

iAPBS

1.0.0

Generated by Doxygen 1.5.8

Wed Nov 18 14:47:49 2009

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Chapter 1

Directory Hierarchy

1.1 Directories

This directory hierarchy is sorted roughly, but not completely, alphabetically:

src 5

Chapter 2

File Index

2.1 File List

Here is a list of all documented files with brief descriptions:

| | |
|---|----|
| apbs_driver.c (The main iAPBS driver code) | 7 |
| apbs_driver.h (Header file for the main iAPBS driver) | 11 |

Chapter 3

Directory Documentation

3.1 /tmp/iapbs-1.0.0/src/ Directory Reference

Files

- file [apbs_driver.c](#)
The main iAPBS driver code.
- file [apbs_driver.h](#)
Header file for the main iAPBS driver.
- file **wrapper.f**
- file **wrapper_inc.f**

Chapter 4

File Documentation

4.1 apbs_driver.c File Reference

The main iAPBS driver code.

```
#include "apbs/apbs.h"
#include "apbs/nosh.h"
#include "apbs/mgparm.h"
#include "apbs/pbeparm.h"
#include "apbs/femparm.h"
#include "apbs/routines.h"
#include "apbs_driver.h"
```

Defines

- #define `MAX_BUF_SIZE` 4096
Buffer size for internal APBS string input.

Functions

- int `apbsdrv_` (int *nat, double x[NATOMS], double y[NATOMS], double z[NATOMS], double radius[NATOMS], double charge[NATOMS], double r_param[9], int i_param[25], double grid[3], int dime[3], int pdime[3], double glen[3], double center[3], double cglen[3], double fglen[3], double ccenter[3],

```
double fcenter[3], double *ofrac, int *dbg, double ionq[MAXION], double
ionc[MAXION], double ionr[MAXION], double esEnergy[1], double
npEnergy[1], double apbsdX[NATOMS], double apbsdY[NATOMS], double
apbsdZ[NATOMS], double apbsqfx[NATOMS], double apbsqfy[NATOMS],
double apbsqfz[NATOMS], double apbsibx[NATOMS], double
apbsiby[NATOMS], double apbsibz[NATOMS], double apbsnpx[NATOMS],
double apbsnpy[NATOMS], double apbsnpz[NATOMS], double
apbsdbx[NATOMS], double apbsdby[NATOMS], double apbsdbz[NATOMS])
```

Wrapper iAPBS function.

- char * [setupString](#) (double r_param[9], int i_param[25], double grid[3], int dime[3], double ionq[MAXION], double ionc[MAXION], double ionr[MAXION], double glen[3], double center[3], double cglen[3], double fglen[3], double ccenter[3], double fcenter[3], double *ofrac, int pdime[3], int debug)

Creates APBS input string.

- double [getElecEnergy](#) (Vcom *com, NOsh *nosh, double totEnergy[NOSH_-MAXCALC], int iprint)

Combine and pretty-print energy data.

4.1.1 Detailed Description

The main iAPBS driver code.

Author:

Robert Konecny

Note:

Energy is returned in kJ/mol, forces in kJ/(mol/Å).

Revision

273

Id

[apbs_driver.c](#) 273 2009-05-07 04:06:25Z rok

4.1.2 Function Documentation

4.1.2.1 `int apbsdrv_ (int * nat, double x[NATOMS], double y[NATOMS], double z[NATOMS], double radius[NATOMS], double charge[NATOMS], double r_param[9], int i_param[25], double grid[3], int dime[3], int pdime[3], double glen[3], double center[3], double cglen[3], double fglen[3], double ccenter[3], double fcenter[3], double * ofrac, int * dbg, double ionq[MAXION], double ionc[MAXION], double ionr[MAXION], double esEnergy[1], double npEnergy[1], double apbsdx[NATOMS], double apbsdy[NATOMS], double apbsdz[NATOMS], double apbsqfx[NATOMS], double apbsqfy[NATOMS], double apbsqfz[NATOMS], double apbsibx[NATOMS], double apbsiby[NATOMS], double apbsibz[NATOMS], double apbsnpx[NATOMS], double apbsnpy[NATOMS], double apbsnpz[NATOMS], double apbsdbx[NATOMS], double apbsdby[NATOMS], double apbsdbz[NATOMS])`

Wrapper iAPBS function.

Author:

Robert Konecny

References `getElecEnergy()`, `MAX_BUF_SIZE`, and `setupString()`.

4.1.2.2 `double getElecEnergy (Vcom * com, NOsh * nosh, double totEnergy[NOSH_MAXCALC], int iprint)`

Combine and pretty-print energy data.

Note:

Collect Elect Energy

Author:

Robert Konecny

Parameters:

nosh Communications object

totEnergy Parameters from input file

iprint Array of energies from different calculations Index of energy statement to print

Referenced by `apbsdrv_()`.

4.1.2.3 `char* setupString (double r_param[9], int i_param[25], double grid[3], int dime[3], double ionq[MAXION], double ionc[MAXION], double ionr[MAXION], double glen[3], double center[3], double cglen[3], double fglen[3], double ccenter[3], double fcenter[3], double * ofrac, int pdime[3], int debug)`

Creates APBS input string.

Author:

Robert Konecny

References MAX_BUF_SIZE.

Referenced by apbsdrv_().

4.2 apbs_driver.h File Reference

Header file for the main iAPBS driver.

Defines

- #define [NATOMS](#) 150000
Maximum number of atoms.

Functions

- VEXTERNC int [apbsdrv_](#) (int *nat, double x[NATOMS], double y[NATOMS], double z[NATOMS], double radius[NATOMS], double charge[NATOMS], double r_param[9], int i_param[25], double grid[3], int dime[3], int pdime[3], double glen[3], double center[3], double cglen[3], double fglen[3], double ccenter[3], double fcenter[3], double *ofrac, int *dbg, double ionq[MAXION], double ionc[MAXION], double ionr[MAXION], double esEnergy[NOSH_MAXCALC], double npEnergy[NOSH_MAXCALC], double apbsdxdx[NATOMS], double apbsdy[NATOMS], double apbsdz[NATOMS], double apbsqfx[NATOMS], double apbsqfy[NATOMS], double apbsqfz[NATOMS], double apbsibx[NATOMS], double apbsiby[NATOMS], double apbsibz[NATOMS], double apbsnpx[NATOMS], double apbsnpy[NATOMS], double apbsnpz[NATOMS], double apsdbx[NATOMS], double apsdby[NATOMS], double apsdzbz[NATOMS])
Wrapper iAPBS function.
- VEXTERNC int [iforceMG](#) (Vmem *mem, NOsh *nosh, PBEparm *pbeparm, MGparm *mgparm, Vpmg *pmg, int *nforce, AtomForce **atomForce, Valist *alist[NOSH_MAXMOL], int debug)
Calculate forces from MG solution.
- double [getElecEnergy](#) (Vcom *com, NOsh *nosh, double totEnergy[NOSH_MAXCALC], int iprint)
Combine and pretty-print energy data.
- char * [setupString](#) (double r_param[7], int i_param[21], double grid[3], int dime[3], double ionq[MAXION], double ionc[MAXION], double ionr[MAXION], double glen[3], double center[3], double cglen[3], double fglen[3], double ccenter[3], double fcenter[3], double *ofrac, int pdime[3], int debug)
Creates APBS input string.

4.2.1 Detailed Description

Header file for the main iAPBS driver.

Author:

Robert Konecny

Version:

Id

[apbs_driver.h](#) 273 2009-05-07 04:06:25Z rok

4.2.2 Function Documentation

4.2.2.1 `VEXTERNC int apbsdrv_ (int * nat, double x[NATOMS], double y[NATOMS], double z[NATOMS], double radius[NATOMS], double charge[NATOMS], double r_param[9], int i_param[25], double grid[3], int dime[3], int pdime[3], double glen[3], double center[3], double cglen[3], double fglen[3], double ccenter[3], double fcenter[3], double * ofrac, int * dbg, double ionq[MAXION], double ionc[MAXION], double ionr[MAXION], double esEnergy[NOSH_MAXCALC], double npEnergy[NOSH_MAXCALC], double apbsdx[NATOMS], double apbsdy[NATOMS], double apbsdz[NATOMS], double apbsqfx[NATOMS], double apbsqfy[NATOMS], double apbsqfz[NATOMS], double apbsibx[NATOMS], double apbsiby[NATOMS], double apbsibz[NATOMS], double apbsnpx[NATOMS], double apbsnpy[NATOMS], double apbsnpz[NATOMS], double apbsdbx[NATOMS], double apbsdby[NATOMS], double apbsdbz[NATOMS])`

Wrapper iAPBS function.

Author:

Robert Konecny

Parameters:

- nat* Number of atoms
- x* Atomic coordinate (x)
- y* Atomic coordinate (y)
- z* Atomic coordinate (z)

radius Atomic radii
charge Atomic charges
r_param Input APBS parameters (real values)
i_param Input APBS parameters (integer values)
grid Grid spacing
dime Grid dimensions
pdime Grid of processors to be used in calculation
glen Grid side lengths
center Grid center
cglen Coarse grid side lengths
fglen Fine grid side lengths
ccenter Coarse grid center
fcenter Fine grid center
ofrac Overlap fraction between procs
dbg Debug verbosity flag
ionq Mobile ion charge
ionc Mobile ion concentration
ionr Mobile ion radius
esEnergy Electrostatic energy
npEnergy Non-polar energy
apbsdx Total electrostatic force per atom (x coordinate)
apbsdy Total electrostatic force per atom (y coordinate)
apbsdz Total electrostatic force per atom (z coordinate)
apbsqfx Fixed charge force (x)
apbsqfy Fixed charge force (y)
apbsqfz Fixed charge force (z)
apbsibx Ionic boundary force (x)
apbsiby Ionic boundary force (y)
apbsibz Ionic boundary force (z)
apbsnpx Non-polar force (x)
apbsnpy Non-polar force (y)
apbsnpz Non-polar force (z)
apbsdbx Dielectric boundary force (x)
apbsdby Dielectric boundary force (y)
apbsdbz Dielectric boundary force (z)

Returns:

1 if successful, 0 otherwise

4.2.2.2 `double getElecEnergy (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

Note:

Collect Elect Energy

Author:

Robert Konecny

Parameters:

nosh Communications object

totEnergy Parameters from input file

iprint Array of energies from different calculations Index of energy statement to print

Referenced by `apbsdrv_()`.

4.2.2.3 `VEXTERNC int iforceMG (Vmem * mem, NOsh * nosh, PBEparm * pbeparm, MGparm * mgparm, Vpmg * pmg, int * nforce, AtomForce ** atomForce, Valist * alist[NOSH_MAXMOL], int debug)`

Calculate forces from MG solution.

Author:

Robert Konecny (based on `forceMG`)

Parameters:

mem Memory management object

nosh Parameters from input file

pbeparm Generic PBE parameters

mgparm MG-specific parameters

pmg MG object
nforce 0 => no forces, 1 => net forces, >1 => number of forces (1 per atom)
atomForce Pointer to array of force objects
alist List of atom lists
debug verbosity flag

Returns:

1 if successful, 0 otherwise

4.2.2.4 `char* setupString (double r_param[7], int i_param[21], double grid[3], int dime[3], double ionq[MAXION], double ionc[MAXION], double ionr[MAXION], double glen[3], double center[3], double cglen[3], double fglen[3], double ccenter[3], double fcenter[3], double * ofrac, int pdime[3], int debug)`

Creates APBS input string.

Author:

Robert Konecny

Parameters:

r_param Input APBS parameters (real values)
i_param Input APBS parameters (integer values)
grid Grid spacing
dime Grid dimensions
ionq Mobile ion charge
ionc Mobile ion concentration
ionr Mobile ion radius
glen Grid side lengths
center Grid center
cglen Coarse grid side lengths
fglen Fine grid side lengths
ccenter Coarse grid center
fcenter Fine grid center
ofrac Overlap fraction between procs
pdime Grid of processors to be used in calculation
debug Debug verbosity level.

Returns:

the input string

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