Voro++

Generated by Doxygen 1.5.7

Mon Nov 3 18:02:17 2008

Contents

Chapter 1

Voro++ class reference manual

1.1 Introduction

Voro++ is a software library for carrying out 3D cell-based calculations of the Voronoi tessellation. It is primarily designed for applications in physics and materials science, where the Voronoi tessellation can be a useful tool in analyzing particle systems.

Voro++ is comprised of several C++ classes, and is designed to be incorporated into other programs. This manual provides a reference for every function in the class structure. For a general overview of the program, see the Voro++ website at http://math.lbl.gov/voro++/ and in particular the example programs at http://math.lbl.gov/voro++/examples/ that demonstrate many of the library's features.

1.2 C++ class structure

The code is structured around two main C++ classes. The voronoicell class contains all of the routines for constructing a single Voronoi cell. It represents the cells as a collection of vertices that are connected by edges. The command init() can be used to initialize a cell as a large rectangular box. The Voronoi cell can then be computed by repeatedly cutting it with planes that correspond to the perpendicular bisectors between on point and its neighbors. The command plane() will recompute the cell after cutting with a single plane. Once the cell is computed, it can be drawn using commands such as draw_gnuplot() and draw_pov(), or its volume can be computed using the volume() command.

The container class represents a 3D rectangular box of particles. The constructor for this class sets up the coordinate ranges, sets whether each direction is periodic or not, and divides the box into a rectangular subgrid of regions. Particles can be added to the container using the put() command, that adds a particle's position and an integer numerical ID label, to the container by adding it to the corresponding region. The command import() can be used to read in large numbers of particles from a text file. The compute_cell() function creates a single Voronoi cell for a particle in the container, by making use of the voronoicell class, and constructing the cell by making calls to the plane() routine to account for neighboring points. Various commands such as store_cell_volumes() and draw_cells_gnuplot() can be used to calculate and draw the cells in the entire container or in a subregion.

1.3 Extra functionality and the use of templates

The library also supports the Voronoi radical tessellation, by using the container_poly class that is a variant of the container class where the put() command accepts an additional argument for the particle radius. To create this without repeating large parts of the code, the library makes use of templates. The source code is structured around a general template called container_base. There are then two small classes called radius_mono and radius_poly that handle all of the routines for the regular and radical tessellations respectively. The container class is created as the instantiation of the container_base template with the radius_mono class, and the container_poly class is the instantiation of the container_base template with the radius_poly class. Since the different instances are created during the program compilation and since all of the functions of radius_mono and radius_poly are declared inline, this approach should result in minimal overhead with a good compiler.

Similarly, the voronoicell class is constructed around a template called voronoicell_base. The voronoicell class is an instantiation of this template using the neighbor_none class, that does not compute any neighbor information. A variant called voronoicell_neighbor is also available, that makes use of the neighbor_track class to additionally carry out neighbor tracking during the cell construction.

1.4 Wall computation

Wall computations are handled by making use of a pure virtual wall class. Specific wall types are derived from this class, and have a routine called point_inside() that tests to see if a point is inside a wall or not, and a routine called cut_cell() that cuts a cell according to the wall's position. The walls can be added to the container using the add_wall() command, and these are called each time a compute_cell() command is carried out. At present, wall types for planes, spheres, cylinders, and cones are provided, although custom walls can be added by creating new classes derived from the pure virtual class.

Chapter 2

Class Index

2.1 Class Hierarchy

This inheritance list is sorted roughly, but not completely, alphabetically:

Chapter 3

Class Index

3.1 Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

Chapter 4

Class Documentation

4.1 container_base< r_option > Class Template Reference

A class representing the whole simulation region.

`#include <container.hh>`

Public Member Functions

- container_base (fpoint xa, fpoint xb, fpoint ya, fpoint yb, fpoint za, fpoint zb, int xn, int yn, int zn, bool xper, bool yper, bool zper, int memi)
- ~container_base ()
- void draw_particles (const char *filename)
- void draw_particles ()
- void draw_particles (ostream &os)
- void draw_particles_pov (const char *filename)
- void draw_particles_pov ()
- void draw_particles_pov (ostream &os)
- void import (istream &is)
- void import ()
- void import (const char *filename)
- void region_count ()
- void clear ()
- void draw_cells_gnuplot (const char *filename, fpoint xmin, fpoint xmax, fpoint ymin, fpoint ymax, fpoint zmin, fpoint zmax)
- void draw_cells_gnuplot (const char *filename)
- void draw_cells_pov (const char *filename, fpoint xmin, fpoint xmax, fpoint ymin, fpoint ymax, fpoint zmin, fpoint zmax)
- void draw_cells_pov (const char *filename)
- void store_cell_volumes (fpoint *bb)
- fpoint packing_fraction (fpoint *bb, fpoint cx, fpoint cy, fpoint cz, fpoint r)
- fpoint packing_fraction (fpoint *bb, fpoint xmin, fpoint xmax, fpoint ymin, fpoint ymax, fpoint zmin, fpoint zmax)
- fpoint sum_cell_volumes ()

- void compute_all_cells ()
- void print_all (ostream &os)
- void print_all ()
- void print_all (const char *filename)
- void print_all_neighbor (ostream &os)
- void print_all_neighbor ()
- void print_all_neighbor (const char *filename)
- template<class n_option >
  bool compute_cell_sphere (voronoicell_base< n_option > &c, int i, int j, int k, int ijk, int s)
- template<class n_option >
  bool compute_cell_sphere (voronoicell_base< n_option > &c, int i, int j, int k, int ijk, int s, fpoint x, fpoint y, fpoint z)
- template<class n_option >
  bool compute_cell (voronoicell_base< n_option > &c, int i, int j, int k, int ijk, int s)
- template<class n_option >
  bool compute_cell (voronoicell_base< n_option > &c, int i, int j, int k, int ijk, int s, fpoint x, fpoint y, fpoint z)
- void put (int n, fpoint x, fpoint y, fpoint z)
- void put (int n, fpoint x, fpoint y, fpoint z, fpoint r)
- void add_wall (wall &w)
- bool point_inside (fpoint x, fpoint y, fpoint z)
- bool point_inside_walls (fpoint x, fpoint y, fpoint z)

Protected Member Functions

- template<class n_option >
  void print_all (ostream &os, voronoicell_base< n_option > &c)
- template<class n_option >
  bool initialize_voronoicell (voronoicell_base< n_option > &c, fpoint x, fpoint y, fpoint z)
- void add_particle_memory (int i)
- void add_list_memory ()

Protected Attributes

- const fpoint ax
- const fpoint bx
- const fpoint ay
- const fpoint by
- const fpoint az
- const fpoint bz
- const fpoint xsp
- const fpoint ysp
- const fpoint zsp
- const int nx
- const int ny
- const int nz
- const int nxy
- const int nxyz

- const int hx
- const int hy
- const int hz
- const int hxy
- const int hxyz
- const bool xperiodic
- const bool yperiodic
- const bool zperiodic
- int * co
- int * mem
- int ** id
- unsigned int * mask
- int * sl
- unsigned int mv
- int s_start
- int s_end
- int s_size
- fpoint ** p
- wall ** walls
- int wall_number
- int current_wall_size
- r_option radius
- int sz
- fpoint * mrad

Friends

- class facets_loop
- class radius_poly

4.1.1 Detailed Description

template<class r_option> class container_base< r_option >

A class representing the whole simulation region.

The container class represents the whole simulation region. The container constructor sets up the geometry and periodicity, and divides the geometry into rectangular grid of blocks, each of which handles the particles in a particular area. Routines exist for putting in particles, importing particles from standard input, and carrying out Voronoi calculations.

Definition at line 30 of file container.hh.

4.1.2 Constructor & Destructor Documentation

4.1.2.1 template<class r_option > container_base< r_option >::container_base (fpoint *xa*, fpoint *xb*, fpoint *ya*, fpoint *yb*, fpoint *za*, fpoint *zb*, int *xn*, int *yn*, int *zn*, bool *xper*, bool *yper*, bool *zper*, int *memi*) [inline]

Container constructor. The first six arguments set the corners of the box to be (xa,ya,za) and (xb,yb,zb). The box is then divided into an nx by ny by nz grid of blocks, set by the following three arguments. The next three arguments are booleans, which set the periodicity in each direction. The final argument sets the amount of memory allocated to each block.

Definition at line 16 of file container.cc.

4.1.2.2 template<class r_option > container_base< r_option >::~container_base () [inline]

Container destructor - free memory.

Definition at line 131 of file container.cc.

4.1.3 Member Function Documentation

4.1.3.1 template<class r_option > void container_base< r_option >::add_list_memory () [inline, protected]

Add list memory.

Definition at line 264 of file container.cc.

4.1.3.2 template<class r_option > void container_base< r_option >::add_particle_memory (int *i*) [inline, protected]

Increase memory for a particular region.

Definition at line 246 of file container.cc.

4.1.3.3 template<class r_option > void container_base< r_option >::add_wall (wall & *w*) [inline]

Adds a wall to the container.

Parameters:

← *&w* a wall object to be added.

Definition at line 1372 of file container.cc.

4.1.3.4 template<class r_option > void container_base< r_option >::clear () [inline]

Clears a container of particles.

Definition at line 318 of file container.cc.

4.1.3.5 template<class r_option > void container_base< r_option >::compute_all_cells () [inline]

This function computes all the cells in the container, but does nothing with the output. It is useful for measuring the pure computation time of the Voronoi algorithm, without any extraneous calculations, such as volume evaluation or cell output.

Definition at line 389 of file container.cc.

4.1.3.6 template<class r_option > template<class n_option > bool container_base< r_option >::compute_cell (voronoicell_base< n_option > & *c*, int *i*, int *j*, int *k*, int *ijk*, int *s*, fpoint *x*, fpoint *y*, fpoint *z*) [inline]

This routine computes a Voronoi cell for a single particle in the container. It can be called by the user, but is also forms the core part of several of the main functions, such as store_cell_volumes(), print_all(), and the drawing routines. The algorithm constructs the cell by testing over the neighbors of the particle, working outwards until it reaches those particles which could not possibly intersect the cell. For maximum efficiency, this algorithm is divided into three parts. In the first section, the algorithm tests over the blocks which are in the immediate vicinity of the particle, by making use of one of the precomputed worklists. The code then continues to test blocks on the worklist, but also begins to construct a list of neighboring blocks outside the worklist which may need to be test. In the third section, the routine starts testing these neighboring blocks, evaluating whether or not a particle in them could possibly intersect the cell. For blocks that intersect the cell, it tests the particles in that block, and then adds the block neighbors to the list of potential places to consider.

Parameters:

- ← *&c* a reference to a voronoicell object.
- ← ***(i,j,k)*** the coordinates of the block that the test particle is in.
- ← ***ijk*** the index of the block that the test particle is in, set to i+nx∗(j+ny∗k).
- ← ***s*** the index of the particle within the test block.
- ← ***(x,y,z)*** The coordinates of the particle.
- ← ***s*** the index of the particle within the test block.

Definition at line 706 of file container.cc.

4.1.3.7 template<class r_option > template<class n_option > bool container_base< r_option >::compute_cell (voronoicell_base< n_option > & *c*, int *i*, int *j*, int *k*, int *ijk*, int *s*) [inline]

A overloaded version of compute_cell, that sets up the x, y, and z variables. It can be run by the user, and it is also called multiple times by the functions print_all(), store_cell_volumes(), and the output routines.

Parameters:

- ← *&c* a reference to a voronoicell object.
- ← ***(i,j,k)*** the coordinates of the block that the test particle is in.
- ← ***ijk*** the index of the block that the test particle is in, set to i+nx∗(j+ny∗k).
- ← ***s*** the index of the particle within the test block.

Definition at line 675 of file container.cc.

4.1.3.8 template<class r_option > template<class n_option > bool container_base< r_option >::compute_cell_sphere (voronoicell_base< n_option > & *c*, int *i*, int *j*, int *k*, int *ijk*, int *s*, fpoint *x*, fpoint *y*, fpoint *z*) [inline]

This routine is a simpler alternative to compute_cell(), that constructs the cell by testing over successively larger spherical shells of particles. For a container that is homogeneously filled with particles, this routine runs as fast as compute_cell(). However, it rapidly becomes inefficient for cases when the particles are not homogeneously distributed, or where parts of the container might not be filled. In that case, the spheres may grow very large before being cut off, leading to poor efficiency.

Parameters:

← *&c* a reference to a voronoicell object.
← *(i,j,k)* the coordinates of the block that the test particle is in.
← *ijk* the index of the block that the test particle is in, set to i+nx∗(j+ny∗k).
← *s* the index of the particle within the test block.
← *(x,y,z)* The coordinates of the particle.

Definition at line 618 of file container.cc.

4.1.3.9 template<class r_option > template<class n_option > bool container_base< r_option >::compute_cell_sphere (voronoicell_base< n_option > & *c*, int *i*, int *j*, int *k*, int *ijk*, int *s*) [inline]

A overloaded version of compute_cell_sphere(), that sets up the x, y, and z variables.

Parameters:

← *&c* a reference to a voronoicell object.
← *(i,j,k)* the coordinates of the block that the test particle is in.
← *ijk* the index of the block that the test particle is in, set to i+nx∗(j+ny∗k).
← *s* the index of the particle within the test block.

Definition at line 659 of file container.cc.

4.1.3.10 template<class r_option > void container_base< r_option >::draw_cells_gnuplot (const char ∗ *filename*) [inline]

If only a filename is supplied to draw_cells_gnuplot(), then assume that we are calculating the entire simulation region.

Definition at line 349 of file container.cc.

4.1.3.11 template<class r_option > void container_base< r_option >::draw_cells_gnuplot (const char ∗ *filename*, fpoint *xmin*, fpoint *xmax*, fpoint *ymin*, fpoint *ymax*, fpoint *zmin*, fpoint *zmax*) [inline]

Computes the Voronoi cells for all particles within a box with corners (xmin,ymin,zmin) and (xmax,ymax,zmax), and saves the output in a format that can be read by gnuplot.

Definition at line 327 of file container.cc.

4.1.3.12 template<class r_option > void container_base< r_option >::draw_cells_pov (const char * *filename*) [inline]

If only a filename is supplied to draw_cells_pov(), then assume that we are calculating the entire simulation region.

Definition at line 380 of file container.cc.

4.1.3.13 template<class r_option > void container_base< r_option >::draw_cells_pov (const char * *filename*, fpoint *xmin*, fpoint *xmax*, fpoint *ymin*, fpoint *ymax*, fpoint *zmin*, fpoint *zmax*) [inline]

Computes the Voronoi cells for all particles within a box with corners (xmin,ymin,zmin) and (xmax,ymax,zmax), and saves the output in a format that can be read by gnuplot.

Definition at line 357 of file container.cc.

4.1.3.14 template<class r_option > void container_base< r_option >::draw_particles (ostream & *os*) [inline]

Dumps all the particle positions and identifies to a file.

Definition at line 147 of file container.cc.

4.1.3.15 template<class r_option > void container_base< r_option >::draw_particles () [inline]

An overloaded version of the draw_particles() routine, that just prints to standard output.

Definition at line 161 of file container.cc.

4.1.3.16 template<class r_option > void container_base< r_option >::draw_particles (const char * *filename*) [inline]

An overloaded version of the draw_particles() routine, that outputs the particle positions to a file.

Parameters:

← *filename* the file to write to.

Definition at line 169 of file container.cc.

4.1.3.17 template<class r_option > void container_base< r_option >::draw_particles_pov (ostream & *os*) [inline]

Dumps all the particle positions in the POV-Ray format.

Definition at line 178 of file container.cc.

4.1.3.18 template<class r_option > void container_base< r_option >::draw_particles_pov () [inline]

An overloaded version of the draw_particles_pov() routine, that just prints to standard output.

Definition at line 194 of file container.cc.

4.1.3.19 template<class r_option > void container_base< r_option >::draw_particles_pov (const char * *filename*) [inline]

An overloaded version of the draw_particles_pov() routine, that outputs the particle positions to a file.

Parameters:

← ***filename*** the file to write to.

Definition at line 202 of file container.cc.

4.1.3.20 template<class r_option > void container_base< r_option >::import (const char * *filename*) [inline]

An overloaded version of the import routine, that reads in particles from a particular file.

Parameters:

← ***filename*** The name of the file to read from.

Definition at line 298 of file container.cc.

4.1.3.21 template<class r_option > void container_base< r_option >::import () [inline]

An overloaded version of the import routine, that reads the standard input.

Definition at line 290 of file container.cc.

4.1.3.22 template<class r_option > void container_base< r_option >::import (istream & *is*) [inline]

Import a list of particles from standard input.

Definition at line 283 of file container.cc.

4.1.3.23 template<class r_option > template<class n_option > bool container_base< r_option >::initialize_voronoicell (voronoicell_base< n_option > & *c*, fpoint *x*, fpoint *y*, fpoint *z*) [inline, protected]

Initialize the Voronoi cell to be the entire container. For non-periodic coordinates, this is set by the position of the walls. For periodic coordinates, the space is equally divided in either direction from the particle's initial position. That makes sense since those boundaries would be made by the neighboring periodic images of this particle.

Definition at line 567 of file container.cc.

4.1.3.24 template<class r_option > fpoint container_base< r_option >::packing_fraction (fpoint * *bb*, fpoint *xmin*, fpoint *xmax*, fpoint *ymin*, fpoint *ymax*, fpoint *zmin*, fpoint *zmax*) [inline]

Computes the local packing fraction at a point, by summing the volumes of all particles within test box, and dividing by the sum of their Voronoi volumes that were previous computed using the store_cell_volumes() function.

Parameters:

← ∗*bb* an array holding the Voronoi volumes of the particles.

← *(xmin,ymin,zmin)* the minimum coordinates of the box.

← *(xmax,ymax,zmax)* the maximum coordinates of the box.

Definition at line 450 of file container.cc.

4.1.3.25 template<class r_option > fpoint container_base< r_option >::packing_fraction (fpoint * *bb*, fpoint *cx*, fpoint *cy*, fpoint *cz*, fpoint *r*) [inline]

Computes the local packing fraction at a point, by summing the volumes of all particles within a test sphere, and dividing by the sum of their Voronoi volumes that were previous computed using the store_cell_volumes() function.

Parameters:

← ∗*bb* an array holding the Voronoi volumes of the particles.

← *(cx,cy,cz)* the center of the test sphere.

← *r* the radius of the test sphere.

Definition at line 423 of file container.cc.

4.1.3.26 template<class r_option > bool container_base< r_option >::point_inside (fpoint *x*, fpoint *y*, fpoint *z*) [inline]

This function tests to see if a given vector lies within the container bounds and any walls.

Parameters:

← *(x,y,z)* The position vector to be tested.

Returns:

True if the point is inside the container, false if the point is outside.

Definition at line 585 of file container.cc.

4.1.3.27 template<class r_option > bool container_base< r_option >::point_inside_walls (fpoint *x*, fpoint *y*, fpoint *z*) [inline]

This function tests to see if a give vector lies within the walls that have been added to the container, but does not specifically check whether the vector lies within the container bounds.

Parameters:

← ***(x,y,z)*** The position vector to be tested.

Returns:

True if the point is inside the container, false if the point is outside.

Definition at line 597 of file container.cc.

4.1.3.28 template<class r_option > template<class n_option > void container_base< r_option >::print_all (ostream & *os*, voronoicell_base< n_option > & *c*) [inline, protected]

Prints a list of all particle labels, positions, and Voronoi volumes to the standard output.

Definition at line 485 of file container.cc.

4.1.3.29 template<class r_option > void container_base< r_option >::print_all (const char * *filename*) [inline]

An overloaded version of print_all(), which outputs the result to a particular file.

Parameters:

← ***filename*** The name fo the file to write to.

Definition at line 523 of file container.cc.

4.1.3.30 template<class r_option > void container_base< r_option >::print_all () [inline]

An overloaded version of print_all(), which just prints to standard output.

Definition at line 514 of file container.cc.

4.1.3.31 template<class r_option > void container_base< r_option >::print_all (ostream & *os*) [inline]

Prints a list of all particle labels, positions, and Voronoi volumes to the standard output.

Definition at line 507 of file container.cc.

4.1.3.32 template<class r_option > void container_base< r_option >::print_all_neighbor (const char * *filename*) [inline]

An overloaded version of print_all_neighbor(), which outputs the result to a particular file

Parameters:

← ***filename*** The name of the file to write to.

Definition at line 552 of file container.cc.

4.1.3.33 template<class r_option > void container_base< r_option >::print_all_neighbor () [inline]

An overloaded version of print_all_neighbor(), which just prints to standard output.

Definition at line 543 of file container.cc.

4.1.3.34 template<class r_option > void container_base< r_option >::print_all_neighbor (ostream & *os*) [inline]

Prints a list of all particle labels, positions, Voronoi volumes, and a list of neighboring particles to an output stream.

Parameters:

← ***os*** The output stream to print to.

Definition at line 535 of file container.cc.

4.1.3.35 template<class r_option > void container_base< r_option >::put (int *n*, fpoint *x*, fpoint *y*, fpoint *z*, fpoint *r*) [inline]

Put a particle into the correct region of the container.

Parameters:

← ***n*** The numerical ID of the inserted particle.
← ***(x,y,z)*** The position vector of the inserted particle.
← ***r*** The radius of the particle.

Definition at line 230 of file container.cc.

4.1.3.36 template<class r_option > void container_base< r_option >::put (int *n*, fpoint *x*, fpoint *y*, fpoint *z*) [inline]

Put a particle into the correct region of the container.

Definition at line 211 of file container.cc.

4.1.3.37 template<class r_option > void container_base< r_option >::region_count () [inline]

Outputs the number of particles within each region.

Definition at line 307 of file container.cc.

4.1.3.38 template<class r_option > void container_base< r_option >::store_cell_volumes (fpoint * *bb*) [inline]

Computes the Voronoi volumes for all the particles, and stores the results according to the particle label in the fpoint array bb.

Definition at line 401 of file container.cc.

4.1.3.39 template<class r_option > fpoint container_base< r_option >::sum_cell_volumes () [inline]

Computes the Voronoi volumes for all the particles, and stores the results according to the particle label in the fpoint array bb.

Definition at line 472 of file container.cc.

4.1.4 Member Data Documentation

4.1.4.1 template<class r_option > const fpoint container_base< r_option >::ax [protected]

The minimum x coordinate of the container.

Definition at line 75 of file container.hh.

4.1.4.2 template<class r_option > const fpoint container_base< r_option >::ay [protected]

The minimum y coordinate of the container.

Definition at line 79 of file container.hh.

4.1.4.3 template<class r_option > const fpoint container_base< r_option >::az [protected]

The minimum z coordinate of the container.

Definition at line 83 of file container.hh.

4.1.4.4 template<class r_option > const fpoint container_base< r_option >::bx [protected]

The maximum x coordinate of the container.

Definition at line 77 of file container.hh.

4.1.4.5 template<class r_option > const fpoint container_base< r_option >::by [protected]

The maximum y coordinate of the container.

Definition at line 81 of file container.hh.

4.1.4.6 template<class r_option > const fpoint container_base< r_option >::bz [protected]

The maximum z coordinate of the container.

Definition at line 85 of file container.hh.

4.1.4.7 template<class r_option > int* container_base< r_option >::co [protected]

This array holds the number of particles within each computational box of the container.

Definition at line 132 of file container.hh.

4.1.4.8 template<class r_option > int container_base< r_option >::current_wall_size [protected]

The current amount of memory allocated for walls.

Definition at line 168 of file container.hh.

4.1.4.9 template<class r_option > const int container_base< r_option >::hx [protected]

The number of boxes in the x direction for the searching mask.

Definition at line 109 of file container.hh.

4.1.4.10 template<class r_option > const int container_base< r_option >::hxy [protected]

A constant, set to the value of hx multiplied by hy, which is used in the routines which step through mask boxes in sequence.

Definition at line 117 of file container.hh.

4.1.4.11 template<class r_option > const int container_base< r_option >::hxyz [protected]

A constant, set to the value of hx∗hy∗hz, which is used in the routines which step through mask boxes in sequence.

Definition at line 120 of file container.hh.

4.1.4.12 template<class r_option > const int container_base< r_option >::hy [protected]

The number of boxes in the y direction for the searching mask.

Definition at line 111 of file container.hh.

4.1.4.13 template<class r_option > const int container_base< r_option >::hz [protected]

The number of boxes in the z direction for the searching mask.

Definition at line 113 of file container.hh.

4.1.4.14 template<class r_option > int∗∗ container_base< r_option >::id [protected]

This array holds the numerical IDs of each particle in each computational box.

Definition at line 141 of file container.hh.

4.1.4.15 template<class r_option > unsigned int∗ container_base< r_option >::mask [protected]

This array is used as a mask.

Definition at line 143 of file container.hh.

4.1.4.16 template<class r_option > int* container_base< r_option >::mem [protected]

This array holds the maximum amount of particle memory for each computational box of the container. If the number of particles in a particular box ever approaches this limit, more is allocated using the add_particle_memory() function.

Definition at line 138 of file container.hh.

4.1.4.17 template<class r_option > fpoint* container_base< r_option >::mrad [protected]

An array to hold the minimum distances associated with the worklists. This array is initialized during container construction, by the initialize_radii() routine.

Definition at line 189 of file container.hh.

4.1.4.18 template<class r_option > unsigned int container_base< r_option >::mv [protected]

This sets the current value being used to mark tested blocks in the mask.

Definition at line 149 of file container.hh.

4.1.4.19 template<class r_option > const int container_base< r_option >::nx [protected]

The number of boxes in the x direction.

Definition at line 96 of file container.hh.

4.1.4.20 template<class r_option > const int container_base< r_option >::nxy [protected]

A constant, set to the value of nx multiplied by ny, which is used in the routines which step through boxes in sequence.

Definition at line 104 of file container.hh.

4.1.4.21 template<class r_option > const int container_base< r_option >::nxyz [protected]

A constant, set to the value of nx*ny*nz, which is used in the routines which step through boxes in sequence.

Definition at line 107 of file container.hh.

4.1.4.22 template<class r_option > const int container_base< r_option >::ny [protected]

The number of boxes in the y direction.

Definition at line 98 of file container.hh.

4.1.4.23 template<class r_option > const int container_base< r_option >::nz [protected]

The number of boxes in the z direction.

Definition at line 100 of file container.hh.

4.1.4.24 template<class r_option > fpoint** container_base< r_option >::p [protected]

A two dimensional array holding particle positions. For the derived container_poly class, this also holds particle radii.

Definition at line 161 of file container.hh.

4.1.4.25 template<class r_option > r_option container_base< r_option >::radius [protected]

This object contains all the functions for handling how the particle radii should be treated. If the template is instantiated with the radius_mono class, then this object contains mostly blank routines that do nothing to the cell computation, to compute the basic Voronoi diagram. If the template is instantiated with the radius_poly calls, then this object provides routines for modifying the Voronoi cell computation in order to create the radical Voronoi tessellation.

Definition at line 178 of file container.hh.

4.1.4.26 template<class r_option > int container_base< r_option >::s_end [protected]

The position of the last element on the search list to be considered.

Definition at line 155 of file container.hh.

4.1.4.27 template<class r_option > int container_base< r_option >::s_size [protected]

The current size of the search list.

Definition at line 157 of file container.hh.

4.1.4.28 template<class r_option > int container_base< r_option >::s_start [protected]

The position of the first element on the search list to be considered.

Definition at line 152 of file container.hh.

4.1.4.29 template<class r_option > int* container_base< r_option >::sl [protected]

This array is used to store the list of blocks to test during the Voronoi cell computation.

Definition at line 146 of file container.hh.

4.1.4.30 template<class r_option > int container_base< r_option >::sz [protected]

The amount of memory in the array structure for each particle. This is set to 3 when the basic class is initialized, so that the array holds (x,y,z) positions. If the container class is initialized as part of the derived class container_poly, then this is set to 4, to also hold the particle radii.

Definition at line 185 of file container.hh.

4.1.4.31 template<class r_option > int container_base< r_option >::wall_number [protected]

The current number of wall objects, initially set to zero.
Definition at line 166 of file container.hh.

4.1.4.32 template<class r_option > wall** container_base< r_option >::walls [protected]

This array holds pointers to any wall objects that have been added to the container.
Definition at line 164 of file container.hh.

4.1.4.33 template<class r_option > const bool container_base< r_option >::xperiodic [protected]

A boolean value that determines if the x coordinate in periodic or not.
Definition at line 123 of file container.hh.

4.1.4.34 template<class r_option > const fpoint container_base< r_option >::xsp [protected]

The inverse box length in the x direction, set to nx/(bx-ax).
Definition at line 88 of file container.hh.

4.1.4.35 template<class r_option > const bool container_base< r_option >::yperiodic [protected]

A boolean value that determines if the y coordinate in periodic or not.
Definition at line 126 of file container.hh.

4.1.4.36 template<class r_option > const fpoint container_base< r_option >::ysp [protected]

The inverse box length in the y direction, set to ny/(by-ay).
Definition at line 91 of file container.hh.

4.1.4.37 template<class r_option > const bool container_base< r_option >::zperiodic [protected]

A boolean value that determines if the z coordinate in periodic or not.
Definition at line 129 of file container.hh.

4.1.4.38 template<class r_option > const fpoint container_base< r_option >::zsp [protected]

The inverse box length in the z direction, set to nz/(bz-az).
Definition at line 94 of file container.hh.
The documentation for this class was generated from the following files:

- container.hh

- container.cc
- worklist.cc

4.2 facets_loop Class Reference

A class to handle loops on regions of the container handling non-periodic and periodic boundary conditions.

`#include <container.hh>`

Public Member Functions

- template<class r_option >
  facets_loop (container_base< r_option > *q)
- int init (fpoint vx, fpoint vy, fpoint vz, fpoint r, fpoint &px, fpoint &py, fpoint &pz)
- int init (fpoint xmin, fpoint xmax, fpoint ymin, fpoint ymax, fpoint zmin, fpoint zmax, fpoint &px, fpoint &py, fpoint &pz)
- int inc (fpoint &px, fpoint &py, fpoint &pz)

Public Attributes

- int ip
- int jp
- int kp

4.2.1 Detailed Description

A class to handle loops on regions of the container handling non-periodic and periodic boundary conditions.

Many of the container routines require scanning over a rectangular sub-grid of blocks, and the routines for handling this are stored in the facets_loop class. A facets_loop class can first be initialized to either calculate the subgrid which is within a distance r of a vector (vx,vy,vz), or a subgrid corresponding to a rectangular box. The routine inc() can then be successively called to step through all the blocks within this subgrid.

Definition at line 296 of file container.hh.

4.2.2 Constructor & Destructor Documentation

4.2.2.1 template<class r_option > facets_loop::facets_loop (container_base< r_option > * *q*) [inline]

Creates a facets_loop object, by pulling the necesssary constants about the container geometry from a pointer to the current container class.

Definition at line 1261 of file container.cc.

4.2.3 Member Function Documentation

4.2.3.1 int facets_loop::inc (fpoint & *px*, fpoint & *py*, fpoint & *pz*) [inline]

Returns the next block to be tested in a loop, and updates the periodicity vector if necessary.

Definition at line 1336 of file container.cc.

4.2.3.2 int facets_loop::init (fpoint *xmin*, fpoint *xmax*, fpoint *ymin*, fpoint *ymax*, fpoint *zmin*, fpoint *zmax*, fpoint & *px*, fpoint & *py*, fpoint & *pz*) [inline]

Initializes a facets_loop object, by finding all blocks which overlap the box with corners (xmin,ymin,zmin) and (xmax,ymax,zmax). It returns the first block which is to be tested, and sets the periodic displacement vector (px,py,pz) accordingly.

Definition at line 1304 of file container.cc.

4.2.3.3 int facets_loop::init (fpoint *vx*, fpoint *vy*, fpoint *vz*, fpoint *r*, fpoint & *px*, fpoint & *py*, fpoint & *pz*) [inline]

Initializes a facets_loop object, by finding all blocks which are within a distance r of the vector (vx,vy,vz). It returns the first block which is to be tested, and sets the periodic displacement vector (px,py,pz) accordingly.

Definition at line 1270 of file container.cc.

4.2.4 Member Data Documentation

4.2.4.1 int facets_loop::ip

The current block index in the x direction, referencing a real cell in the range 0 to nx-1.

Definition at line 305 of file container.hh.

4.2.4.2 int facets_loop::jp

The current block index in the y direction, referencing a real cell in the range 0 to ny-1.

Definition at line 308 of file container.hh.

4.2.4.3 int facets_loop::kp

The current block index in the z direction, referencing a real cell in the range 0 to nz-1.

Definition at line 311 of file container.hh.

The documentation for this class was generated from the following files:

- container.hh
- container.cc

4.3 fatal_error Struct Reference

Structure for printing fatal error messages and exiting.

`#include <cell.hh>`

Public Member Functions

- fatal_error (const char *p)

4.3.1 Detailed Description

Structure for printing fatal error messages and exiting.

Structure for printing fatal error messages and exiting.

Definition at line 20 of file cell.hh.

4.3.2 Constructor & Destructor Documentation

4.3.2.1 fatal_error::fatal_error (const char * p) [inline]

This routine prints an error message to the standard error.

Parameters:

← ***p*** The message to print.

Definition at line 23 of file cell.hh.

The documentation for this struct was generated from the following file:

- cell.hh

4.4 neighbor_none Class Reference

A class passed to the voronoicell_base template to switch off neighbor computation.

`#include <cell.hh>`

Public Member Functions

- neighbor_none (voronoicell_base< neighbor_none > *ivc)
- void allocate (int i, int m)
- void add_memory_vertices (int i)
- void add_memory_vorder (int i)
- void init ()
- void init_octahedron ()
- void init_tetrahedron ()
- void set_pointer (int p, int n)
- void copy (int a, int b, int c, int d)
- void set (int a, int b, int c)
- void set_aux1 (int k)
- void copy_aux1 (int a, int b)
- void copy_aux1_shift (int a, int b)
- void set_aux2_copy (int a, int b)
- void copy_pointer (int a, int b)
- void set_to_aux1 (int j)
- void set_to_aux2 (int j)
- void print_edges (int i)
- void allocate_aux1 (int i)
- void switch_to_aux1 (int i)
- void copy_to_aux1 (int i, int m)
- void set_to_aux1_offset (int k, int m)
- void print (ostream &os, int i, int j)
- void label_facets ()
- void neighbors (ostream &os)
- void check_facets ()

4.4.1 Detailed Description

A class passed to the voronoicell_base template to switch off neighbor computation.

This is a class full of empty routines for neighbor computation. If the voronoicell_base template is instantiated with this class, then it has the effect of switching off all neighbor computation. Since all these routines are declared inline, it should have the effect of a zero speed overhead in the resulting code.

Definition at line 248 of file cell.hh.

4.4.2 Constructor & Destructor Documentation

4.4.2.1 neighbor_none::neighbor_none (voronoicell_base< neighbor_none > * *ivc*) [inline]

This is a blank constructor.
Definition at line 251 of file cell.hh.

4.4.3 Member Function Documentation

4.4.3.1 void neighbor_none::add_memory_vertices (int *i*) [inline]

This is a blank placeholder function that does nothing.
Definition at line 255 of file cell.hh.

4.4.3.2 void neighbor_none::add_memory_vorder (int *i*) [inline]

This is a blank placeholder function that does nothing.
Definition at line 257 of file cell.hh.

4.4.3.3 void neighbor_none::allocate (int *i*, int *m*) [inline]

This is a blank placeholder function that does nothing.
Definition at line 253 of file cell.hh.

4.4.3.4 void neighbor_none::allocate_aux1 (int *i*) [inline]

This is a blank placeholder function that does nothing.
Definition at line 287 of file cell.hh.

4.4.3.5 void neighbor_none::check_facets () [inline]

This is a blank placeholder function that does nothing.
Definition at line 301 of file cell.hh.

4.4.3.6 void neighbor_none::copy (int *a*, int *b*, int *c*, int *d*) [inline]

This is a blank placeholder function that does nothing.
Definition at line 267 of file cell.hh.

4.4.3.7 void neighbor_none::copy_aux1 (int *a*, int *b*) [inline]

This is a blank placeholder function that does nothing.
Definition at line 273 of file cell.hh.

4.4.3.8 void neighbor_none::copy_aux1_shift (int *a*, int *b*) [inline]

This is a blank placeholder function that does nothing.
Definition at line 275 of file cell.hh.

4.4.3.9 void neighbor_none::copy_pointer (int *a*, int *b*) [inline]

This is a blank placeholder function that does nothing.
Definition at line 279 of file cell.hh.

4.4.3.10 void neighbor_none::copy_to_aux1 (int *i*, int *m*) [inline]

This is a blank placeholder function that does nothing.
Definition at line 291 of file cell.hh.

4.4.3.11 void neighbor_none::init () [inline]

This is a blank placeholder function that does nothing.
Definition at line 259 of file cell.hh.

4.4.3.12 void neighbor_none::init_octahedron () [inline]

This is a blank placeholder function that does nothing.
Definition at line 261 of file cell.hh.

4.4.3.13 void neighbor_none::init_tetrahedron () [inline]

This is a blank placeholder function that does nothing.
Definition at line 263 of file cell.hh.

4.4.3.14 void neighbor_none::label_facets () [inline]

This is a blank placeholder function that does nothing.
Definition at line 297 of file cell.hh.

4.4.3.15 void neighbor_none::neighbors (ostream & *os*) [inline]

This is a blank placeholder function that does nothing.
Definition at line 299 of file cell.hh.

4.4.3.16 void neighbor_none::print (ostream & *os*, int *i*, int *j*) [inline]

This is a blank placeholder function that does nothing.
This routine is a placeholder which just prints the ID of a vertex.

Parameters:

← ***os*** The output stream to write to.
← ***i*** The ID of a vertex.
← ***j*** The particular plane of interest (ignored in this routine).

Definition at line 1779 of file cell.cc.

4.4.3.17 void neighbor_none::print_edges (int *i*) [inline]

This is a blank placeholder function that does nothing.
Definition at line 285 of file cell.hh.

4.4.3.18 void neighbor_none::set (int *a*, int *b*, int *c*) [inline]

This is a blank placeholder function that does nothing.
Definition at line 269 of file cell.hh.

4.4.3.19 void neighbor_none::set_aux1 (int *k*) [inline]

This is a blank placeholder function that does nothing.
Definition at line 271 of file cell.hh.

4.4.3.20 void neighbor_none::set_aux2_copy (int *a*, int *b*) [inline]

This is a blank placeholder function that does nothing.
Definition at line 277 of file cell.hh.

4.4.3.21 void neighbor_none::set_pointer (int *p*, int *n*) [inline]

This is a blank placeholder function that does nothing.
Definition at line 265 of file cell.hh.

4.4.3.22 void neighbor_none::set_to_aux1 (int *j*) [inline]

This is a blank placeholder function that does nothing.
Definition at line 281 of file cell.hh.

4.4.3.23 void neighbor_none::set_to_aux1_offset (int *k*, int *m*) [inline]

This is a blank placeholder function that does nothing.

Definition at line 293 of file cell.hh.

4.4.3.24 void neighbor_none::set_to_aux2 (int *j*) [inline]

This is a blank placeholder function that does nothing.

Definition at line 283 of file cell.hh.

4.4.3.25 void neighbor_none::switch_to_aux1 (int *i*) [inline]

This is a blank placeholder function that does nothing.

Definition at line 289 of file cell.hh.

The documentation for this class was generated from the following files:

- cell.hh
- cell.cc

4.5 neighbor_track Class Reference

A class passed to the voronoicell_base template to switch on the neighbor computation.

`#include <cell.hh>`

Public Member Functions

- neighbor_track (voronoicell_base< neighbor_track > *ivc)
- ~neighbor_track ()
- void allocate (int i, int m)
- void add_memory_vertices (int i)
- void add_memory_vorder (int i)
- void init ()
- void init_octahedron ()
- void init_tetrahedron ()
- void set_pointer (int p, int n)
- void copy (int a, int b, int c, int d)
- void set (int a, int b, int c)
- void set_aux1 (int k)
- void copy_aux1 (int a, int b)
- void copy_aux1_shift (int a, int b)
- void set_aux2_copy (int a, int b)
- void copy_pointer (int a, int b)
- void set_to_aux1 (int j)
- void set_to_aux2 (int j)
- void print_edges (int i)
- void allocate_aux1 (int i)
- void switch_to_aux1 (int i)
- void copy_to_aux1 (int i, int m)
- void set_to_aux1_offset (int k, int m)
- void print (ostream &os, int i, int j)
- void label_facets ()
- void neighbors (ostream &os)
- void check_facets ()

Public Attributes

- int ** mne
- int ** ne
- voronoicell_base< neighbor_track > * vc

4.5.1 Detailed Description

A class passed to the voronoicell_base template to switch on the neighbor computation.

This class encapsulates all the routines which are required to carry out the neighbor tracking. If the voronoicell_base template is instantiated with this class, then the neighbor computation is enabled. All these routines are simple and declared inline, so they should be directly integrated into the functions in the voronoicell class during compilation, without zero function call overhead.

Definition at line 313 of file cell.hh.

4.5.2 Constructor & Destructor Documentation

4.5.2.1 neighbor_track::neighbor_track (voronoicell_base< neighbor_track > * *ivc*)

This constructs the neighbor_track class, within a current voronoicell_neighbor class. It allocates memory for neighbor storage in a similar way to the voronoicell constructor.

Definition at line 1988 of file cell.cc.

4.5.2.2 neighbor_track::~neighbor_track ()

The destructor for the neighbor_track class deallocates the arrays for neighbor tracking.

Definition at line 1999 of file cell.cc.

4.5.3 Member Function Documentation

4.5.3.1 void neighbor_track::add_memory_vertices (int *i*) [inline]

This increases the size of the ne[] array.

Parameters:

← ***i*** the new size of the array.

Definition at line 2014 of file cell.cc.

4.5.3.2 void neighbor_track::add_memory_vorder (int *i*) [inline]

This increases the size of the maximum allowable vertex order in the neighbor tracking.

Definition at line 2023 of file cell.cc.

4.5.3.3 void neighbor_track::allocate (int *i*, int *m*) [inline]

This allocates a single array for neighbor tracking.

Parameters:

← ***i*** the vertex order of the array to be extended.

← ***m*** the size of the array to be extended.

Definition at line 2008 of file cell.cc.

4.5.3.4 void neighbor_track::allocate_aux1 (int *i*) [inline]

This allocates a new array and sets the auxilliary pointer to it.

Definition at line 2141 of file cell.cc.

4.5.3.5 void neighbor_track::check_facets () [inline]

This routine checks to make sure the neighbor information of each facets is consistent.

Definition at line 2165 of file cell.cc.

4.5.3.6 void neighbor_track::copy (int *a*, int *b*, int *c*, int *d*) [inline]

This is a basic operation to copy ne[c][d] to ne[a][b].

Definition at line 2082 of file cell.cc.

4.5.3.7 void neighbor_track::copy_aux1 (int *a*, int *b*) [inline]

This is a basic operation to copy a neighbor into paux1.

Definition at line 2099 of file cell.cc.

4.5.3.8 void neighbor_track::copy_aux1_shift (int *a*, int *b*) [inline]

This is a basic operation to copy a neighbor into paux1 with a shift. It is used in the delete_connection() routine of the voronoicell class.

Definition at line 2105 of file cell.cc.

4.5.3.9 void neighbor_track::copy_pointer (int *a*, int *b*) [inline]

This is a basic routine to copy ne[b] into ne[a].

Definition at line 2117 of file cell.cc.

4.5.3.10 void neighbor_track::copy_to_aux1 (int *i*, int *m*) [inline]

This routine copies neighbor information into the auxilliary pointer.

Definition at line 2154 of file cell.cc.

4.5.3.11 void neighbor_track::init () [inline]

This initializes the neighbor information for a rectangular box and is called during the initiailization routine for the voronoicell class.

Definition at line 2033 of file cell.cc.

4.5.3.12 void neighbor_track::init_octahedron () [inline]

This initializes the neighbor information for an octahedron. The eight initial faces are assigned ID numbers from -1 to -8.

Definition at line 2050 of file cell.cc.

4.5.3.13 void neighbor_track::init_tetrahedron () [inline]

This initializes the neighbor information for an tetrahedron. The four initial faces are assigned ID numbers from -1 to -4.

Definition at line 2064 of file cell.cc.

4.5.3.14 void neighbor_track::label_facets () [inline]

This routine labels the facets in an arbitrary order, starting from one.

Definition at line 2223 of file cell.cc.

4.5.3.15 void neighbor_track::neighbors (ostream & *os*) [inline]

This routine provides a list of plane IDs.

Parameters:

← *&os* An output stream to write to.

Definition at line 2195 of file cell.cc.

4.5.3.16 void neighbor_track::print (ostream & *os*, int *i*, int *j*) [inline]

This routine prints out a bracketed pair showing a vertex number, and the corresponding neighbor information.

Parameters:

← *os* The output stream to write to.

← *i* The vertex number to print.

← *j* The index of the neighbor information to print.

Definition at line 2257 of file cell.cc.

4.5.3.17 void neighbor_track::print_edges (int *i*) [inline]

This prints out the neighbor information for vertex i.

Definition at line 2132 of file cell.cc.

4.5.3.18 void neighbor_track::set (int *a*, int *b*, int *c*) [inline]

This is a basic operation to carry out ne[a][b]=c.

Definition at line 2087 of file cell.cc.

4.5.3.19 void neighbor_track::set_aux1 (int *k*) [inline]

This is a basic operation to set the auxiliary pointer paux1.

Parameters:

← ***k*** the order of the vertex to point to.

Definition at line 2094 of file cell.cc.

4.5.3.20 void neighbor_track::set_aux2_copy (int *a*, int *b*) [inline]

This routine sets the second auxiliary pointer to a new section of memory, and then copies existing neighbor information into it.

Definition at line 2111 of file cell.cc.

4.5.3.21 void neighbor_track::set_pointer (int *p*, int *n*) [inline]

This is a basic operation to set a new pointer in the ne[] array.

Parameters:

← ***p*** the index in the ne[] array to set.
← ***n*** the order of the vertex.

Definition at line 2077 of file cell.cc.

4.5.3.22 void neighbor_track::set_to_aux1 (int *j*) [inline]

This sets ne[j] to the first auxilliary pointer.

Definition at line 2122 of file cell.cc.

4.5.3.23 void neighbor_track::set_to_aux1_offset (int *k*, int *m*) [inline]

This sets ne[k] to the auxillary pointer with an offset.

Definition at line 2159 of file cell.cc.

4.5.3.24 void neighbor_track::set_to_aux2 (int *j*) [inline]

This sets ne[j] to the second auxilliary pointer.

Definition at line 2127 of file cell.cc.

4.5.3.25 void neighbor_track::switch_to_aux1 (int *i*) [inline]

This deletes a particular neighbor array and switches the pointer to the auxilliary pointer.

Definition at line 2147 of file cell.cc.

4.5.4 Member Data Documentation

4.5.4.1 int** neighbor_track::mne

This two dimensional array holds the neighbor information associated with each vertex. mne[p] is a one dimensional array which holds all of the neighbor informations for vertices of order p.

Definition at line 319 of file cell.hh.

4.5.4.2 int** neighbor_track::ne

This is a two dimensional array that holds the neighbor information associated with each vertex. ne[i] points to a one-dimensional array in mne[nu[i]]. ne[i][j] holds the neighbor information associated with the jth edge of vertex i. It is set to the ID number of the plane that made the face that is clockwise from the jth edge.

Definition at line 326 of file cell.hh.

4.5.4.3 voronoicell_base<neighbor_track>* neighbor_track::vc

This is a pointer back to the voronoicell class which created this class. It is used to reference the members of that class in computations.

Definition at line 332 of file cell.hh.

The documentation for this class was generated from the following files:

- cell.hh
- cell.cc

4.6 radius_mono Class Reference

A class encapsulating all routines specifically needed in the standard Voronoi tessellation.

`#include <container.hh>`

Public Member Functions

- radius_mono (container_base< radius_mono > *icc)
- void import (istream &is)
- void store_radius (int i, int j, fpoint r)
- void clear_max ()
- void init (int s, int i)
- fpoint volume (int ijk, int s)
- fpoint cutoff (fpoint lrs)
- fpoint scale (fpoint rs, int t, int q)
- void print (ostream &os, int ijk, int q)
- void rad (ostream &os, int l, int c)

Public Attributes

- const int mem_size

4.6.1 Detailed Description

A class encapsulating all routines specifically needed in the standard Voronoi tessellation.

This class encapsulates all the routines that are required for carrying out a standard Voronoi tessellation that would be appropriate for a monodisperse system. When the container class is instantiated using this class, all information about particle radii is switched off. Since all these functions are declared inline, there should be no loss of speed.

Definition at line 228 of file container.hh.

4.6.2 Constructor & Destructor Documentation

4.6.2.1 radius_mono::radius_mono (container_base< radius_mono > * *icc*) [inline]

This constructor sets a pointer back to the container class that created it, and initializes the mem_size constant to 3.

Definition at line 237 of file container.hh.

4.6.3 Member Function Documentation

4.6.3.1 void radius_mono::clear_max () [inline]

This is a blank placeholder function that does nothing.

Definition at line 242 of file container.hh.

4.6.3.2 fpoint radius_mono::cutoff (fpoint *lrs*) [inline]

This routine is called when deciding when to terminate the computation of a Voronoi cell. For the monodisperse case, this routine just returns the same value that is passed to it.

Parameters:

← ***lrs*** a cutoff radius for the cell computation.

Returns:

The same value passed to it.

Definition at line 1448 of file container.cc.

4.6.3.3 void radius_mono::import (istream & *is*) [inline]

Imports a list of particles from an input stream for the monodisperse case where no radius information is expected.

Parameters:

← ***&is*** an input stream to read from.

Definition at line 1401 of file container.cc.

4.6.3.4 void radius_mono::init (int *s*, int *i*) [inline]

This is a blank placeholder function that does nothing.

Definition at line 244 of file container.hh.

4.6.3.5 void radius_mono::print (ostream & *os*, int *ijk*, int *q*) [inline]

This is a blank placeholder function that does nothing.

Definition at line 249 of file container.hh.

4.6.3.6 void radius_mono::rad (ostream & *os*, int *l*, int *c*) [inline]

Prints the radius of particle, by just supplying a generic value of "s".

Parameters:

← ***&os*** the output stream to write to.

← ***l*** the region to consider.

← ***c*** the number of the particle within the region.

Definition at line 1456 of file container.cc.

4.6.3.7 fpoint radius_mono::scale (fpoint *rs*, int *t*, int *q*) [inline]

Applies a blank scaling to the position of a cutting plane.

Parameters:

← ***rs*** the distance between the Voronoi cell and the cutting plane.

← ***t*** the region to consider

← ***q*** the number of the particle within the region.

Returns:

The scaled position, which for this case, is equal to rs.

Definition at line 1503 of file container.cc.

4.6.3.8 void radius_mono::store_radius (int *i*, int *j*, fpoint *r*) [inline]

This is a blank placeholder function that does nothing.

Definition at line 240 of file container.hh.

4.6.3.9 fpoint radius_mono::volume (int *ijk*, int *s*) [inline]

Returns the scaled volume of a particle, which is always set to 0.125 for the monodisperse case where particles are taken to have unit diameter.

Parameters:

← ***ijk*** the region to consider.

← ***s*** the number of the particle within the region.

Returns:

The cube of the radius of the particle, which is 0.125 in this case.

Definition at line 1475 of file container.cc.

4.6.4 Member Data Documentation

4.6.4.1 const int radius_mono::mem_size

The number of floating point numbers allocated for each particle in the container, set to 3 for this case for the x, y, and z positions.

Definition at line 233 of file container.hh.

The documentation for this class was generated from the following files:

- container.hh
- container.cc

4.7 radius_poly Class Reference

A class encapsulating all routines specifically needed in the Voronoi radical tessellation.

`#include <container.hh>`

Public Member Functions

- radius_poly (container_base< radius_poly > *icc)
- void import (istream &is)
- void store_radius (int i, int j, fpoint r)
- void clear_max ()
- void init (int ijk, int s)
- fpoint volume (int ijk, int s)
- fpoint cutoff (fpoint lrs)
- fpoint scale (fpoint rs, int t, int q)
- void print (ostream &os, int ijk, int q)
- void rad (ostream &os, int l, int c)

Public Attributes

- const int mem_size

4.7.1 Detailed Description

A class encapsulating all routines specifically needed in the Voronoi radical tessellation.

This class encapsulates all the routines that are required for carrying out the radical Voronoi tessellation that is appropriate for polydisperse sphere. When the container class is instantiated with this class, information about particle radii is switched on.

Definition at line 262 of file container.hh.

4.7.2 Constructor & Destructor Documentation

4.7.2.1 radius_poly::radius_poly (container_base< radius_poly > * *icc*) [inline]

This constructor sets a pointer back to the container class that created it, and initializes the mem_size constant to 4.

Definition at line 271 of file container.hh.

4.7.3 Member Function Documentation

4.7.3.1 void radius_poly::clear_max () [inline]

Clears the stored maximum radius.

Definition at line 1394 of file container.cc.

4.7.3.2 fpoint radius_poly::cutoff (fpoint *lrs*) [inline]

This routine is called when deciding when to terminate the computation of a Voronoi cell. For the Voronoi radical tessellation for a polydisperse case, this routine multiplies the cutoff value by the scaling factor that was precomputed in the init() routine.

Parameters:

← ***lrs*** a cutoff radius for the cell computation.

Returns:

The value scaled by the factor mul.

Definition at line 1439 of file container.cc.

4.7.3.3 void radius_poly::import (istream & *is*) [inline]

Imports a list of particles from an input stream for the polydisperse case, where both positions and particle radii are both stored.

Parameters:

← ***&is*** an input stream to read from.

Definition at line 1413 of file container.cc.

4.7.3.4 void radius_poly::init (int *ijk*, int *s*) [inline]

Initializes the radius_poly class for a new Voronoi cell calculation, by computing the radial cut-off value, based on the current particle's radius and the maximum radius of any particle in the packing.

Parameters:

← ***ijk*** the region to consider.

← ***s*** the number of the particle within the region.

Definition at line 1427 of file container.cc.

4.7.3.5 void radius_poly::print (ostream & *os*, int *ijk*, int *q*) [inline]

Prints the radius of a particle to an open file stream.

Parameters:

← ***&os*** an open file stream.

← ***ijk*** the region to consider.

← ***q*** the number of the particle within the region.

Definition at line 1511 of file container.cc.

4.7.3.6 void radius_poly::rad (ostream & *os*, int *l*, int *c*) [inline]

Prints the radius of a particle to an open output stream.

Parameters:

← *&os* the output stream to write to.
← *l* the region to consider.
← *c* the number of the particle within the region.

Definition at line 1464 of file container.cc.

4.7.3.7 fpoint radius_poly::scale (fpoint *rs*, int *t*, int *q*) [inline]

Scales the position of a plane according to the relative sizes of the particle radii.

Parameters:

← *rs* the distance between the Voronoi cell and the cutting plane.
← *t* the region to consider
← *q* the number of the particle within the region.

Returns:

The scaled position.

Definition at line 1494 of file container.cc.

4.7.3.8 void radius_poly::store_radius (int *i*, int *j*, fpoint *r*) [inline]

Sets the radius of the jth particle in region i to r, and updates the maximum particle radius.

Parameters:

← *i* the region of the particle to consider.
← *j* the number of the particle within the region.
← *r* the radius to set.

Definition at line 1388 of file container.cc.

4.7.3.9 fpoint radius_poly::volume (int *ijk*, int *s*) [inline]

Returns the scaled volume of a particle.

Parameters:

← *ijk* the region to consider.
← *s* the number of the particle within the region.

Returns:

The cube of the radius of the particle.

Definition at line 1483 of file container.cc.

4.7.4 Member Data Documentation

4.7.4.1 const int radius_poly::mem_size

The number of floating point numbers allocated for each particle in the container, set to 4 for this case for the x, y, and z positions, plus the radius.

Definition at line 267 of file container.hh.

The documentation for this class was generated from the following files:

- container.hh
- container.cc

4.8 suretest Class Reference

A class to reliably carry out floating point comparisons, storing marginal cases for future reference.

`#include <cell.hh>`

Public Member Functions

- suretest ()
- ~suretest ()
- void init (fpoint x, fpoint y, fpoint z, fpoint rsq)
- int test (int n, fpoint &ans)

Public Attributes

- fpoint * p

4.8.1 Detailed Description

A class to reliably carry out floating point comparisons, storing marginal cases for future reference.

Floating point comparisons can be unreliable on some processor architectures, and can produce unpredictable results. On a number of popular Intel processors, floating point numbers are held to higher precision when in registers than when in memory. When a register is swapped from a register to memory, a truncation error, and in some situations this can create circumstances where for two numbers c and d, the program finds c>d first, but later c<d. The programmer has no control over when the swaps between memory and registers occur, and recompiling with slightly different code can give different results. One solution to avoid this is to force the compiler to evaluate everything in memory (e.g. by using the -ffloat-store option in the GNU C++ compiler) but this could be viewed overkill, since it slows the code down, and the extra register precision is useful.

In the plane cutting routine of the voronoicell class, we need to reliably know whether a vertex lies inside, outside, or on the cutting plane, since if it changed during the tracing process there would be confusion. This class makes these tests reliable, by storing the results of marginal cases, where the vertex lies within tolerance2 of the cutting plane. If that vertex is tested again, then code looks up the value of the table in a buffer, rather than doing the floating point comparison again. Only vertices which are close to the plane are stored and tested, so this routine should create minimal computational overhead.

Definition at line 52 of file cell.hh.

4.8.2 Constructor & Destructor Documentation

4.8.2.1 suretest::suretest ()

Initializes the suretest class and creates a buffer for marginal points.

Definition at line 1679 of file cell.cc.

4.8.2.2 suretest::~suretest ()

Suretest destructor to free memory allocation.

Definition at line 1684 of file cell.cc.

4.8.3 Member Function Documentation

4.8.3.1 void suretest::init (fpoint *x*, fpoint *y*, fpoint *z*, fpoint *rsq*) [inline]

Sets up the suretest class with a particular test plane, and removes any special cases from the table.

Definition at line 1690 of file cell.cc.

4.8.3.2 int suretest::test (int *n*, fpoint & *ans*) [inline]

Definition at line 1695 of file cell.cc.

4.8.4 Member Data Documentation

4.8.4.1 fpoint* suretest::p

This is a pointer to the array in the voronoicell class which holds the vertex coordinates.

Definition at line 55 of file cell.hh.

The documentation for this class was generated from the following files:

- cell.hh
- cell.cc

4.9 voronoicell_base< n_option > Class Template Reference

A class encapsulating all the routines for storing and calculating a single Voronoi cell.

`#include <cell.hh>`

Public Member Functions

- voronoicell_base ()
- ~voronoicell_base ()
- void init (fpoint xmin, fpoint xmax, fpoint ymin, fpoint ymax, fpoint zmin, fpoint zmax)
- void init_octahedron (fpoint l)
- void init_tetrahedron (fpoint x0, fpoint y0, fpoint z0, fpoint x1, fpoint y1, fpoint z1, fpoint x2, fpoint y2, fpoint z2, fpoint x3, fpoint y3, fpoint z3)
- void init_test (int n)
- void add_vertex (fpoint x, fpoint y, fpoint z, int a)
- void add_vertex (fpoint x, fpoint y, fpoint z, int a, int b)
- void add_vertex (fpoint x, fpoint y, fpoint z, int a, int b, int c)
- void add_vertex (fpoint x, fpoint y, fpoint z, int a, int b, int c, int d)
- void add_vertex (fpoint x, fpoint y, fpoint z, int a, int b, int c, int d, int e)
- void draw_pov (ostream &os, fpoint x, fpoint y, fpoint z)
- void draw_pov (const char *filename, fpoint x, fpoint y, fpoint z)
- void draw_pov (fpoint x, fpoint y, fpoint z)
- void draw_pov_mesh (ostream &os, fpoint x, fpoint y, fpoint z)
- void draw_pov_mesh (const char *filename, fpoint x, fpoint y, fpoint z)
- void draw_pov_mesh (fpoint x, fpoint y, fpoint z)
- void draw_gnuplot (ostream &os, fpoint x, fpoint y, fpoint z)
- void draw_gnuplot (const char *filename, fpoint x, fpoint y, fpoint z)
- void draw_gnuplot (fpoint x, fpoint y, fpoint z)
- void check_relations ()
- void check_duplicates ()
- void construct_relations ()
- fpoint volume ()
- fpoint maxradsq ()
- void print_edges ()
- void perturb (fpoint r)
- void facets (ostream &os)
- void facets ()
- void facets (const char *filename)
- void facet_statistics (ostream &os)
- void facet_statistics ()
- void facet_statistics (const char *filename)
- bool nplane (fpoint x, fpoint y, fpoint z, fpoint rs, int p_id)
- bool nplane (fpoint x, fpoint y, fpoint z, int p_id)
- bool plane (fpoint x, fpoint y, fpoint z, fpoint rs)
- bool plane (fpoint x, fpoint y, fpoint z)
- bool plane_intersects (fpoint x, fpoint y, fpoint z, fpoint rs)
- bool plane_intersects_guess (fpoint x, fpoint y, fpoint z, fpoint rs)
- void label_facets ()
- void neighbors (ostream &os)
- void check_facets ()

Public Attributes

- int ** ed
- int * nu
- int current_vertices
- int current_vertex_order
- int current_delete_size
- int current_delete2_size
- fpoint * pts
- int p
- int up
- suretest sure

Friends

- class neighbor_track

4.9.1 Detailed Description

template<class n_option> class voronoicell_base< n_option >

A class encapsulating all the routines for storing and calculating a single Voronoi cell.

This class encapsulates all the routines for storing and calculating a single Voronoi cell. The cell can first be initialized by the init() function to be a rectangular box. The box can then be successively cut by planes using the plane function. Other routines exist for outputting the cell, computing its volume, or finding the largest distance of a vertex from the cell center. The cell is described by two arrays. pts[] is a floating point array which holds the vertex positions. ed[] holds the table of edges, and also a relation table that determines how two vertices are connected to one another. The relation table is redundant, but helps speed up the computation. The function check_relations() checks that the relational table is valid.

Definition at line 94 of file cell.hh.

4.9.2 Constructor & Destructor Documentation

4.9.2.1 template<class n_option > voronoicell_base< n_option >::voronoicell_base () [inline]

Constructs a Voronoi cell and sets up the initial memory.

Definition at line 11 of file cell.cc.

4.9.2.2 template<class n_option > voronoicell_base< n_option >::~voronoicell_base () [inline]

The voronoicell destructor deallocates all the dynamic memory.

Definition at line 42 of file cell.cc.

4.9.3 Member Function Documentation

4.9.3.1 template<class n_option > void voronoicell_base< n_option >::add_vertex (fpoint *x*, fpoint *y*, fpoint *z*, int *a*, int *b*, int *c*, int *d*, int *e*) [inline]

Adds an order 5 vertex to the memory structure, and specifies its edges.

Definition at line 484 of file cell.cc.

4.9.3.2 template<class n_option > void voronoicell_base< n_option >::add_vertex (fpoint *x*, fpoint *y*, fpoint *z*, int *a*, int *b*, int *c*, int *d*) [inline]

Adds an order 4 vertex to the memory structure, and specifies its edges.

Definition at line 474 of file cell.cc.

4.9.3.3 template<class n_option > void voronoicell_base< n_option >::add_vertex (fpoint *x*, fpoint *y*, fpoint *z*, int *a*, int *b*, int *c*) [inline]

Adds an order 3 vertex to the memory structure, and specifies its edges.

Definition at line 464 of file cell.cc.

4.9.3.4 template<class n_option > void voronoicell_base< n_option >::add_vertex (fpoint *x*, fpoint *y*, fpoint *z*, int *a*, int *b*) [inline]

Adds an order 2 vertex to the memory structure, and specifies its edges.

Definition at line 454 of file cell.cc.

4.9.3.5 template<class n_option > void voronoicell_base< n_option >::add_vertex (fpoint *x*, fpoint *y*, fpoint *z*, int *a*) [inline]

Adds an order one vertex to the memory structure, and specifies its edge.

Parameters:

← ***(x,y,z)*** are the coordinates of the vertex

← ***a*** is the first and only edge of this vertex

Definition at line 444 of file cell.cc.

4.9.3.6 template<class n_option > void voronoicell_base< n_option >::check_duplicates () [inline]

This routine checks for any two vertices that are connected by more than one edge. The plane algorithm is designed so that this should not happen, so any occurrences are most likely errors. Note that the routine is O(p), so running it every time the plane routine is called will result in a significant slowdown.

Definition at line 511 of file cell.cc.

4.9.3.7 template<class n_option > void voronoicell_base< n_option >::check_facets () [inline]

If the template is instantiated with the neighbor tracking turned on, then this routine will check that the neighbor information is consistent, by tracing around every facet, and ensuring that all the neighbor information for that facet refers to the same neighbor. If the neighbor tracking isn't turned on, this routine does nothing.

Definition at line 1888 of file cell.cc.

4.9.3.8 template<class n_option > void voronoicell_base< n_option >::check_relations () [inline]

Checks that the relational table of the Voronoi cell is accurate, and prints out any errors. This algorithm is O(p), so running it every time the plane routine is called will result in a significant slowdown.

Definition at line 496 of file cell.cc.

4.9.3.9 template<class n_option > void voronoicell_base< n_option >::construct_relations () [inline]

Constructs the relational table if the edges have been specified.

Definition at line 524 of file cell.cc.

4.9.3.10 template<class n_option > void voronoicell_base< n_option >::draw_gnuplot (fpoint *x*, fpoint *y*, fpoint *z*) [inline]

An overloaded version of the draw_gnuplot routine, that prints to the standard output.

Parameters:

← ***(x,y,z)*** A displacement vector to be added to the cell's position.

Definition at line 1602 of file cell.cc.

4.9.3.11 template<class n_option > void voronoicell_base< n_option >::draw_gnuplot (const char * *filename*, fpoint *x*, fpoint *y*, fpoint *z*) [inline]

An overloaded version of the draw_gnuplot routine that writes directly to a file.

Parameters:

← ***filename*** The name of the file to write to.

← ***(x,y,z)*** A displacement vector to be added to the cell's position.

Definition at line 1590 of file cell.cc.

4.9.3.12 template<class n_option > void voronoicell_base< n_option >::draw_gnuplot (ostream & *os*, fpoint *x*, fpoint *y*, fpoint *z*) [inline]

Outputs the edges of the Voronoi cell (in gnuplot format) to an output stream.

Parameters:

← ***os*** A reference to an output stream to write to.

← ***(x,y,z)*** A displacement vector to be added to the cell's position.

Definition at line 1573 of file cell.cc.

4.9.3.13 template<class n_option > void voronoicell_base< n_option >::draw_pov (fpoint *x*, fpoint *y*, fpoint *z*) [inline]

An overloaded version of the draw_pov routine, that outputs the edges of the Voronoi cell (in POV-Ray format) to standard output.

Parameters:

← ***(x,y,z)*** A displacement vector to be added to the cell's position.

Definition at line 1564 of file cell.cc.

4.9.3.14 template<class n_option > void voronoicell_base< n_option >::draw_pov (const char * *filename*, fpoint *x*, fpoint *y*, fpoint *z*) [inline]

An overloaded version of the draw_pov routine, that outputs the edges of the Voronoi cell (in POV-Ray format) to a file.

Parameters:

← ***filename*** The file to write to.

← ***(x,y,z)*** A displacement vector to be added to the cell's position.

Definition at line 1552 of file cell.cc.

4.9.3.15 template<class n_option > void voronoicell_base< n_option >::draw_pov (ostream & *os*, fpoint *x*, fpoint *y*, fpoint *z*) [inline]

Outputs the edges of the Voronoi cell (in POV-Ray format) to an open file stream, displacing the cell by an amount (x,y,z).

Parameters:

← ***os*** A output stream to write to.

← ***(x,y,z)*** A displacement vector to be added to the cell's position.

Definition at line 1534 of file cell.cc.

4.9.3.16 template<class n_option > void voronoicell_base< n_option >::draw_pov_mesh (fpoint *x*, fpoint *y*, fpoint *z*) [inline]

An overloaded version of the draw_pov_mesh routine, that prints to the standard output.

Parameters:

← ***(x,y,z)*** A displacement vector to be added to the cell's position.

Definition at line 1666 of file cell.cc.

4.9.3.17 template<class n_option > void voronoicell_base< n_option >::draw_pov_mesh (const char * *filename*, fpoint *x*, fpoint *y*, fpoint *z*) [inline]

An overloaded version of the draw_pov_mesh routine, that writes directly to a file.

Parameters:

← ***filename*** A filename to write to.

← ***(x,y,z)*** A displacement vector to be added to the cell's position.

Definition at line 1654 of file cell.cc.

4.9.3.18 template<class n_option > void voronoicell_base< n_option >::draw_pov_mesh (ostream & *os*, fpoint *x*, fpoint *y*, fpoint *z*) [inline]

Outputs the Voronoi cell in the POV mesh2 format, described in section 1.3.2.2 of the POV-Ray documentation. The mesh2 output consists of a list of vertex vectors, followed by a list of triangular faces. The routine also makes use of the optional inside_vector specification, which makes the mesh object solid, so the the POV-Ray Constructive Solid Geometry (CSG) can be applied.

Parameters:

← ***os*** An output stream to write to.

← ***(x,y,z)*** A displacement vector to be added to the cell's position.

Definition at line 1616 of file cell.cc.

4.9.3.19 template<class n_option > void voronoicell_base< n_option >::facet_statistics (const char * *filename*) [inline]

An overloaded version of facet_statistics() which outputs the results to a file.

Parameters:

← ***filename*** The name of the file to write to.

Definition at line 1858 of file cell.cc.

4.9.3.20 template<class n_option > void voronoicell_base< n_option >::facet_statistics () [inline]

An overloaded version of facet_statistics() which outputs the results to standard output.

Definition at line 1850 of file cell.cc.

4.9.3.21 template<class n_option > void voronoicell_base< n_option >::facet_statistics (ostream & *os*) [inline]

Examines all the facets, and evaluates them by the number of vertices that they have.

Parameters:

← ***os*** An open output stream to write to.

Definition at line 1804 of file cell.cc.

4.9.3.22 template<class n_option > void voronoicell_base< n_option >::facets (const char * *filename*) [inline]

An overloaded version of facets(), which outputs the results to a file.

Parameters:

← ***filename*** The name of the file to write to.

Definition at line 1793 of file cell.cc.

4.9.3.23 template<class n_option > void voronoicell_base< n_option >::facets () [inline]

An overloaded version of facets() which output the results to the standard output.

Definition at line 1786 of file cell.cc.

4.9.3.24 template<class n_option > void voronoicell_base< n_option >::facets (ostream & *os*) [inline]

Prints out a list of all the facets and their vertices. If the neighbor option is defined, it lists each cutting plane.

Definition at line 1745 of file cell.cc.

4.9.3.25 template<class n_option > void voronoicell_base< n_option >::init (fpoint *xmin*, fpoint *xmax*, fpoint *ymin*, fpoint *ymax*, fpoint *zmin*, fpoint *zmax*) [inline]

Initializes a Voronoi cell as a rectangular box with the given dimensions

Definition at line 194 of file cell.cc.

4.9.3.26 template<class n_option > void voronoicell_base< n_option >::init_octahedron (fpoint *l*) [inline]

Initializes a Voronoi cell as a regular octahedron.

Parameters:

← ***l*** The distance from the octahedron center to a vertex. Six vertices are initialized at (-l,0,0), (l,0,0), (0,-l,0), (0,l,0), (0,0,-l), and (0,0,l).

Definition at line 224 of file cell.cc.

4.9.3.27 template<class n_option > void voronoicell_base< n_option >::init_test (int *n*) [inline]

Initializes an arbitrary test object using the add_vertex() and construct_relations() routines. See the source code for information about the specific objects.

Parameters:

← ***n*** the number of the test object (from 0 to 9)

Definition at line 275 of file cell.cc.

4.9.3.28 template<class n_option > void voronoicell_base< n_option >::init_tetrahedron (fpoint *x0*, fpoint *y0*, fpoint *z0*, fpoint *x1*, fpoint *y1*, fpoint *z1*, fpoint *x2*, fpoint *y2*, fpoint *z2*, fpoint *x3*, fpoint *y3*, fpoint *z3*) [inline]

Initializes a Voronoi cell as a tetrahedron. It assumes that the normal to the face for the first three vertices points inside.

Parameters:

(x0,y0,z0) A position vector for the first vertex.

(x1,y1,z1) A position vector for the second vertex.

(x2,y2,z2) A position vector for the third vertex.

(x3,y3,z3) A position vector for the fourth vertex.

Definition at line 252 of file cell.cc.

4.9.3.29 template<class n_option > void voronoicell_base< n_option >::label_facets () [inline]

If the template is instantiated with the neighbor tracking turned on, then this routine will label all the facets of the current cell. Otherwise this routine does nothing.

Definition at line 1869 of file cell.cc.

4.9.3.30 template<class n_option > fpoint voronoicell_base< n_option >::maxradsq () [inline]

Computes the maximum radius squared of a vertex from the center of the cell. It can be used to determine when enough particles have been testing an all planes that could cut the cell have been considered.

Returns:

The maximum radius squared of a vertex.

Definition at line 1519 of file cell.cc.

4.9.3.31 template<class n_option > void voronoicell_base< n_option >::neighbors (ostream & *os*) [inline]

If the template is instantiated with the neighbor tracking turned on, then this routine will print out a list of all the neighbors of a given cell. Otherwise, this routine does nothing.

Parameters:

← ***os*** An open output stream to write to.

Definition at line 1878 of file cell.cc.

4.9.3.32 template<class n_option > bool voronoicell_base< n_option >::nplane (fpoint *x*, fpoint *y*, fpoint *z*, int *p_id*) [inline]

This routine calculates the modulus squared of the vector before passing it to the main nplane() routine with full arguments.

Parameters:

← ***(x,y,z)*** The vector to cut the cell by.

← ***p_id*** The plane ID (for neighbor tracking only).

Definition at line 1444 of file cell.cc.

4.9.3.33 template<class n_option > bool voronoicell_base< n_option >::nplane (fpoint *x*, fpoint *y*, fpoint *z*, fpoint *rsq*, int *p_id*) [inline]

Cuts the Voronoi cell by a particle whose center is at a separation of (x,y,z) from the cell center. The value of rsq should be initially set to $x^2+y^2+z^2$.

Definition at line 541 of file cell.cc.

4.9.3.34 template<class n_option > void voronoicell_base< n_option >::perturb (fpoint *r*) [inline]

Randomly perturbs the points in the Voronoi cell by an amount r.

Definition at line 1672 of file cell.cc.

4.9.3.35 template<class n_option > bool voronoicell_base< n_option >::plane (fpoint *x*, fpoint *y*, fpoint *z*) [inline]

Cuts a Voronoi cell using the influence of a particle at (x,y,z), first calculating the modulus squared of this vector before passing it to the main nplane() routine. Zero is supplied as the plane ID, which will be ignored unless neighbor tracking is enabled.

Parameters:

← ***(x,y,z)*** The vector to cut the cell by.

Definition at line 1425 of file cell.cc.

4.9.3.36 template<class n_option > bool voronoicell_base< n_option >::plane (fpoint *x*, fpoint *y*, fpoint *z*, fpoint *rsq*) [inline]

This version of the plane routine just makes up the plane ID to be zero. It will only be referenced if neighbor tracking is enabled.

Parameters:

← ***(x,y,z)*** The vector to cut the cell by.

← ***rsq*** The modulus squared of the vector.

Definition at line 1435 of file cell.cc.

4.9.3.37 template<class n_option > bool voronoicell_base< n_option >::plane_intersects (fpoint *x*, fpoint *y*, fpoint *z*, fpoint *rsq*) [inline]

This routine tests to see whether the cell intersects a plane by starting from the guess point up. If up intersects, then it immediately returns true. Otherwise, it calls the plane_intersects_track() routine.

Parameters:

← ***(x,y,z)*** The normal vector to the plane.

← ***rsq*** The distance along this vector of the plane.

Returns:

false if the plane does not intersect the plane, true if it does.

Definition at line 1899 of file cell.cc.

4.9.3.38 template<class n_option > bool voronoicell_base< n_option >::plane_intersects_guess (fpoint *x*, fpoint *y*, fpoint *z*, fpoint *rsq*) [inline]

This routine tests to see if a cell intersects a plane. It first tests a random sample of approximately sqrt(p)/4 points. If any of those are intersect, then it immediately returns true. Otherwise, it takes the closest point and passes that to plane_intersect_track() routine.

Parameters:

← ***(x,y,z)*** The normal vector to the plane.

← ***rsq*** The distance along this vector of the plane.

Returns:

false if the plane does not intersect the plane, true if it does.

Definition at line 1913 of file cell.cc.

4.9.3.39 template<class n_option > void voronoicell_base< n_option >::print_edges () [inline]

Prints the vertices, their edges, the relation table, and also notifies if any glaring memory errors are visible.

Definition at line 1726 of file cell.cc.

4.9.3.40 template<class n_option > fpoint voronoicell_base< n_option >::volume () [inline]

Calculates the volume of the Voronoi cell, by decomposing the cell into tetrahedra extending outward from the zeroth vertex, which are evaluated using a scalar triple product.

Returns:

A floating point number holding the calculated volume.

Definition at line 1474 of file cell.cc.

4.9.4 Member Data Documentation

4.9.4.1 template<class n_option > int voronoicell_base< n_option >::current_delete2_size

This sets the size of the auxiliary delete stack.

Definition at line 132 of file cell.hh.

4.9.4.2 template<class n_option > int voronoicell_base< n_option >::current_delete_size

This sets the size of the main delete stack.

Definition at line 130 of file cell.hh.

4.9.4.3 template<class n_option > int voronoicell_base< n_option >::current_vertex_order

This holds the current maximum allowed order of a vertex, which sets the size of the mem, mep, and mec arrays. If a vertex is created with more vertices than this, the arrays are dynamically extended using the add_memory_vorder routine.

Definition at line 128 of file cell.hh.

4.9.4.4 template<class n_option > int voronoicell_base< n_option >::current_vertices

This holds the current size of the arrays ed and nu, which hold the vertex information. If more vertices are created than can fit in this array, then it is dynamically extended using the add_memory_vertices routine.

Definition at line 122 of file cell.hh.

4.9.4.5 template<class n_option > int** voronoicell_base< n_option >::ed

This is a two dimensional array that holds information about the edge connections of the vertices that make up the cell. The two dimensional array is not allocated in the usual method. To account for the fact the different vertices have different orders, and thus require different amounts of storage, the elementss of ed[i] point to one-dimensional arrays in the mep[] array of different sizes.

More specifically, if vertex i has order m, then ed[i] points to a one-dimensional array in mep[m] that has 2*m+1 entries. The first m elements hold the neighboring edges, so that the jth edge of vertex i is held in ed[i][j]. The next m elements hold a table of relations which is redundant but helps speed up the

computation. It satisfies the relation ed[ed[i][j]][ed[i][m+j]]=i. The final entry holds a back pointer, so that ed[i+2∗m]=i. These are used when rearranging the memory.

Definition at line 113 of file cell.hh.

4.9.4.6 template<class n_option > int* voronoicell_base< n_option >::nu

This array holds the order of the vertices in the Voronoi cell. This array is dynamically allocated, with its current size held by current_vertices.

Definition at line 117 of file cell.hh.

4.9.4.7 template<class n_option > int voronoicell_base< n_option >::p

This sets the total number of vertices in the current cell.

Definition at line 138 of file cell.hh.

4.9.4.8 template<class n_option > fpoint* voronoicell_base< n_option >::pts

This in an array with size 3∗current_vertices for holding the positions of the vertices.

Definition at line 135 of file cell.hh.

4.9.4.9 template<class n_option > suretest voronoicell_base< n_option >::sure

This is a class used in the plane routine for carrying out reliable comparisons of whether points in the cell are inside, outside, or on the current cutting plane.

Definition at line 149 of file cell.hh.

4.9.4.10 template<class n_option > int voronoicell_base< n_option >::up

This is the index of particular point in the cell, which is used to start the tracing routines for plane intersection and cutting. These routines will work starting from any point, but it's often most efficient to start from the last point considered, since in many cases, the cell construction algorithm may consider many planes with similar vectors concurrently.

Definition at line 145 of file cell.hh.

The documentation for this class was generated from the following files:

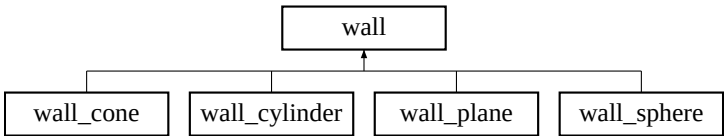
- cell.hh
- cell.cc

4.10 wall Class Reference

Pure virtual class from which wall objects are derived.

`#include <container.hh>`

Inheritance diagram for wall::



Public Member Functions

- virtual bool point_inside (fpoint x, fpoint y, fpoint z)=0
- virtual bool cut_cell (voronoicell_base< neighbor_none > &c, fpoint x, fpoint y, fpoint z)=0
- virtual bool cut_cell (voronoicell_base< neighbor_track > &c, fpoint x, fpoint y, fpoint z)=0

4.10.1 Detailed Description

Pure virtual class from which wall objects are derived.

This is a pure virtual class for a generic wall object. A wall object can be specified by deriving a new class from this and specifying the functions.

Definition at line 329 of file container.hh.

4.10.2 Member Function Documentation

4.10.2.1 virtual bool wall::cut_cell (voronoicell_base< neighbor_track > & *c*, fpoint *x*, fpoint *y*, fpoint *z*) [pure virtual]

A pure virutal function for cutting a cell with neighbor-tracking enabled with a wall.

Implemented in wall_sphere, wall_plane, wall_cylinder, and wall_cone.

4.10.2.2 virtual bool wall::cut_cell (voronoicell_base< neighbor_none > & *c*, fpoint *x*, fpoint *y*, fpoint *z*) [pure virtual]

A pure virutal function for cutting a cell without neighbor-tracking with a wall.

Implemented in wall_sphere, wall_plane, wall_cylinder, and wall_cone.

4.10.2.3 virtual bool wall::point_inside (fpoint *x*, fpoint *y*, fpoint *z*) [pure virtual]

A pure virtual function for testing whether a point is inside the wall object.

Implemented in wall_sphere, wall_plane, wall_cylinder, and wall_cone.

The documentation for this class was generated from the following file:

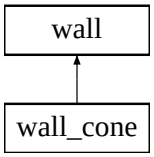
- container.hh

4.11 wall_cone Struct Reference

A class representing a conical wall object.

`#include <wall.hh>`

Inheritance diagram for wall_cone::



Public Member Functions

- wall_cone (fpoint ixc, fpoint iyc, fpoint izc, fpoint ixa, fpoint iya, fpoint iza, fpoint ang, int iw_id=-99)
- bool point_inside (fpoint x, fpoint y, fpoint z)
- template<class n_option >
  bool cut_cell_base (voronoicell_base< n_option > &c, fpoint x, fpoint y, fpoint z)
- bool cut_cell (voronoicell_base< neighbor_none > &c, fpoint x, fpoint y, fpoint z)
- bool cut_cell (voronoicell_base< neighbor_track > &c, fpoint x, fpoint y, fpoint z)

4.11.1 Detailed Description

A class representing a conical wall object.

This class respresents a cone wall object.

Definition at line 85 of file wall.hh.

4.11.2 Constructor & Destructor Documentation

4.11.2.1 wall_cone::wall_cone (fpoint *ixc*, fpoint *iyc*, fpoint *izc*, fpoint *ixa*, fpoint *iya*, fpoint *iza*, fpoint *ang*, int *iw_id* = `-99`) `[inline]`

Constructs a cone wall object.

Parameters:

← ***(ixc,iyc,izc)*** the apex of the cone.

← ***(ixa,iya,iza)*** a vector pointing along the axis of the cone.

← ***ang*** the angle (in radians) of the cone, measured from the axis.

← ***iw_id*** an ID number to associate with the wall for neighbor tracking.

Definition at line 95 of file wall.hh.

4.11.3 Member Function Documentation

4.11.3.1 bool wall_cone::cut_cell (voronoicell_base< neighbor_track > & *c*, fpoint *x*, fpoint *y*, fpoint *z*) [inline, virtual]

A pure virutal function for cutting a cell with neighbor-tracking enabled with a wall.

Implements wall.

Definition at line 103 of file wall.hh.

4.11.3.2 bool wall_cone::cut_cell (voronoicell_base< neighbor_none > & *c*, fpoint *x*, fpoint *y*, fpoint *z*) [inline, virtual]

A pure virutal function for cutting a cell without neighbor-tracking with a wall.

Implements wall.

Definition at line 102 of file wall.hh.

4.11.3.3 template<class n_option > bool wall_cone::cut_cell_base (voronoicell_base< n_option > & *c*, fpoint *x*, fpoint *y*, fpoint *z*) [inline]

Cuts a cell by the cone wall object. The conical wall is approximated by a single plane applied at the point on the cone which is closest to the center of the cell. This works well for particle arrangements that are packed against the wall, but loses accuracy for sparse particle distributions.

Parameters:

← *&c* the Voronoi cell to be cut.

← *(x,y,z)* the location of the Voronoi cell.

Returns:

true if the cell still exists, false if the cell is deleted.

Definition at line 105 of file wall.cc.

4.11.3.4 bool wall_cone::point_inside (fpoint *x*, fpoint *y*, fpoint *z*) [virtual]

Tests to see whether a point is inside the cone wall object.

Parameters:

← *(x,y,z)* the vector to test.

Returns:

true if the point is inside, false if the point is outside.

Implements wall.

Definition at line 85 of file wall.cc.

The documentation for this struct was generated from the following files:

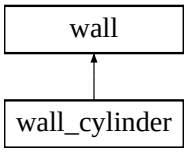
- wall.hh
- wall.cc

4.12 wall_cylinder Struct Reference

A class representing a cylindrical wall object.

`#include <wall.hh>`

Inheritance diagram for wall_cylinder::



Public Member Functions

- wall_cylinder (fpoint ixc, fpoint iyc, fpoint izc, fpoint ixa, fpoint iya, fpoint iza, fpoint irc, int iw_id=-99)
- bool point_inside (fpoint x, fpoint y, fpoint z)
- template<class n_option >
  bool cut_cell_base (voronoicell_base< n_option > &c, fpoint x, fpoint y, fpoint z)
- bool cut_cell (voronoicell_base< neighbor_none > &c, fpoint x, fpoint y, fpoint z)
- bool cut_cell (voronoicell_base< neighbor_track > &c, fpoint x, fpoint y, fpoint z)

4.12.1 Detailed Description

A class representing a cylindrical wall object.

This class respresents a open cylinder wall object.

Definition at line 58 of file wall.hh.

4.12.2 Constructor & Destructor Documentation

4.12.2.1 wall_cylinder::wall_cylinder (fpoint *ixc*, fpoint *iyc*, fpoint *izc*, fpoint *ixa*, fpoint *iya*, fpoint *iza*, fpoint *irc*, int *iw_id* = -99) [inline]

Constructs a cylinder wall object.

Parameters:

← ***(ixc,iyc,izc)*** a point on the axis of the cylinder.

← ***(ixa,iya,iza)*** a vector pointing along the direction of the cylinder.

← ***irc*** the radius of the cylinder

← ***iw_id*** an ID number to associate with the wall for neighbor tracking.

Definition at line 68 of file wall.hh.

4.12.3 Member Function Documentation

4.12.3.1 bool wall_cylinder::cut_cell (voronoicell_base< neighbor_track > & *c*, fpoint *x*, fpoint *y*, fpoint *z*) [inline, virtual]

A pure virutal function for cutting a cell with neighbor-tracking enabled with a wall.

Implements wall.

Definition at line 75 of file wall.hh.

4.12.3.2 bool wall_cylinder::cut_cell (voronoicell_base< neighbor_none > & *c*, fpoint *x*, fpoint *y*, fpoint *z*) [inline, virtual]

A pure virutal function for cutting a cell without neighbor-tracking with a wall.

Implements wall.

Definition at line 74 of file wall.hh.

4.12.3.3 template<class n_option > bool wall_cylinder::cut_cell_base (voronoicell_base< n_option > & *c*, fpoint *x*, fpoint *y*, fpoint *z*) [inline]

Cuts a cell by the cylindrical wall object. The cylindrical wall is approximated by a single plane applied at the point on the cylinder which is closest to the center of the cell. This works well for particle arrangements that are packed against the wall, but loses accuracy for sparse particle distributions.

Parameters:

← *&c* the Voronoi cell to be cut.

← *(x,y,z)* the location of the Voronoi cell.

Returns:

true if the cell still exists, false if the cell is deleted.

Definition at line 70 of file wall.cc.

4.12.3.4 bool wall_cylinder::point_inside (fpoint *x*, fpoint *y*, fpoint *z*) [virtual]

Tests to see whether a point is inside the cylindrical wall object.

Parameters:

← *(x,y,z)* the vector to test.

Returns:

true if the point is inside, false if the point is outside.

Implements wall.

Definition at line 54 of file wall.cc.

The documentation for this struct was generated from the following files:

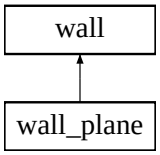
- wall.hh
- wall.cc

4.13 wall_plane Struct Reference

A class representing a plane wall object.

`#include <wall.hh>`

Inheritance diagram for wall_plane::



Public Member Functions

- wall_plane (fpoint ixc, fpoint iyc, fpoint izc, fpoint iac, int iw_id=-99)
- bool point_inside (fpoint x, fpoint y, fpoint z)
- template<class n_option >
  bool cut_cell_base (voronoicell_base< n_option > &c, fpoint x, fpoint y, fpoint z)
- bool cut_cell (voronoicell_base< neighbor_none > &c, fpoint x, fpoint y, fpoint z)
- bool cut_cell (voronoicell_base< neighbor_track > &c, fpoint x, fpoint y, fpoint z)

4.13.1 Detailed Description

A class representing a plane wall object.

This class represents a single plane wall object.

Definition at line 36 of file wall.hh.

4.13.2 Constructor & Destructor Documentation

4.13.2.1 wall_plane::wall_plane (fpoint *ixc*, fpoint *iyc*, fpoint *izc*, fpoint *iac*, int *iw_id* = -99) [inline]

Constructs a plane wall object

Parameters:

← ***(ixc,iyc,izc)*** a normal vector to the plane.

← ***iac*** a displacement along the normal vector.

← ***iw_id*** an ID number to associate with the wall for neighbor tracking.

Definition at line 43 of file wall.hh.

4.13.3 Member Function Documentation

4.13.3.1 bool wall_plane::cut_cell (voronoicell_base< neighbor_track > & *c*, fpoint *x*, fpoint *y*, fpoint *z*) [inline, virtual]

A pure virutal function for cutting a cell with neighbor-tracking enabled with a wall.

Implements wall.

Definition at line 49 of file wall.hh.

4.13.3.2 bool wall_plane::cut_cell (voronoicell_base< neighbor_none > & *c*, fpoint *x*, fpoint *y*, fpoint *z*) [inline, virtual]

A pure virutal function for cutting a cell without neighbor-tracking with a wall.

Implements wall.

Definition at line 48 of file wall.hh.

4.13.3.3 template<class n_option > bool wall_plane::cut_cell_base (voronoicell_base< n_option > & *c*, fpoint *x*, fpoint *y*, fpoint *z*) [inline]

Cuts a cell by the plane wall object.

Parameters:

← *&c* the Voronoi cell to be cut.
← *(x,y,z)* the location of the Voronoi cell.

Returns:

true if the cell still exists, false if the cell is deleted.

Definition at line 46 of file wall.cc.

4.13.3.4 bool wall_plane::point_inside (fpoint *x*, fpoint *y*, fpoint *z*) [virtual]

Tests to see whether a point is inside the plane wall object.

Parameters:

← *(x,y,z)* the vector to test.

Returns:

true if the point is inside, false if the point is outside.

Implements wall.

Definition at line 37 of file wall.cc.

The documentation for this struct was generated from the following files:

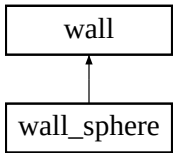
- wall.hh
- wall.cc

4.14 wall_sphere Struct Reference

A class representing a spherical wall object.

`#include <wall.hh>`

Inheritance diagram for wall_sphere::



Public Member Functions

- wall_sphere (fpoint ixc, fpoint iyc, fpoint izc, fpoint irc, int iw_id=-99)
- bool point_inside (fpoint x, fpoint y, fpoint z)
- template<class n_option >
  bool cut_cell_base (voronoicell_base< n_option > &c, fpoint x, fpoint y, fpoint z)
- bool cut_cell (voronoicell_base< neighbor_none > &c, fpoint x, fpoint y, fpoint z)
- bool cut_cell (voronoicell_base< neighbor_track > &c, fpoint x, fpoint y, fpoint z)

4.14.1 Detailed Description

A class representing a spherical wall object.

This class represents a spherical wall object.

Definition at line 13 of file wall.hh.

4.14.2 Constructor & Destructor Documentation

4.14.2.1 wall_sphere::wall_sphere (fpoint *ixc*, fpoint *iyc*, fpoint *izc*, fpoint *irc*, int *iw_id* = `-99`) `[inline]`

Constructs a spherical wall object.

Parameters:

← ***iw_id*** an ID number to associate with the wall for neighbor tracking.

← ***(ixc,iyc,izc)*** a position vector for the sphere's center.

← ***irc*** the radius of the sphere.

Definition at line 21 of file wall.hh.

4.14.3 Member Function Documentation

4.14.3.1 bool wall_sphere::cut_cell (voronoicell_base< neighbor_track > & *c*, fpoint *x*, fpoint *y*, fpoint *z*) [inline, virtual]

A pure virutal function for cutting a cell with neighbor-tracking enabled with a wall.

Implements wall.

Definition at line 27 of file wall.hh.

4.14.3.2 bool wall_sphere::cut_cell (voronoicell_base< neighbor_none > & *c*, fpoint *x*, fpoint *y*, fpoint *z*) [inline, virtual]

A pure virutal function for cutting a cell without neighbor-tracking with a wall.

Implements wall.

Definition at line 26 of file wall.hh.

4.14.3.3 template<class n_option > bool wall_sphere::cut_cell_base (voronoicell_base< n_option > & *c*, fpoint *x*, fpoint *y*, fpoint *z*) [inline]

Cuts a cell by the sphere wall object. The spherical wall is approximated by a single plane applied at the point on the sphere which is closest to the center of the cell. This works well for particle arrangements that are packed against the wall, but loses accuracy for sparse particle distributions.

Parameters:

← *&c* the Voronoi cell to be cut.

← *(x,y,z)* the location of the Voronoi cell.

Returns:

true if the cell still exists, false if the cell is deleted.

Definition at line 24 of file wall.cc.

4.14.3.4 bool wall_sphere::point_inside (fpoint *x*, fpoint *y*, fpoint *z*) [virtual]

Tests to see whether a point is inside the sphere wall object.

Parameters:

← *(x,y,z)* the vector to test.

Returns:

true if the point is inside, false if the point is outside.

Implements wall.

Definition at line 12 of file wall.cc.

The documentation for this struct was generated from the following files:

- wall.hh
- wall.cc

Index