowIn.m_grid[2] = apolparm->grid[2];
05180     geoflowIn.m_gamma = apolparm->gamma;
05181     geoflowIn.m_pdie = pbeparm->pdie ;
05182     geoflowIn.m_sdie = pbeparm->sdie ;
05183     geoflowIn.m_press = apolparm->press ;
05184     geoflowIn.m_tol = parm->etol;
05185     geoflowIn.m_bconc = apolparm->bconc ;
05186     geoflowIn.m_vdwdispersion = parm->vdw;
05187     geoflowIn.m_etolSolvation = .01 ; // to be added?
05188
05189     // debug
05190     //printGeometricFlowStruct( geoflowIn );
05191
05192     //printf("num mols: %i\n", nosh->nmol);
05193     struct GeometricFlowOutput geoflowOut =
05194         runGeometricFlowWrapAPBS( geoflowIn, molecules[0] );
05195
05196     Vnm_tprint( 1, " Global net energy = %1.12E\n", geoflowOut.m_totalSolvation);
05197     Vnm_tprint( 1, " Global net ELEC energy = %1.12E\n", geoflowOut.m_elecSolvation);
05198     Vnm_tprint( 1, " Global net APOL energy = %1.12E\n", geoflowOut.m_nonpolarSolvation);
05199
05200     Vnm_tstop(APBS_TIMER_SOLVER, "Solver timer");
05201
05202     return 1;
05203 }
05204 }
05205
05206 #endif
05207
05208 #ifdef ENABLE_PBAM
05209
05213 VPUBLIC int solvePBAM( Valist* molecules[NOSH_MAXMOL],
```

```

05214                                     NOsh *nosh,
05215                                     PBEparm *pbeparm,
05216                                     PBAMparm *parm )
05217 {
05218     if (nosh != VNULL) {
05219         if (nosh->bogus) return 1;
05220     }
05221
05222     int i, j;
05223     Vnm_tstart(APBS_TIMER_SOLVER, "Solver timer");
05224     PBAMInput pbamIn = getPBAMParams();
05225
05226     pbamIn.nmol_ = nosh->nmol;
05227
05228     // change any of the parameters you want...
05229     pbamIn.temp_ = pbeparm->temp;
05230     if (fabs(pbamIn.temp_-0.0) < 1e-3)
05231     {
05232         printf("No temperature specified. Setting to 298.15K\n");
05233         pbamIn.temp_ = 298.15;
05234     }
05235
05236     // Dielectrics
05237     pbamIn.idiel_ = pbeparm->pdie;
05238     pbamIn.sdiel_ = pbeparm->sdiel;
05239
05240     // Salt conc
05241     pbamIn.salt_ = parm->salt;
05242
05243     // Runtime: can be energyforce, electrostatics etc
05244     strncpy(pbamIn.runType_, parm->runtype, CHR_MAXLEN);
05245     strncpy(pbamIn.runName_, parm->runname, CHR_MAXLEN);
05246
05247     pbamIn.randOrient_ = parm->setrandorient;
05248
05249     pbamIn.boxLen_ = parm->pbcbboxlen;
05250     pbamIn.pbcType_ = parm->setpbcs;
05251
05252     pbamIn.setunits_ = parm->setunits;
05253     if(parm->setunits == 1) strncpy(pbamIn.units_, parm->units, CHR_MAXLEN);
05254
05255     // Electrostatic stuff
05256     if (parm->setgridpt) pbamIn.gridPts_ = parm->gridpt;
05257     strncpy(pbamIn.map3D_, parm->map3dname, CHR_MAXLEN);
05258     pbamIn.grid2Dct_ = parm->grid2Dct;
05259     for (i=0; i<pbamIn.grid2Dct_; i++)
05260     {
05261         strncpy(pbamIn.grid2D_[i], parm->grid2Dname[i], CHR_MAXLEN);
05262         strncpy(pbamIn.grid2Dax_[i], parm->grid2Dax[i], CHR_MAXLEN);
05263         pbamIn.grid2Dloc_[i] = parm->grid2Dloc[i];
05264     }
05265     strncpy(pbamIn.dxname_, parm->dxname, CHR_MAXLEN);
05266
05267     // Dynamics stuff
05268     pbamIn.ntraj_ = parm->ntraj;
05269     strncpy(pbamIn.termCombine_, parm->termcombine, CHR_MAXLEN);
05270
05271     pbamIn.termct_ = parm->termct;
05272     pbamIn.contct_ = parm->confilct;
05273
05274     if (strcmp(pbamIn.runType_, "dynamics", 8)== 0)
05275     {
05276         if (pbamIn.nmol_ > parm->diffct)
05277         {
05278             Vnm_tprint(2, "You need more diffusion information!\n");
05279             return 0;
05280         }
05281
05282         for (i=0; i<pbamIn.nmol_; i++)
05283         {
05284             if (parm->xyzct[i] < parm->ntraj)
05285             {
05286                 Vnm_tprint(2, "For molecule %d, you are missing trajectory!\n", i+1);
05287                 return 0;
05288             } else {
05289                 for (j=0; j<pbamIn.ntraj_; j++)
05290                 {
05291                     strncpy(pbamIn.xyzfil_[i][j], parm->xyzfil[i][j], CHR_MAXLEN);
05292                 }
05293             }
05294         }
05295     }

```



```
05295
05296     for (i=0; i<pbamIn.nmol_; i++)
05297     {
05298         strncpy(pbamIn.moveType_[i], parm->moveType[i], CHR_MAXLEN);
05299         pbamIn.transDiff_[i] = parm->transDiff[i];
05300         pbamIn.rotDiff_[i] = parm->rotDiff[i];
05301     }
05302
05303     for (i=0; i<pbamIn.termct_; i++)
05304     {
05305         strncpy(pbamIn.termnam_[i], parm->termnam[i], CHR_MAXLEN);
05306         pbamIn.termnu_[i][0] = parm->termnu[i][0];
05307         pbamIn.termval_[i] = parm->termVal[i];
05308     }
05309
05310     for (i=0; i<pbamIn.contct_; i++)
05311     {
05312         strncpy(pbamIn.confil_[i], parm->confil[i], CHR_MAXLEN);
05313     }
05314 }
05315
05316 // debug
05317 printPBAMStruct( pbamIn );
05318
05319 // Run the darn thing
05320 PBAMOutput pbamOut = runPBAMWrapAPBS( pbamIn, molecules, nosh->nmol );
05321
05322 Vnm_tprint(1, "\n\nReturning to APBS caller...\n\n");
05323
05324 if (!strcmp(pbamIn.runType_, "dynamics", 8) &&
05325     strcmp(pbamIn.runType_, "energyforce", 11)) {
05326
05327     if (!strcmp(pbamIn.units_, "kcalmol", 7)) { //scale to kJmol is 4.18400
05328
05329         Vnm_tprint(1, "Interaction energy in kCal/mol...\n\n");
05330
05331         for (int i = 0; i < PBAMPARM_MAXMOL; i++) {
05332             Vnm_tprint(1, " Molecule %d: Global net ELEC energy = %1.12E\n",
05333                 i+1, pbamOut.energies_[i]);
05334             Vnm_tprint(1, " Force = (%1.6E, %1.6E, %1.6E)\n\n",
05335                 pbamOut.forces_[i][0], pbamOut.forces_[i][1],
05336                 pbamOut.forces_[i][2]);
05337             if (pbamOut.energies_[i+1] == 0.) break;
05338         }
05339     } else if (!strcmp(pbamIn.units_, "Jmol", 4)) { //scale to kJmol is 0.001
05340
05341         Vnm_tprint(1, "Interaction energy in J/mol...\n\n");
05342
05343         for (int i = 0; i < PBAMPARM_MAXMOL; i++) {
05344             Vnm_tprint(1, " Molecule %d: Global net ELEC energy = %1.12E\n",
05345                 i+1, pbamOut.energies_[i]);
05346             Vnm_tprint(1, " Force = (%1.6E, %1.6E, %1.6E)\n\n",
05347                 pbamOut.forces_[i][0], pbamOut.forces_[i][1],
05348                 pbamOut.forces_[i][2]);
05349             if (pbamOut.energies_[i+1] == 0.) break;
05350         }
05351     } else { // if (!strcmp(pbamIn.units_, "kT", 2)) //scale to kJmol is 2.478 @ 298K
05352         // or 0.008315436242 * 298
05353
05354         Vnm_tprint(1, "Interaction energy in kT @ %6.2f K...\n\n", pbamIn.temp_);
05355
05356         for (int i = 0; i < PBAMPARM_MAXMOL; i++) {
05357             Vnm_tprint(1, " Molecule %d: Global net ELEC energy = %1.12E\n",
05358                 i+1, pbamOut.energies_[i]);
05359             Vnm_tprint(1, " Force = (%1.6E, %1.6E, %1.6E)\n\n",
05360                 pbamOut.forces_[i][0], pbamOut.forces_[i][1],
05361                 pbamOut.forces_[i][2]);
05362             if (pbamOut.energies_[i+1] == 0.) break;
05363         }
05364     }
05365 }
05366
05367 Vnm_tstop(APBS_TIMER_SOLVER, "Solver timer");
05368
05369 return 1;
05370
05371 }
05372
05373 #endif
```

```
05376
05377 #ifndef ENABLE_PBSAM
05378
05382 VPUBLIC int solvePBSAM( Valist* molecules[NOSH_MAXMOL],
05383                        NOsh *nosh,
05384                        PBEparam *pbeparm,
05385                        PBAMparam *param,
05386                        PBSAMparam *sampparm )
05387 {
05388     printf("solvePBSAM!!!\n");
05389     char fname_tp[VMAX_ARGLEN];
05390     if (nosh != VNULL) {
05391         if (nosh->bogus) return 1;
05392     }
05393
05394     int i, j, k, ierr;
05395     Vnm_tstart(APBS_TIMER_SOLVER, "Solver timer");
05396     PBSAMInput pbsamIn = getPBSAMParams();
05397     PBAMInput pbamIn; // = getPBAMParams();
05398
05399     pbamIn.nmol_ = nosh->nmol;
05400
05401     // change any of the parameters you want...
05402     pbamIn.temp_ = pbeparm->temp;
05403     if (fabs(pbamIn.temp_-0.0) < 1e-3)
05404     {
05405         printf("No temperature specified. Setting to 298.15K\n");
05406         pbamIn.temp_ = 298.15;
05407     }
05408
05409     // Dielectrics
05410     pbamIn.idiel_ = pbeparm->pdie;
05411     pbamIn.sdiel_ = pbeparm->sdie;
05412
05413     // Salt conc
05414     pbamIn.salt_ = param->salt;
05415
05416     // Runtype: can be energyforce, electrostatics etc
05417     strncpy(pbamIn.runType_, param->runtype, CHR_MAXLEN);
05418     strncpy(pbamIn.runName_, param->runname, CHR_MAXLEN);
05419
05420     pbamIn.setunits_ = param->setunits;
05421     if (param->setunits == 1) strncpy(pbamIn.units_, param->units, CHR_MAXLEN);
05422     pbamIn.randOrient_ = param->setrandorient;
05423
05424     pbamIn.boxLen_ = param->pbcbboxlen;
05425     pbamIn.pbcType_ = param->setpbcs;
05426
05427     // Electrostatic stuff
05428     if (param->setgridpt) pbamIn.gridPts_ = param->gridpt;
05429     strncpy(pbamIn.map3D_, param->map3dname, CHR_MAXLEN);
05430     pbamIn.grid2Dct_ = param->grid2Dct;
05431     for (i=0; i<pbamIn.grid2Dct; i++)
05432     {
05433         strncpy(pbamIn.grid2D_[i], param->grid2Dname[i], CHR_MAXLEN);
05434         strncpy(pbamIn.grid2Dax_[i], param->grid2Dax[i], CHR_MAXLEN);
05435         pbamIn.grid2Dloc_[i] = param->grid2Dloc[i];
05436     }
05437     strncpy(pbamIn.dlname_, param->dlname, CHR_MAXLEN);
05438
05439     // Dynamics stuff
05440     pbamIn.ntraj_ = param->ntraj;
05441     strncpy(pbamIn.termCombine_, param->termcombine, CHR_MAXLEN);
05442
05443     pbamIn.termct_ = param->termct;
05444     pbamIn.contct_ = param->confilct;
05445
05446     if (strncmp(pbamIn.runType_, "dynamics", 8) == 0)
05447     {
05448         if (pbamIn.nmol_ > param->diffct)
05449         {
05450             Vnm_tprint(2, "You need more diffusion information!\n");
05451             return 0;
05452         }
05453
05454         for (i=0; i<pbamIn.nmol_; i++)
05455         {
05456             if (param->xyzct[i] < param->ntraj)
05457             {
05458                 Vnm_tprint(2, "For molecule %d, you are missing trajectory!\n", i+1);
05459                 return 0;
05460             }
05461         }
05462     }
05463 }
```

```

05460     } else {
05461         for (j=0; j<pbamIn.ntraj_; j++)
05462         {
05463             strncpy(pbamIn.xyzfil_[i][j], parm->xyzfil[i][j], CHR_MAXLEN);
05464         }
05465     }
05466 }
05467
05468 for (i=0; i<pbamIn.nmol_; i++)
05469 {
05470     strncpy(pbamIn.moveType_[i], parm->moveType[i], CHR_MAXLEN);
05471     pbamIn.transDiff_[i] = parm->transDiff[i];
05472     pbamIn.rotDiff_[i] = parm->rotDiff[i];
05473 }
05474
05475 for (i=0; i<pbamIn.termct_; i++)
05476 {
05477     strncpy(pbamIn.termnam_[i], parm->termnam[i], CHR_MAXLEN);
05478     pbamIn.termnu_[i][0] = parm->termnu[i][0];
05479     pbamIn.termval_[i] = parm->termVal[i];
05480 }
05481
05482 for (i=0; i<pbamIn.contct_; i++)
05483 {
05484     strncpy(pbamIn.confil_[i], parm->confil[i], CHR_MAXLEN);
05485 }
05486 }
05487
05488 // SAM details
05489 pbsamIn.tolsp_ = samparm->tolsp;
05490 pbsamIn.imatct_ = samparm->imatct;
05491 pbsamIn.expct_ = samparm->expct;
05492 for (i=0; i<samparm->surfct; i++)
05493 {
05494     strncpy(pbsamIn.surffil_[i], samparm->surffil[i], CHR_MAXLEN);
05495 }
05496 for (i=0; i<samparm->imatct; i++)
05497 {
05498     strncpy(pbsamIn.imatfil_[i], samparm->imatfil[i], CHR_MAXLEN);
05499 }
05500 for (i=0; i<samparm->expct; i++)
05501 {
05502     strncpy(pbsamIn.expfil_[i], samparm->expfil[i], CHR_MAXLEN);
05503 }
05504
05505 // Running MSMS if the MSMS flag is used
05506 if (samparm->setmsms == 1) {
05507     for (i=0; i<pbamIn.nmol_; i++) {
05508         // find a clever way to use prefix of molecule name for msms outputs
05509         for (j=0; j < VMAX_ARGLEN; j++)
05510             if (nosh->molpath[i][j] == '\0') break;
05511
05512         // assume terminated by '.pqr' -> 4 char, want to term w/ '.xyzr'
05513         //char xyzr[j+2], surf[j+2], outname[j-4];
05514         char xyzr[VMAX_ARGLEN], surf[VMAX_ARGLEN], outname[VMAX_ARGLEN];
05515         for( k=0; k < j - 4; k++)
05516         {
05517             xyzr[k] = nosh->molpath[i][k];
05518             outname[k] = nosh->molpath[i][k];
05519             surf[k] = nosh->molpath[i][k];
05520         }
05521         outname[k] = '\0';
05522         xyzr[k] = '.'; surf[k] = '.';
05523         xyzr[k+1] = 'x'; surf[k+1] = 'v';
05524         xyzr[k+2] = 'y'; surf[k+2] = 'e';
05525         xyzr[k+3] = 'z'; surf[k+3] = 'r';
05526         xyzr[k+4] = 'r'; surf[k+4] = 't';
05527         xyzr[k+5] = '\0'; surf[k+5] = '\0';
05528
05529         // write an XYZR file from xyzr data
05530         FILE *fp;
05531         fp=fopen(xyzr, "w");
05532         Vatom *atom;
05533         for(k=0; k< Valist_getNumberAtoms(molecules[i]); k++)
05534         {
05535             atom = Valist_getAtom(molecules[i],k);
05536             fprintf(fp, "%.4f %.4f %.4f %.4f\n", Vatom_getPosition(atom)[0],
05537                 Vatom_getPosition(atom)[1],
05538                 Vatom_getPosition(atom)[2],
05539                 Vatom_getRadius(atom));
05540         }

```

```

05541     }
05542     fclose(fp);
05543
05544     #ifdef _WIN32
05545         sprintf(fname_tp, "msms.exe -if %s -prob %f -dens %f -of %s",
05546                 xyzr, samparm->probe_radius, samparm->density, outname);
05547     #else
05548         sprintf(fname_tp, "msms -if %s -prob %f -dens %f -of %s",
05549                 xyzr, samparm->probe_radius, samparm->density, outname);
05550     #endif
05551
05552     printf("%s\n", fname_tp);
05553
05554     printf("Running MSMS...\n");
05555     ierr = system(fname_tp);
05556
05557     strncpy(pbsamIn.surffil_[i], surf, CHR_MAXLEN);
05558 }
05559 }
05560
05561 // debug
05562 printPBSAMStruct( pbamIn, pbsamIn );
05563
05564 // Run the darn thing
05565 PBAMOutput pbamOut = runPBSAMWrapAPBS(pbamIn, pbsamIn, molecules, nosh->nmol);
05566
05567 Vnm_tprint(1, "\n\nReturning to APBS caller...\n\n");
05568
05569 if (!strcmp(pbamIn.runType_, "dynamics", 8) &&
05570     strcmp(pbamIn.runType_, "energyforce", 11)) {
05571
05572     if (!strcmp(pbamIn.units_, "kcalmol", 7)) { //scale to kJmol is 4.18400
05573
05574         Vnm_tprint(1, "Interaction energy in kCal/mol...\n\n");
05575
05576         for (int i = 0; i < PBAMPARM_MAXMOL; i++) {
05577             Vnm_tprint(1, "  Molecule %d: Global net ELEC energy = %1.12E\n",
05578                         i+1, pbamOut.energies_[i]);
05579             Vnm_tprint(1, "          Force = (%1.6E, %1.6E, %1.6E)\n\n",
05580                         pbamOut.forces_[i][0], pbamOut.forces_[i][1],
05581                         pbamOut.forces_[i][2]);
05582             if (pbamOut.energies_[i+1] == 0.) break;
05583         }
05584     } else if (!strcmp(pbamIn.units_, "Jmol", 4)) { //scale to kJmol is 0.001
05585
05586         Vnm_tprint(1, "Interaction energy in J/mol...\n\n");
05587
05588         for (int i = 0; i < PBAMPARM_MAXMOL; i++) {
05589             Vnm_tprint(1, "  Molecule %d: Global net ELEC energy = %1.12E\n",
05590                         i+1, pbamOut.energies_[i]);
05591             Vnm_tprint(1, "          Force = (%1.6E, %1.6E, %1.6E)\n\n",
05592                         pbamOut.forces_[i][0], pbamOut.forces_[i][1],
05593                         pbamOut.forces_[i][2]);
05594             if (pbamOut.energies_[i+1] == 0.) break;
05595         }
05596     } else { // if (!strcmp(pbamIn.units_, "kT", 2)) //scale to kJmol is 2.478 @ 298K
05597         // or 0.008315436242 * 298
05598
05599         Vnm_tprint(1, "Interaction energy in kT @ %6.2f K...\n\n", pbamIn.temp_);
05600
05601         for (int i = 0; i < PBAMPARM_MAXMOL; i++) {
05602             Vnm_tprint(1, "  Molecule %d: Global net ELEC energy = %1.12E\n",
05603                         i+1, pbamOut.energies_[i]);
05604             Vnm_tprint(1, "          Force = (%1.6E, %1.6E, %1.6E)\n\n",
05605                         pbamOut.forces_[i][0], pbamOut.forces_[i][1],
05606                         pbamOut.forces_[i][2]);
05607             if (pbamOut.energies_[i+1] == 0.) break;
05608         }
05609     }
05610 }
05611 }
05612 }
05613 }
05614
05615 Vnm_tstop(APBS_TIMER_SOLVER, "Solver timer");
05616
05617 return 1;
05618 }
05619
05620 #endif

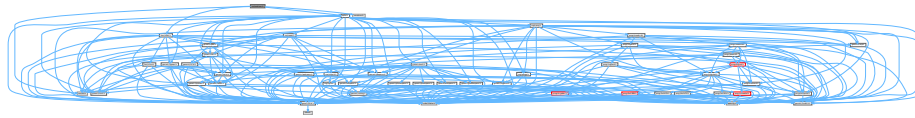
```

9.152 src/routines.h File Reference

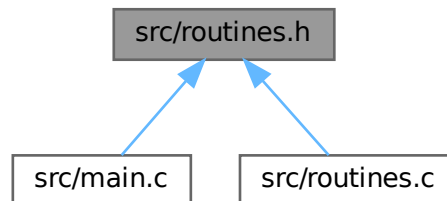
Header file for front end auxiliary routines.

```
#include "apbs.h"
#include "mc/mc.h"
#include "fem/vfetk.h"
#include "mcx/mcx.h"
```

Include dependency graph for routines.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [AtomForce](#)
Structure to hold atomic forces.

Macros

- #define [APBSRC](#) 13
Return code for APBS during failure.

Typedefs

- typedef struct [AtomForce](#) [AtomForce](#)
Define [AtomForce](#) type.

Functions

- VEXTERNC [Vparam](#) * [loadParameter](#) ([NOsh](#) *nosh)
Loads and returns parameter object.
- VEXTERNC int [loadMolecules](#) ([NOsh](#) *nosh, [Vparam](#) *param, [Valist](#) *alist[[NOSH_MAXMOL](#)])
Load the molecules given in NOsh into atom lists.

- VEXTERNC void `killMolecules` (`NOsh *nosh`, `Valist *alist[NOSH_MAXMOL]`)
Destroy the loaded molecules.
- VEXTERNC int `loadDielMaps` (`NOsh *nosh`, `Vgrid *dielXMap[NOSH_MAXMOL]`, `Vgrid *dielYMap[NOSH_MAXMOL]`, `Vgrid *dielZMap[NOSH_MAXMOL]`)
Load the dielectric maps given in NOsh into grid objects.
- VEXTERNC void `killDielMaps` (`NOsh *nosh`, `Vgrid *dielXMap[NOSH_MAXMOL]`, `Vgrid *dielYMap[NOSH_MAXMOL]`, `Vgrid *dielZMap[NOSH_MAXMOL]`)
Destroy the loaded dielectric.
- VEXTERNC int `loadKappaMaps` (`NOsh *nosh`, `Vgrid *kappa[NOSH_MAXMOL]`)
Load the kappa maps given in NOsh into grid objects.
- VEXTERNC void `killKappaMaps` (`NOsh *nosh`, `Vgrid *kappa[NOSH_MAXMOL]`)
Destroy the loaded kappa maps.
- VEXTERNC int `loadPotMaps` (`NOsh *nosh`, `Vgrid *pot[NOSH_MAXMOL]`)
Load the potential maps given in NOsh into grid objects.
- VEXTERNC void `killPotMaps` (`NOsh *nosh`, `Vgrid *pot[NOSH_MAXMOL]`)
Destroy the loaded potential maps.
- VEXTERNC int `loadChargeMaps` (`NOsh *nosh`, `Vgrid *charge[NOSH_MAXMOL]`)
Load the charge maps given in NOsh into grid objects.
- VEXTERNC void `killChargeMaps` (`NOsh *nosh`, `Vgrid *charge[NOSH_MAXMOL]`)
Destroy the loaded charge maps.
- VEXTERNC void `printPBE Parm` (`PBE Parm *pbeparm`)
Print out generic PBE params loaded from input.
- VEXTERNC void `printMG Parm` (`MG Parm *mgparm`, `double realCenter[3]`)
Print out MG-specific params loaded from input.
- VEXTERNC int `initMG` (`int icalc`, `NOsh *nosh`, `MG Parm *mgparm`, `PBE Parm *pbeparm`, `double realCenter[3]`, `Vpbe *pbe[NOSH_MAXCALC]`, `Valist *alist[NOSH_MAXMOL]`, `Vgrid *dielXMap[NOSH_MAXMOL]`, `Vgrid *dielYMap[NOSH_MAXMOL]`, `Vgrid *dielZMap[NOSH_MAXMOL]`, `Vgrid *kappaMap[NOSH_MAXMOL]`, `Vgrid *chargeMap[NOSH_MAXMOL]`, `Vpmgp *pmgp[NOSH_MAXCALC]`, `Vpmg *pmg[NOSH_MAXCALC]`, `Vgrid *potMap[NOSH_MAXMOL]`)
Initialize an MG calculation.
- VEXTERNC void `killMG` (`NOsh *nosh`, `Vpbe *pbe[NOSH_MAXCALC]`, `Vpmgp *pmgp[NOSH_MAXCALC]`, `Vpmg *pmg[NOSH_MAXCALC]`)
Kill structures initialized during an MG calculation.
- VEXTERNC int `solveMG` (`NOsh *nosh`, `Vpmg *pmg`, `MG Parm_CalcType type`)
Solve the PBE with MG.
- VEXTERNC int `setPartMG` (`NOsh *nosh`, `MG Parm *mgparm`, `Vpmg *pmg`)
Set MG partitions for calculating observables and performing I/O.
- VEXTERNC int `energyMG` (`NOsh *nosh`, `int icalc`, `Vpmg *pmg`, `int *nenergy`, `double *totEnergy`, `double *qf←Energy`, `double *qmEnergy`, `double *dielEnergy`)
Calculate electrostatic energies from MG solution.
- VEXTERNC void `killEnergy` ()
Kill arrays allocated for energies.
- VEXTERNC int `forceMG` (`Vmem *mem`, `NOsh *nosh`, `PBE Parm *pbeparm`, `MG Parm *mgparm`, `Vpmg *pmg`, `int *nforce`, `AtomForce **atomForce`, `Valist *alist[NOSH_MAXMOL]`)
Calculate forces from MG solution.
- VEXTERNC void `killForce` (`Vmem *mem`, `NOsh *nosh`, `int nforce[NOSH_MAXCALC]`, `AtomForce *atom←Force[NOSH_MAXCALC]`)
Free memory from MG force calculation.

- VEXTERNC void `storeAtomEnergy` (`Vpmg` *pmg, int icalc, double **atomEnergy, int *nenergy)
Store energy in arrays for future use.
- VEXTERNC int `writedataFlat` (`NOSH` *nosh, `Vcom` *com, const char *fname, double totEnergy[`NOSH_MAXCALC`], double qfEnergy[`NOSH_MAXCALC`], double qmEnergy[`NOSH_MAXCALC`], double dielEnergy[`NOSH_MAXCALC`], int nenergy[`NOSH_MAXCALC`], double *atomEnergy[`NOSH_MAXCALC`], int nforce[`NOSH_MAXCALC`], `AtomForce` *atomForce[`NOSH_MAXCALC`])
Write out information to a flat file.
- VEXTERNC int `writedataXML` (`NOSH` *nosh, `Vcom` *com, const char *fname, double totEnergy[`NOSH_MAXCALC`], double qfEnergy[`NOSH_MAXCALC`], double qmEnergy[`NOSH_MAXCALC`], double dielEnergy[`NOSH_MAXCALC`], int nenergy[`NOSH_MAXCALC`], double *atomEnergy[`NOSH_MAXCALC`], int nforce[`NOSH_MAXCALC`], `AtomForce` *atomForce[`NOSH_MAXCALC`])
Write out information to an XML file.
- VEXTERNC int `writedataMG` (int rank, `NOSH` *nosh, `PBEparm` *pbeparm, `Vpmg` *pmg)
Write out observables from MG calculation to file.
- VEXTERNC int `writematMG` (int rank, `NOSH` *nosh, `PBEparm` *pbeparm, `Vpmg` *pmg)
Write out operator matrix from MG calculation to file.
- VEXTERNC double `returnEnergy` (`Vcom` *com, `NOSH` *nosh, double totEnergy[`NOSH_MAXCALC`], int iprint)
Access net local energy.
- VEXTERNC int `printEnergy` (`Vcom` *com, `NOSH` *nosh, double totEnergy[`NOSH_MAXCALC`], int iprint)
Combine and pretty-print energy data (deprecated...see printElecEnergy)
- VEXTERNC int `printElecEnergy` (`Vcom` *com, `NOSH` *nosh, double totEnergy[`NOSH_MAXCALC`], int iprint)
Combine and pretty-print energy data.
- VEXTERNC int `printApolEnergy` (`NOSH` *nosh, int iprint)
Combine and pretty-print energy data.
- VEXTERNC int `printForce` (`Vcom` *com, `NOSH` *nosh, int nforce[`NOSH_MAXCALC`], `AtomForce` *atom←
Force[`NOSH_MAXCALC`], int i)
Combine and pretty-print force data (deprecated...see printElecForce)
- VEXTERNC int `printElecForce` (`Vcom` *com, `NOSH` *nosh, int nforce[`NOSH_MAXCALC`], `AtomForce` *atom←
Force[`NOSH_MAXCALC`], int i)
Combine and pretty-print force data.
- VEXTERNC int `printApolForce` (`Vcom` *com, `NOSH` *nosh, int nforce[`NOSH_MAXCALC`], `AtomForce` *atom←
Force[`NOSH_MAXCALC`], int i)
Combine and pretty-print force data.
- VEXTERNC void `startVio` ()
Wrapper to start MALOC Vio layer.
- VEXTERNC int `energyAPOL` (`APOLparm` *apolparm, double sasa, double sav, double atomsasa[], double atomwcaEnergy[], int numatoms)
Calculate non-polar energies.
- VEXTERNC int `forceAPOL` (`Vacc` *acc, `Vmem` *mem, `APOLparm` *apolparm, int *nforce, `AtomForce` **atom←
Force, `Valist` *alist, `Vclist` *clist)
Calculate non-polar forces.
- VEXTERNC int `initAPOL` (`NOSH` *nosh, `Vmem` *mem, `Vparam` *param, `APOLparm` *apolparm, int *nforce, `AtomForce` **atomForce, `Valist` *alist)
Upperlevel routine to the non-polar energy and force routines.
- VEXTERNC void `printFEPARM` (int icalc, `NOSH` *nosh, `FEParm` *feparm, `Vfetk` *fetk[`NOSH_MAXCALC`])
Print out FE-specific params loaded from input.
- VEXTERNC int `energyFE` (`NOSH` *nosh, int icalc, `Vfetk` *fetk[`NOSH_MAXCALC`], int *nenergy, double *totEnergy, double *qfEnergy, double *qmEnergy, double *dielEnergy)
Calculate electrostatic energies from FE solution.

- `VPUBLIC Vrc_Codes initFE (int icalc, NOsh *nosh, FEMparm *feparm, PBEparm *pbeparm, Vpbe *pbe[NOSH_MAXCALC], Valist *alist[NOSH_MAXMOL], Vfetk *fetk[NOSH_MAXCALC])`
Initialize FE solver objects.
- `VEXTERNC void killFE (NOsh *nosh, Vpbe *pbe[NOSH_MAXCALC], Vfetk *fetk[NOSH_MAXCALC], Gem *gem[NOSH_MAXMOL])`
Kill structures initialized during an FE calculation.
- `VEXTERNC int preRefineFE (int i, FEMparm *feparm, Vfetk *fetk[NOSH_MAXCALC])`
Pre-refine mesh before solve.
- `VEXTERNC int partFE (int i, NOsh *nosh, FEMparm *feparm, Vfetk *fetk[NOSH_MAXCALC])`
Partition mesh (if applicable)
- `VEXTERNC int solveFE (int i, PBEparm *pbeparm, FEMparm *feparm, Vfetk *fetk[NOSH_MAXCALC])`
Solve-estimate-refine.
- `VEXTERNC int postRefineFE (int icalc, FEMparm *feparm, Vfetk *fetk[NOSH_MAXCALC])`
Estimate error, mark mesh, and refine mesh after solve.
- `VEXTERNC int writedataFE (int rank, NOsh *nosh, PBEparm *pbeparm, Vfetk *fetk)`
Write FEM data to files.
- `VEXTERNC Vrc_Codes loadMeshes (NOsh *nosh, Gem *gm[NOSH_MAXMOL])`
Load the meshes given in NOsh into geometry objects.
- `VEXTERNC void killMeshes (NOsh *nosh, Gem *alist[NOSH_MAXMOL])`
Destroy the loaded meshes.

9.152.1 Detailed Description

Header file for front end auxiliary routines.

Author

Nathan Baker

Version

\$Id\$

Attention

```
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* APBS -- Adaptive Poisson-Boltzmann Solver
*
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*
*
```

Definition in file [routines.h](#).

9.153 routines.h

[Go to the documentation of this file.](#)

```

00001
00061 #ifndef _APBSROUTINES_H_
00062 #define _APBSROUTINES_H_
00063
00064 #include "apbs.h"
00065
00066 #ifdef HAVE_MC_H
00067 #    include "mc/mc.h"
00068 #    include "fem/vfetk.h"
00069 #endif
00070 #ifdef HAVE_MCX_H
00071 #    include "mcx/mcx.h"
00072 #endif
00073
00074 #ifdef ENABLE_BEM
00075 #    include "TABIPBstruct.h"
00076 #endif
00077
00078 #ifdef ENABLE_GEOFLOW
00079 #    include "GeometricFlowWrap.h"
00080 #endif
00081
00082 #if defined(ENABLE_PBAM) || defined(ENABLE_PBSAM)
00083 #    include "PBAMWrap.h"
00084 #endif
00085
00086 #ifdef ENABLE_PBSAM
00087 #    include "PBSAMWrap.h"
00088 #endif
00089
00093 #define APBSRC 13
00094
00099 struct AtomForce {
00100     double ibForce[3];
00101     double qfForce[3];
00102     double dbForce[3];
00103     double sasaForce[3];
00104     double savForce[3];
00105     double wcaForce[3];
00106 };
00107
00111 typedef struct AtomForce AtomForce;
00112
```

```

00118 VEXTERNC Vparam* loadParameter(
00119     Nosh *nosh
00121 );
00122
00128 VEXTERNC int loadMolecules(
00129     Nosh *nosh,
00130     Vparam *param,
00132     Valist *alist[NOSH_MAXMOL]
00134 );
00135
00142 VEXTERNC void killMolecules(Nosh *nosh, Valist *alist[NOSH_MAXMOL]);
00143
00153 VEXTERNC int loadDielMaps(Nosh *nosh,
00154     Vgrid *dielXMap[NOSH_MAXMOL],
00155     Vgrid *dielYMap[NOSH_MAXMOL],
00156     Vgrid *dielZMap[NOSH_MAXMOL]
00157 );
00158
00167 VEXTERNC void killDielMaps(Nosh *nosh, Vgrid *dielXMap[NOSH_MAXMOL],
00168     Vgrid *dielYMap[NOSH_MAXMOL], Vgrid *dielZMap[NOSH_MAXMOL]);
00169
00177 VEXTERNC int loadKappaMaps(Nosh *nosh, Vgrid *kappa[NOSH_MAXMOL]);
00178
00185 VEXTERNC void killKappaMaps(Nosh *nosh, Vgrid *kappa[NOSH_MAXMOL]);
00186
00194 VEXTERNC int loadPotMaps(Nosh *nosh, Vgrid *pot[NOSH_MAXMOL]);
00195
00202 VEXTERNC void killPotMaps(Nosh *nosh, Vgrid *pot[NOSH_MAXMOL]);
00203
00211 VEXTERNC int loadChargeMaps(Nosh *nosh, Vgrid *charge[NOSH_MAXMOL]);
00212
00219 VEXTERNC void killChargeMaps(Nosh *nosh, Vgrid *charge[NOSH_MAXMOL]);
00220
00226 VEXTERNC void printPBEPARM(PBEparm *pbeparm);
00227
00234 VEXTERNC void printMGPARM(MGparm *mgparm, double realCenter[3]);
00235
00241 VEXTERNC int initMG(
00242     int icalc,
00243     Nosh *nosh,
00244     MGparm *mgparm,
00245     PBEparm *pbeparm,
00246     double realCenter[3],
00247     Vpbe *pbe[NOSH_MAXCALC],
00248     Valist *alist[NOSH_MAXMOL],
00249     Vgrid *dielXMap[NOSH_MAXMOL],
00250     Vgrid *dielYMap[NOSH_MAXMOL],
00251     Vgrid *dielZMap[NOSH_MAXMOL],
00252     Vgrid *kappaMap[NOSH_MAXMOL],
00253     Vgrid *chargeMap[NOSH_MAXMOL],
00254     Vpmgp *pmgp[NOSH_MAXCALC],
00255     Vpmg *pmg[NOSH_MAXCALC],
00256     Vgrid *potMap[NOSH_MAXMOL]
00257 );
00258
00264 VEXTERNC void killMG(
00265     Nosh *nosh,
00266     Vpbe *pbe[NOSH_MAXCALC],
00267     Vpmgp *pmgp[NOSH_MAXCALC],
00268     Vpmg *pmg[NOSH_MAXCALC]
00269 );
00270
00279 VEXTERNC int solveMG(Nosh *nosh, Vpmg *pmg, MGparm_CalcType type);
00280
00289 VEXTERNC int setPartMG(Nosh *nosh, MGparm *mgparm, Vpmg *pmg);
00290
00304 VEXTERNC int energyMG(Nosh *nosh, int icalc, Vpmg *pmg,
00305     int *nenergy, double *totEnergy, double *qfEnergy, double *qmEnergy,
00306     double *dielEnergy);
00307
00312 VEXTERNC void killEnergy();
00313
00327 VEXTERNC int forceMG(Vmem *mem, Nosh *nosh, PBEparm *pbeparm, MGparm *mgparm,
00328     Vpmg *pmg, int *nforce, AtomForce **atomForce, Valist *alist[NOSH_MAXMOL]);
00329
00338 VEXTERNC void killForce(Vmem *mem, Nosh *nosh, int nforce[NOSH_MAXCALC],
00339     AtomForce *atomForce[NOSH_MAXCALC]);
00340
00345 VEXTERNC void storeAtomEnergy(
00346     Vpmg *pmg,
00347     int icalc,

```

```
00348         double **atomEnergy,
00349         int *nenergy
00350     );
00351
00368 VEXTERNC int writedataFlat(Nosh *nosh, Vcom *com, const char *fname,
00369         double totEnergy[NOSH_MAXCALC], double qfEnergy[NOSH_MAXCALC],
00370         double qmEnergy[NOSH_MAXCALC], double dielEnergy[NOSH_MAXCALC],
00371         int nenergy[NOSH_MAXCALC], double *atomEnergy[NOSH_MAXCALC],
00372         int nforce[NOSH_MAXCALC], AtomForce *atomForce[NOSH_MAXCALC]);
00373
00390 VEXTERNC int writedataXML(Nosh *nosh, Vcom *com, const char *fname,
00391         double totEnergy[NOSH_MAXCALC], double qfEnergy[NOSH_MAXCALC],
00392         double qmEnergy[NOSH_MAXCALC], double dielEnergy[NOSH_MAXCALC],
00393         int nenergy[NOSH_MAXCALC], double *atomEnergy[NOSH_MAXCALC],
00394         int nforce[NOSH_MAXCALC], AtomForce *atomForce[NOSH_MAXCALC]);
00395
00405 VEXTERNC int writedataMG(int rank, Nosh *nosh, PBEparm *pbeparm, Vpmg *pmg);
00406
00416 VEXTERNC int writematMG(int rank, Nosh *nosh, PBEparm *pbeparm, Vpmg *pmg);
00417
00427 VEXTERNC double returnEnergy(Vcom *com, Nosh *nosh, double totEnergy[NOSH_MAXCALC], int iprint);
00428
00434 VEXTERNC int printEnergy(
00435         Vcom *com,
00436         Nosh *nosh,
00437         double totEnergy[NOSH_MAXCALC],
00439         int iprint
00440     );
00441
00447 VEXTERNC int printElecEnergy(
00448         Vcom *com,
00449         Nosh *nosh,
00450         double totEnergy[NOSH_MAXCALC],
00452         int iprint
00453     );
00454
00460 VEXTERNC int printApolEnergy(
00461         Nosh *nosh,
00462         int iprint
00463     );
00464
00470 VEXTERNC int printForce(
00471         Vcom *com,
00472         Nosh *nosh,
00473         int nforce[NOSH_MAXCALC],
00474         AtomForce *atomForce[NOSH_MAXCALC],
00475         int i
00476     );
00477
00483 VEXTERNC int printElecForce(
00484         Vcom *com,
00485         Nosh *nosh,
00486         int nforce[NOSH_MAXCALC],
00487         AtomForce *atomForce[NOSH_MAXCALC],
00488         int i
00489     );
00490
00496 VEXTERNC int printApolForce(
00497         Vcom *com,
00498         Nosh *nosh,
00499         int nforce[NOSH_MAXCALC],
00500         AtomForce *atomForce[NOSH_MAXCALC],
00501         int i
00502     );
00503
00508 VEXTERNC void startVio();
00509
00515 VEXTERNC int energyAPOL(
00516         APOLparm *apolparm,
00517         double sasa,
00518         double sav,
00519         double atomsasa[],
00520         double atomwcaEnergy[],
00521         int numatoms
00522     );
00523
00529 VEXTERNC int forceAPOL(
00530         Vacc *acc,
00531         Vmem *mem,
00532         APOLparm *apolparm,
00533         int *nforce,
```

```

00536             AtomForce **atomForce,
00538             Valist *alist,
00539             Vclist *clist
00540         );
00541
00547 VEXTERNC int initAPOL(
00548     Nosh *nosh,
00549     Vmem *mem,
00550     Vparam *param,
00551     APOLparam *apolparam,
00552     int *nforce,
00553     AtomForce **atomForce,
00554     Valist *alist
00555 );
00556
00557
00558 #ifdef HAVE_MC_H
00559 #include "fem/vfetk.h"
00560
00569 VEXTERNC void printFEPARM(int icalc, Nosh *nosh, FEParm *feparm,
00570     Vfetk *fetk[NOSH_MAXCALC]);
00571
00586 VEXTERNC int energyFE(Nosh* nosh, int icalc, Vfetk *fetk[NOSH_MAXCALC],
00587     int *nenergy, double *totEnergy, double *qfEnergy, double *qmEnergy,
00588     double *dielEnergy);
00589
00597 VEXTERNC Vrc_Codes initFE(
00598     int icalc,
00599     Nosh *nosh,
00600     FEParm *feparm,
00601     PBEparam *pbeparm,
00602     Vpbe *pbe[NOSH_MAXCALC],
00603     Valist *alist[NOSH_MAXMOL],
00604     Vfetk *fetk[NOSH_MAXCALC]
00605 );
00606
00612 VEXTERNC void killFE(
00613     Nosh *nosh,
00614     Vpbe *pbe[NOSH_MAXCALC],
00615     Vfetk *fetk[NOSH_MAXCALC],
00616     Gem *gem[NOSH_MAXMOL]
00617 );
00618
00628 VEXTERNC int preRefineFE(int i,
00629     FEParm *feparm,
00630     Vfetk *fetk[NOSH_MAXCALC]
00631 );
00632
00642 VEXTERNC int partFE(int i, Nosh *nosh, FEParm *feparm,
00643     Vfetk *fetk[NOSH_MAXCALC]);
00644
00654 VEXTERNC int solveFE(int i,
00655     PBEparam *pbeparm,
00656     FEParm *feparm,
00657     Vfetk *fetk[NOSH_MAXCALC]
00658 );
00659
00671 VEXTERNC int postRefineFE(int icalc,
00672     FEParm *feparm,
00673     Vfetk *fetk[NOSH_MAXCALC]
00674 );
00675
00685 VEXTERNC int writedataFE(int rank, Nosh *nosh, PBEparam *pbeparm, Vfetk *fetk);
00686
00692 VEXTERNC Vrc_Codes loadMeshes(
00693     Nosh *nosh,
00694     Gem *gm[NOSH_MAXMOL]
00695 );
00696
00702 VEXTERNC void killMeshes(
00703     Nosh *nosh,
00704     Gem *alist[NOSH_MAXMOL]
00705 );
00706 #endif
00707
00708 #endif
00709
00710
00711
00712 VEXTERNC void printMGPARAM(MGparm *mgparm, double realCenter[3]);
00713

```

```
00714 #ifdef ENABLE_BEM
00720 VEXTERNC int initBEM(
00721     int icalc,
00722     NOsh *nosh,
00723     BEMparm *bemparm,
00724     PBEParm *pbeparm,
00725     Vpbe *pbe[NOSH_MAXCALC]
00726 );
00727
00733 VEXTERNC void killBEM(
00734     NOsh *nosh,
00735     Vpbe *pbe[NOSH_MAXCALC]
00736 );
00737
00746 VEXTERNC int solveBEM(Valist* molecules[NOSH_MAXMOL], NOsh *nosh, PBEParm *pbeparm, BEMparm *bemparm,
    BEMparm_CalcType type);
00747
00756 VEXTERNC int setPartBEM(NOsh *nosh, BEMparm *bemparm);
00757
00771 VEXTERNC int energyBEM(NOsh* nosh, int icalc,
00772     int *nenergy, double *totEnergy, double *qfEnergy, double *qmEnergy,
00773     double *dielEnergy);
00774
00788 VEXTERNC int forceBEM(NOsh *nosh, PBEParm *pbeparm, BEMparm *bemparm,
00789     int *nforce, AtomForce **atomForce, Valist *alist[NOSH_MAXMOL]);
00790
00797 VEXTERNC void printBEMPARM(BEMparm *bemparm);
00798
00808 VEXTERNC int writedataBEM(int rank, NOsh *nosh, PBEParm *pbeparm);
00809
00819 VEXTERNC int writematBEM(int rank, NOsh *nosh, PBEParm *pbeparm);
00820 #endif
00821
00822 #ifdef ENABLE_GEOFLOW
00830 VEXTERNC int solveGeometricFlow(
00831     Valist* molecules[NOSH_MAXMOL],
00832     NOsh *nosh,
00833     PBEParm *pbeparm,
00834     APOLparm *apolparm,
00835     GEOFLOWparm *parm
00836 );
00837 #endif
00838
00839 #ifdef ENABLE_PBAM
00847 VEXTERNC int solvePBAM(
00848     Valist* molecules[NOSH_MAXMOL],
00849     NOsh *nosh,
00850     PBEParm *pbeparm,
00851     PBAMparm *parm
00852 );
00853 #endif
00854
00855 #ifdef ENABLE_PBSAM
00863 VEXTERNC int solvePBSAM(
00864     Valist* molecules[NOSH_MAXMOL],
00865     NOsh *nosh,
00866     PBEParm *pbeparm,
00867     PBAMparm *parm,
00868     PBSAMparm *samparm
00869 );
00870 #endif
```


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