ReMoDy

1.1

Programmer's Guide

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Contents

Chapter 1

ReMoDy Source Code Documentation and User's Guide

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1.0

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1.1 Contents

1.2 Introduction

This is the documentation of the ReMoDy (Reactive Molecular Dynamics) program, which implements the model of reactive molecular dynamics based on the Collision Theory.

1.3 Installation and Execution

1.3.1 Step 1: Extracting the archive

If you have the archive file, like remody.tbz (tar-bzipped) or remody.tgz (tar-gzipped) then files can be retrieved into a current directory as:

tar cvjf remody.tbz

or

tar cvzf remody.tgz

respectively.

1.3.2 Step 2: Compiling

To compile the executable on Linux run make from the remody root directory, where the makefile was saved. Note that the subdirectories src/, run/, and obj/ should be also present.

1.3.3 Step 3: Running

The executables are saved in the run/ directory. It should also contain the example remody.xml and demo.xml files, as well as an initial empty input file empty.dat.gz. To run the program with an OpenGL window active (slow, good for debugging), one can use the command:

./view -f demo.xml empty.dat.gz

This will start the program with the initial parameters read from the demo.xml file and the initial data read from empty.dat.gz file. On startup the program will open the window. One can point at the window with the mouse and press 'f' key to show the frame and 'r' key to run the simulation. Alternatively, one can use 's' key to run iterations step-by-step. Other key functions are described by pressing the '?' key.

To run the program in a batch mode without OpenGL output, one can use this command:

./job -f demo.xml empty.dat.gz &

This will start the run. To change the parameters of the job, one should modify the input xml file accordingly (demo.xml, remody.xml, etc.). A link with the name remody is also set to one of the executables, like

ln -s ./job remody

1.4 Setup

Both view (OpenGL based) and job (batch mode) executables read the configuration xml file. By default the file will have the same name as the executable, for example: job.xml or view.xml. This can be overwritten with the '-f' option. Two example files `remody.xml` and `demo.xml` are provided with the distribution.

The format of the xml file is in most cases self-explanatory with explanations provided in the "title" fields and comments. The main sections include: run, species, domain, and gui.

The **run** section specifies the number of iterations, time steps, output intervals, and the maximum number of molecules to be used.

The **species** section provides the list of species, and reactions between them.

The **domain** section provides the specifications of the boundary conditions and the surface reactions and species.

The **gui** section specifies the parameters used in the OpenGL output window, such as colors, line width, etc.

See also Section Configuration File

1.5 Licencing and Support

The rest of this documentation provides the descriptioin of the structure and functionality of the classes, namespaces, and files of the code.

The code is provided under the GPL licence. Any suggestions/requests can be directed to the developers team at NIFT.

Chapter 2

Configfile

2.1 Configuration File

2.1.1 Invocation

The config file is in XML format. It is loaded at program startup and contains the specification of all the main parameters, grouped in respective sections. An example `syngas.xml` file is provided which includes the setup of syngas reaction on the anode side of a high-temperature solid-oxide fuel cell.

The default name of the config file is <progname>.xml, where <progname> is the name of the executable, such as `view`, `job`, or `remody`. One can override the default name by using -f command line option, like:

remody -f syngas.xml

2.1.2 Sections

The sections are enclosed in XML tag pairs, like <tag>...</tag>. where the tags are as follows:

- `iterations`: specifies the integer number of iterations the code should run
- `time`: several parameters of physical execution time in seconds, such as `start`=start time, `end`=end time, and `step`=time step. The code will run until either the number of iterations as specified in the `iterations` section or the end time is reached.
- `molecules`: integer number equal to the maximum number of molecules that the program will be able to handle. It will determine the memory allocated at the beginning of execution.
- `species`: this section lists all chemical species and reactions between them. Correspondingly, each specie is described in `specie` section as:

1. `specie`: includes such parameters as `mass` in Atomic units [au], `size` in nanometers [nm], and specific heat, `cp` in kJ/(mol∗K). The `specie` tag should also include an attribute `id`, identifying a specie chemical formula, such as CO2, H2O, etc.
2. `reaction`: reaction tag has two attributes: `reactants` and `products`. The reactants tag should contain two species identifiers. Since only elementary (binary) reactions are considered, there should be exactly two identifiers for reactants. Each of the identifiers should correspond to one specie identifiers listed in the list of species. The products attribute should consist of one or two identifiers of reaction products. Also in the reaction section the following parameters are specified:

   `activation` = reaction activation temperature in K,

   `probability` = probability of reaction outcome as given by the `products` attribute. This parameter should always be 1.0 if there is only one reaction with the given reactants. In case of several reactions with the same reactants, but with different products, this parameter should indicate the probability of this particular branch with given reaction products.

   `enthalpy` = enthalpy of reaction in kJ/mol.

- `domain`: The `domain` section consists of the set of parameters describing the geometry and physical properties of the modeled media inside the computational domain, including:

1. `type`: specifies the geometry. Currently only `box` type is supported.
2. `grid`: Specifies parameters of the rectangular grid used in segmentation algorithm for accelerating the interaction scheme. In particular, the `cellsize` parameter determines the size of the grid cell. This size should be selected as small as possible but no less than twice the size of the largest specie.

Decreasing the cell size will speed-up code execution in better than linear proportion of the cell-size (but no better than quadratic). At the same time it will increase memory utilization in proportion to it's 3-rd power. It is not recommended to increase the memory utilization above 90%. One can use Unix 'top' utility to check memory utilization.

3. `energy`: Only used for Lennart-Jones type potentials, currently under development.
4. `bounds`: specifies spatial bounds of the computational domain as: xmin xmax ymin ymax zmin zmax.
5. `bulk`: this section specifies thermodynamic properties and gas composition inside the bulk of the domain. In particular, `temperature` is given in Kelvin [K], and for each specie, its `density` is specified in [kg/m^3].
6. `boundary`: each boundary of the domain contains the description of thermodynamic properties and gas composition on the other side of the boundary in the same format as for the bulk of the domain. In addition to these, the boundary tag should have the boundary identifier `id`-attribute, such as "top", "bottom", "right", "left", "front", and "rear". Also additional boundary tag is `type`, which can be one of: "open", "elastic", and "periodic". In the case of open boundary the molecules can freely cross the boundary, in which case they will be removed from the domain. In case of elastic boundary the molecules will bounce from the boundary like from an elastic wall. For periodic boundaries, the molecules crossing the boundary will reappear from the opposite boundary. Boundary description can also contain the list reactions, between the boundary species given in the same format as in the `species` section.

- `gui`: the gui section describes parameters related to graphical output used when running an OpenGL based version with a visual window output.

1. `translation`: initial translation of the scene.
2. `vector`: parameters for displaying vectors.
3. `frame`: parameters for displaying a domain frame.
4. `mesh`: parameters for displaying mesh. In particular the `node` tag specifies the parameters for displaying particles, or molecules, such as using points or spheres (`type`), etc. Note that using 'spehere' for type may significantly slow-down simulation in GUI mode.

- `xterm`: if set to 1 this parameter will force terminal dumping of certain parameters, like temperature, energy, number of molecules, and species concentrations after every time-step. This can be useful if the time-dependence of concentrations and other parameters needs to be retrieved. In the last case the output can be redirected to a file, which can be processed with the `readlog` utility (see How do I produce time-curves ...?").

Chapter 3

Examples

3.1 Examples

3.1.1 Syngas Simulation Setup

The `syngas.xml` file can be used as an input config file to ReMoDy to simulate the molecular dynamics of syngas including it's interaction with the anode.

- To setup the syngas.xml file read SecConfigfile.
- To start the program loading the `syngas.xml` file, use the command line as:

  ./remody -f syngas.xml

  Note, that the name of your executable can be other than `remody`, such as `view` or `job`, in which case change the command line above accordingly.
- To restart from the previous run data, use the command line:

  ./remody -f syngas.xml remody-<number>.dat.gz

  where `remody-<number>.dat.gz` is the name of the dump file generated by remody.
- To retrieve and post process the data, read FAQs.

Chapter 4

Frequently Asked Questions

4.1 FAQs

- **Q:***"When I run remody with a larger domain the program doesn't run and show me this message:"*

  CAN'T INSERT ELEMENT: Collection OF 99999 IS FULL

  A: Increase the number of molecules above 100000 in <molecules>....</molecules> section of the config file (syngas.xml) You can estimate the number of molecules you should use from the ideal gas law, that is how many molecules you can have in the domain size you selected and increase that number by 10% to avoid that error condition above.

- **Q:** *"How to make the code run faster?"*

  A: When you run the code check how much memory the program is using. For example, you can do it running 'top' from a terminal. If it is using less than 80%, then decrease the parameter inside <**grid**><**cellsize**>**...**</**cellsize**></**grid**> tag. This will make code run a bit faster but it will also increase the memory utilization. It may not even start if you decrease it too much. If the memory utilization is still less than 80%, you can keep decreasing that parameter. Do not decrease it below twice the size of the biggetst molecule in your composition.

- **Q:** *"How do I restart the run?"*

  A: When the code is running it generates output files at regular time interval (physical time, that is) which is set inside <**time**><**output**>**...**</**output**></**time**> tag. The output is dumped to the gzipped-files named like remody-<timestamp>.dat.gz. To restart the run from the output file you should start the run as:

  ./remody -f configfile.xml remody-<timestamp>.dat.gz

- **Q:** *"How do I produce time-curves of various parameters?"*

  A: You can produce time curves for such parameters as temperature (T), number of molecules in the domain (N), average energy per molecule (E), and various specie concentrations. For T,N, and E follow the procedure as described below, using the syntax with an equal sign (=), for species do not use equal sign as described in the following two questions.

- **Q:** *"How do I construct the temperature curve?"*

  A: Run the readlog.py utility with the remody terminal output log file as input. For example, when you start the batch job, use the command like this:

  ./job -f config.xml > job.log &

  This will dump temperature, concentrations, and other parameters into the job.log file every iteration. Then you can run the readlog.py utility to produce the temperature curve file from the log file, like:

  python readlog.py T= < job.log > temp.dat

  where the temp.dat file contains two columns of temperature versus time, which be displayed in gnuplot with a command like:

  plot 'temp.dat' w l

- **Q:** *""* **A:**

- **Q:** *"How do I construct specie concentration time curves?"*

  A: Do similarly as for the temperature curve above, except when running the readlog specify the specie chemical formula as provided in the input xml file, and do not use the equal sign (=) after the specie name as in the case above, like this:

  python readlog.py CO2 < job.log > co2.dat

- **Q:** *"How can I retrieve the results of simulation?"*

  A: Here is how you can produce the results from the simulation run. First check if the run is going with top:

  top

  This will show the table like this:

  ```
  top - 04:29:40 up 42 days, 3:41, 2 users, load average:  1.03,
  1.10, 1.20
  Tasks:  126 total, 3 running, 123 sleeping, 0 stopped, 0 zombie
  Cpu(s):  25.2us, 0.1sy, 0.0ni, 74.7id, 0.0wa, 0.0hi, 0.0si, 0.0st
  Mem:  4031520k total, 3878180k used, 153340k free, 336828k buffers
  Swap:  10241428k total, 1454736k used, 8786692k free, 552436k
  cached
  PID USER PR NI VIRT RES SHR S CPU MEM TIME+ COMMAND
  29283 rolando 25 0 3353m 2.0g 1336 R 100 52.8 9843:09 job
  1 root 15 0 10308 596 544 S 0 0.0 0:04.77 init
  ...
  ```

  There you can see that job is running. Quit it by pressing 'q'-key. Then check how far the run has gone:

  tail -f syngas2.log

  This will show the something like:

  ```
  Time=6.103e-01 Step=2.439e-06 Memory=41% N=8279309 T=1039.63K
  E=1.188e-13J
  H H2 OH H2O CH3 CH4
  5.45126 31.48455 0.00104 18.91287 0.00041 13.87211
  CO2 CO N2
  8.70242 10.84918 10.72622
  ```

  Note that syngas2.log file above was used because the job started with the command:

  ./job -f syngas2.xml job-4.dat.gz 1> syngas2.log 2> syngas2.err &

  If you used a different log file you should use that one above. From the table you can see all the species currently in the simulation. Now you can quit tail -f with pressing ^C (Cntrl.C).

  To produce the time sequence do this:

  1. Run this command:
     python readlog.py H2 < syngas2.log > H2-time.dat
     Note that readlog.py program is in your remody/util directory. This should create the H2-time.dat file.
  2. Check the file with gnuplot:
     gnuplot> plot 'H2-time.dat' w l
     And then you do the same for H2O, CO2, etc.

- **Q:** *"How to produce a spatial distribution along one axis?"*

  A:

1. Check that you have the hist program in run directory: ls hist if you dont, compile it if necessary in your remody/util directory by running make and link it or copy into your run directory, like ln -s ../util/hist .
2. Select the time step for which you want the distribution. For example, for 5 nanoseconds, you should use job-5.dat.gz file.
3. Run the command:

   gunzip job-5.dat.gz -c | grep H2 | grep -v H2O | cut -f 3 | ./hist > H2-5.dat

   This will create the H2-5.dat file, which you can see with gnuplot as:

   plot 'H2-5.dat' w l

   Note, that the line above has 'grep -v H2O' part. This is needed to preclude all H2O molecules from the H2 list. Similarily, when you produce CO distribution, you should use:

   gunzip job-5.dat.gz -c | grep CO | grep -v CO2 | cut -f 3 | ./hist > CO-5.dat

   But to produce H2O or CO2 distributions, you should use:

   gunzip job-5.dat.gz -c | grep H2O | cut -f 3 | ./hist > H2O-5.dat gunzip job-5.dat.gz -c | grep CO2 | cut -f 3 | ./hist > CO2-5.dat

   Then you can produce plot of all of them like:

   plot 'H2-5.dat' w l, 'H2O-5.dat w l, 'CO-5.dat' w l, 'CO2-5.dat' w l

   etc. The same for other nanoseconds. You may need to set the axes labels, like

   set xlabel 'TIME [ns]' set ylabel 'NUMBER OF MOLECULES'

   To save the plot into a png-file, use:

   set term png set output 'concentrations-5ns.png'

   and then run the above plot command again. This will create the concentrations-5ns.png file, which you can include into a presentation or a paper. But don't forget to get the output back to the screen with:

   set output set term x11

   before you try other plot commands, or everything will be written to that png file.

   Of course if you are proficient with Python, you can use the matplotlib module to plot and alalyze the results.

Chapter 5

GUI

5.1 Graphical User Interface

ReMoDy can be compiled in two versions: with and without a graphical user interface (GUI). The former is used to visualize the simulation progress on a small set of data, while the latter is to perform larger-scale simulations where the concurrent visualization is not possible.

After the GUI-enabled version (view) is started, a display window pops up, showing the computational domain. The initial parameters of the scene can be set in the config file (see Sec. Configuration File). The configfile can be reloaded by making the display window active and hitting the 'l' key for 'load'. The keyboard control of the simulation has two modes: *keystroke*, and *commandline*. This is similar to vi text editor in UNIX. Initially the keystroke mode is active.

1. In the keystroke model the single-key-strokes can be used while the display window is active. These include:

- **ESC**: exit. The same as 'q';
- **?**: show help.
- **:**: switch to a terminal command mode (similar to vi). The same as '.';
- **a**: show/hide the axes.
- **b**: show/hide boundary faces of the mesh (not used when mesh is absent).
- **c**: switch the color-scheme.
- **f**: show the box frame.
- **G**: show all the mesh edges.
- **g**: show only the boundary mesh edges.
- **l**: read configuration file.
- **m**: display the menue on the console.
- **N**: show mesh nodes.
- **n**: show boundary vertexes.
- **r**: start/stop the continuous run.
- **s**: perform one step of the simulation. Analogous to '+'.
- **v**: show boundary vectors.
- **w**: dump current window into a xwd file.
- **Z**: zoom-in view.
- **z**: zoom-out view.

1. The command mode is switched from the keystroke mode by hitting the ':' or '.' keys. To switch back from the command mode one has to enter an empty command, that is, press ENTER, while the command line is empty. In the command mode, the command line appears in the terminal windows from which the program has started. The commands one can enter in the command line include:

- **bg**: go to background run mode. During this mode the all controls are disabled.

- **cs**: switch the color scheme.
- **fg**: go to foreground mode.
- **?, h, or help**: show help.
- **r**: run a number of iterations.
- **sp**: toggle between spheres and points in particle (molecule) display.
- **wd**: start/stop window dump every fixed number of iterations.
- **dw**: dump current window picture into a xwd file.
- **e**: exit the program. Also saves current data.
- **q**: quit without saving.
- **.**: quit the command mode. Also hitting ENTER with empty command line.

Chapter 6

Implementation

6.1 Implementation

6.1.1 Collision Detection Scheme

The discretization scheme is based on the combination of the linked cell method (Sec.Linked-Cell Method) with a space-time collision detection scheme (Sec.Space-Time Collision Detection Scheme), which enable to significantly accelerate the execution of the method. To better understand the principle of the method, it has to be compared with the standard time-advancement scheme.

6.1.1.1 Standard Time-Advancement Scheme

In a standard scheme all molecules are advanced using a single global time step. This time step is selected as the minimum time for a molecule to move at the distance of its radius:

$$dt = \frac{d}{v}$$

where 'd' is the on the order of molecule radius and 'v' is the velocity of a molecule. The minimum is sought for all molecules. After each time step the relative positions of all molecules are analyzed to determine if there are any overlaps (collisions) between pairs of molecules.

This choice of time-step, dt, above guarantees that no molecule will miss a collision event. However, since each molecule usually travels much longer distances than its length between the collisions, this scheme leads to unnecessary many steps calculations for an essentially straight trajectory path between the collisions as illustrated in the figure below.

Also, the time step is selected with respect to the smallest molecule, which usually also have the highest velocity. Thus, in the case of a gas mixture, this time-step will be excessively small for bigger and slower moving molecules.

Considering this, and the fact that the molecules travel on straight paths between the collisions, the standard scheme is very inefficient, since it does the majority of computations for molecules undergoing no collisions, but rather traveling on straight paths.

6.1.1.2 Space-Time Collision Detection Scheme

In the new collision detection scheme instead of moving all molecules with the same time step, attempts to move each molecule directly to the site of next collision, avoiding any calculations on the straight path, as shown in the figure.

using a single global time step for all molecules, each molecule has it's own time, and its own time-step. Thus, instead of a 3D position vector and velocity vector, the kinematic parameters for each molecule include a 4D space-time vector (x,y,z,t), velocity vector, (vx,vy,vz) and the time step, dt. The time-step for each molecule is is calculated as the time to the next collision. Thus, one can estimate the time of the next collision event, t_{coll}, for each molecule by adding its current time to its current time step:

$$t_{coll} = t + dt$$

The time-steps of molecules are constantly updated within the loop, where all pairs of molecules are analyzed for possible collisions on the basis of their velocities and radii. If the molecules are found to be heading for a collision, then the time of that collision event is compared to the currently estimated next collision time for each molecule. The time-steps for the molecules are updated if the new collision event is found to occur earlier than both estimated collision events for each molecule. This results in selection of the earliest possible collision events. The collision events also include the collisions with the walls.

In the same loop where the molecular time-steps are updated using collision-detection scheme, the actual collision events are processed for those molecules which are found to be within the interaction distance from each other. In the course of collision molecules change their velocities in compliance to momentum and energy conservation, as well as exchange their kinetic and internal energies according to the equipartition principle, that is, the total energy is equally distributed among the combined degrees of freedom of two molecules.

After the time-steps of all molecules are updated and collisions processed in the collision-detection loop, the molecules enter the time-advance loop, where each molecule is advanced by its time-step to its nearest collision event. These two loops are iterated over and over until the termination time for the simulation.

It should be noted, that the described scheme will not work well, if the times of all molecules start deviate from each other by too large a value, causing some molecules to go too far ahead in time compared with other molecules. Thus, it is necessary to periodically synchronize the molecules, by bringing them all to the same time level. This is done by introducing the global time step, such that all the molecules exceeding the next global time level will not move to the next collisions until all the molecules reach that time level. Then the global time level is incremented by the global time-step and the procedure is repeated. The value of the global time step is selected on the order of molecular mean-free-path:

$$dt = \frac{D}{v}$$

where 'D' is on the order of several mean free-path lengths (or inter-molecular distances). This choice guarantees that the molecular collision times will not go out of sync by too much to cause miscalculations in collision events.

Even though the current scheme is still relying on a global time-step, this time step is by far larger than that used in the standard time-stepping scheme discussed above. This is because in the standard scheme the global time-step is based on molecular size, and in the current scheme it is based on inter-molecular distance, which is far larger than the size of the molecule: $D >> d$. This leads to significant speed-up of calculations compared to the standard time-advance scheme.

6.1.2 Linked-Cell Method

ReMoDy uses interaction acceleration scheme based on linked-cell technique, which is a variant of `Verlet list method` [Verlet L (1967). *Phys. Rev.* **159:** 98-103]. In this method the whole computational domain is divided into box-shaped cells. Only interactions between the molecules from the same or adjacent cells are considered (see Figure).

The size of the grid cells is selected by optimizing the execution speed, and is usually on the order of several mean-free-paths. The method enables to achieve near linear dependence of execution time on the number of molecules. In contrast, looping over all molecules makes execution time proportional to the square of the number of molecules, which makes that impractical for large number of molecules.

6.1.3 Multi-Processor Implementation

The code can be made to run in parallel on multi-core workstations. It uses the shared-memory OpenMP library to distribute processing of the molecules time-advancement and interaction loops among the available CPUs.

The two time-critical loops which run in parallel are time-advancement loop, implemented in subroutine Domain::step(), and interaction loop implemented in Domain::interaction() routine. Before the loops are entered the molecules are indexes sequentially. Each OpenMP thread selects the molecules which has index satisfying the criterion:

$$mod(i_{mol}, N_{threads}) = i_{thread}$$

where $mod(*, *)$ is division by modulus. This way all molecules are distributed equally between active threads. The number of threads is selected as the maximum between the available processors, and the pre-defined constant `'nthreads'`.

In addition to this, in the interaction loop, the locking mechanism is used to prevent simultaneous processing of the same molecules by more than one processor. This can happen because the interaction procedure considers all pairs of molecules, which is done in a double-looping over all molecules. Thus, the selection of molecules from the primary loop, using the mechanism above will not prevent the possibility of simultaneous processing of the same molecule from the secondary loop by more than one processor. The locking mechanism operates by introducing the 'is-locked' flag for each molecule. Inside the nested loop the molecule is considered only when its state is not locked. If this is the case, then the molecule is temporarily locked while its interaction with the primary molecule from the main loop is being processed.

6.1.4 Dynamic Lists

The main data-structures holding molecules are dynamic lists: **Collection** and **Container**. *Collection* is a double-linked list of fixed number of items, with two pointers for each item, pointing to the next and the previous item. The list consist of two parts: active and dead. Each part forms a loop, such that following next or previous pointer from any element across the list will lead back to the same element. The procedure of moving elements between the active and dead parts is very simple, involving only several pointer reassignment operations. The figure below illustrates the operation of removing the active molecule from the computational space and assigning it to the pool of "dead" molecules.

The reverse procedure of "resurrecting" dead molecules and introducing them into the active pool is done in the same manner. This technique enables to avoid expensive memory allocation/deallocation operations, and save time on looping over the list of molecules, since all dead molecules are not in the active list, and are completely ignored by the looping procedure. Thus, no conditional if-statements are necessary, and shorter list sizes can be used.

The *Collection* class is convenient for the dynamic storage of a single collection of items, and is used to store all the molecules in the domain.

Container is a variable size list of pointers to items. Like a *Collection* it is also a double-lined list with the next and previous pointers for each item. But unlike a *Collection*, the *Container* all container lists share the same pool of dead items, or pointers, which can point to any item. Each container list can acquire items from the pool or return them back to the pool.

The *Container* list is convenient to store multiple lists of items where the number of items constantly change. Container lists are used in the implementation of the linked-cell method described below.

Chapter 7

Model

7.1 Physical Model

The physical model of ReMoDy is uses the Collision_theory to describe elementary chemical reactions, and Kinetic theory to describe molecular gas dynamics. Reactions occur probabilistically during molecular collisions, with the probabilities determined by the activation energies and reaction probabilities, if more than one outcome for the reaction exists.

The thermodynamic properties of the gas species include heat capacities which are used to distribute thermal energy among molecular degrees of freedom during the collisions.

7.1.1 Chemical Reactions

The interaction of the two molecules is modeled through the binary collision approximation whereby only two molecules can interact at a time. The interaction between the molecules can be of two kinds: (1) simple mechanical collision, (2) collision with subsequent chemical reaction. The fact of the collision is detected when the distance between the centers of two molecules becomes less than the sum of their radii, and their relative velocities are directed toward each-other.

Collision is modeled in the center-of-mass (CM) frame of reference. The velocities of the two molecules are first recalculated into the CM frame. The total energy of the two molecules is first calculated as their combined internal energy plus their combined kinetic energy in the CM coordinate frame. Chemical reactions are triggered when this energy is in excess of the activation energy for the reaction. In this case the enthalpy of the reaction is added to the total energy. This energy is then redistributed between the degrees of freedom of the product molecules according to the following scheme:

$$energy = KE + IE + enthalpy$$

$$dof_A = DOF(Cp_A)$$
$$dof_B = DOF(Cp_B)$$

where dof_X are total degrees of freedom (kinetic + internal) for molecule X=(A,B), and Cp_X is the specific heat of molecule X. The function DOF(Cp) of coputing the degrees of freedom from the specific heat is defined as:

$$DOF = 3 + (2Cv/R - 3)/2 = 3 + Cv/R - 1.5 = Cv/R + 1.5 = Cp/R + 0.5$$

where $Cv = Cp - R$

The combined kinetic degrees of freedom are 6, then the combined internal degrees of freedom are calculated as:

$$dofi = dof - 6$$

Then for each molecule the ratio of its internal degrees of freedom to the total internal degrees of freedom is computed as:

$$rdofi_A = (dof_A - 3)/dofi$$

$$rdofi_B = 1 - rdofi_A$$

The calculations of energy redistribution between colliding molecules is done in the center-of-mass system (CM). The number of kinetic (translational) degrees of freedom of two colliding molecules in CM system

($dofk_{CM}$) will be less than that in the laboratory system, since the CM system already has 3 translational degrees of freedom associated with its center of mass. Thus, the total number of kinetic degrees of freedom in CM system will be:

$$dofk_{CM} = 6 - 3 = 3$$

And the total number of dof in the CM system will be reduced accordingly: $dof_{CM} = dof - 3$. The number of internal degrees of freedom in CM system remain the same as in the laboratory system: $dofi_{CM} = dofi$.

The procedure for calculating new velocities and internal energies in CM system during the collision of two molecules ('a' and 'b') is as follows:

- The old kinetic energy of the two molecules are computed as:

$$ke_{old} = \frac{ua_{old}^2}{2} + \frac{ub_{old}^2}{2}$$

- It is combined with the old internal energy to form the new total energy in CM system as:

$$e_{old} = ke_{old} + iea + ieb$$

where iea, ieb are the internal energies of molecules a and b respectively.

- The new combined energy (e) of the two molecules is calculated by adding the enthalpy of reaction (h) to the old total energy:

$$e = e_{old} + h$$

- Kinetic energy in the CM system is computed as the share of the new total energy distributed according to degrees of freedom:

$$ke = \frac{dofk_{CM}}{dof_{CM}}\, e$$

$$ie = energy - ke$$

- The new velocities of the molecules in the CM frame are then updated from the old ones. The old velocities were computed according the elastic collision scheme between two hard-balls. So, if the energy was released or absorbed during the reaction, and some of it was absorbed into the internal degrees of freedom, the old velocities should be recalculated. The kinetic-energy is redistributed equally between the two molecules:

$$\frac{ma\, ua^2}{2} = \frac{mb\, ub^2}{2} = \frac{ke}{2}$$

which gives:

$$ua = \sqrt{ke/ma}$$

$$ub = \sqrt{ke/mb}$$

This is used to build the ratio of new to old velocities (see interact(...) function in domain.cc):

$$uratio_A = ua/ua_{old}$$

$$uratio_B = ub/ub_{old}$$

which are used to update the velocity vector for each molecule as:

$$u_X(i) = u_X(i) * uratio_X$$

where i=(x,y,z) is the Cartesian direction of velocity vector. The remaining internal energy, ie, is distribued among the internal degrees of freedom of each molecule X as:

$$InternalEnergy_X = rdofi_X\, ie$$

It should be noted, that in the above calculations, the value of kinetic energy was that computed in CM frame of referecne. This means that he actual kinetic energy of the molecule will have a somewhat higher value that what would be expected from an equal distribution of energy among the internal and exeternal degrees of freedom. Nevertheles, this scheme is considered accurate, since the resistribution of energy is indeed taking place in the center-of-mass reference frame, and this will inevitably lead to a higher contribution of energy to kinetic degrees of freedom.

7.1.2 Cross-Boundary Species

The code provides the possibility of specifying cross-boundary gases, which can enter the computational domain from the other side of the open boundary (the boundary with the type="open" inside the `<boundary>` tag of the XML input file (see Sec.Configuration File).

The algorithm uses the density and temperature to calculate the frequency of injection of molecules of specie, s at the boundary. The injection frequency, f_s per unit area, A is computed as

$$f_s = \frac{N}{\Delta\, t}$$

where $\Delta\, t_s$ is the time interval at which a molecule hits the boundary area A, and N is the number of molecules in a volume with the base A and length $\Delta\, x$ as shown in the figure: The time inteval, $\Delta\, t$, between the collisions can be related to the component of velocity of the molecule of species s, in direction x, v_{sx}, as follows:

$$\Delta\, t = \frac{2\Delta\, x}{v_{sx}}$$

The number of molecules, N can be related to density, ρ, as:

$$N = \frac{\rho}{\mu}\Delta\, x\, A$$

where μ is the mass of one molecule and $A = \Delta\, y\, \Delta\, z$. Thus, the frequency is:

$$f_s = \frac{\rho}{\mu}\Delta\, x\, A\frac{v_{sx}}{2\Delta\, x} = \frac{\rho\, v_{sx}}{2\mu}A$$

Chapter 8

Output

8.1 Output Procedures

There are three data output methods that can be used:

- Compressed snapshots of coordinates, velocities, and internal energies stored in gzipped ASCII format files. The files are dumped at time intervals specified in the input XML file under tag: <time><output>...</output></time> with the file names in format: <task>-<step>.dat.gz, where <task> is the name of the task, which is the same as the name of the executable file (job, view, or any other), and the <step> is the sequence number of the dump, which is automatically incremented for each subsequent dump. The output is performed by `save()` function of Domain class implemented in `domain.cc` file.

- Terminal output of time sequence of average quantities, such as the number of molecules (N), average temperature (T), kinetic (K), internal (I), and total energy (E) per molecule and per degree of freedom. In addition to that is also outputs the physical time (Time) in nanoseconds and memory utilization (Memory). The terminal output can be toggled with <xterm>0,1</xterm> flag in XML file. The output can be captured into a file using redirect command, like:

```
./job > log.log &
```

and post-processed using the Python `readlog.py` utility (see Frequently Asked Questions). The terminal output is performed inside the `Domain::run()` function at every designated time interval.

- The last method is to dump the graphics window in X-Window dump format (XWD) and then convert into one of the common graphics formats, such as png or jpg using standard convert utilities, such as ImageMagic's convert. See also Sec. Graphical User Interface.

Chapter 9

Namespace Index

9.1 Namespace List

Here is a list of all namespaces with brief descriptions:

Chapter 10

Class Index

10.1 Class List

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

Chapter 11

File Index

11.1 File List

Here is a list of all files with brief descriptions:

Chapter 12

Namespace Documentation

12.1 Geom Namespace Reference

Provides some trigeometry functions.

Functions

- void distvec (REAL a[ ], REAL b[ ], REAL c[ ])
- REAL distance (REAL a[ ], REAL b[ ])
- REAL distance (int dim, REAL a[ ], REAL b[ ])
- REAL sclp (REAL a[ ], REAL b[ ])
- REAL length (REAL a[ ])
- REAL area (REAL a[ ], REAL b[ ])
- REAL normalize (REAL a[ ])
- int hash (int i, int j, int n)

12.1.1 Detailed Description

Provides some trigeometry functions.

12.1.2 Function Documentation

12.1.2.1 REAL Geom::area (REAL *a*[ ], REAL *b*[ ])

Definition at line 148 of file model.cc.

References DIM, LENGTH, REAL, and VECP.

Referenced by Domain::Domain(), and Domain::injection().

12.1.2.2 REAL Geom::distance (int *dim*, REAL *a*[ ], REAL *b*[ ])

Definition at line 124 of file model.cc.

References REAL.

12.1.2.3 REAL Geom::distance (REAL *a*[ ], REAL *b*[ ])

Definition at line 116 of file model.cc.

References DIM, and REAL.

12.1.2.4 void Geom::distvec (REAL *a*[ ], REAL *b*[ ], REAL *c*[ ])

Definition at line 113 of file model.cc.

References DIM.

12.1.2.5 int Geom::hash (int *i*, int *j*, int *n*)

Definition at line 137 of file model.cc.

12.1.2.6 REAL Geom::length (REAL *a*[ ])

Definition at line 140 of file model.cc.

References DIM, and REAL.

Referenced by normalize().

12.1.2.7 REAL Geom::normalize (REAL *a*[ ])

Definition at line 108 of file model.cc.

References DIM, length(), and REAL.

12.1.2.8 REAL Geom::sclp (REAL *a*[ ], REAL *b*[ ])

Definition at line 132 of file model.cc.

References DIM, and REAL.

12.2 GridContainer Namespace Reference

Domain Segmentation for Interaction Acceleration.

Functions

- void init (REAL ymin[ ], REAL ymax[ ], REAL radius, Pool< Molecule > *newpool)
- int index (int ind[ ])
- void index (int n, int ind[ ])
- void put (Molecule *node)
- void put (Molecule *node, int icounter)
- Container< Molecule > * get (int ind[ ])
- int * dimensions ()
- bool checkPool (int icell, char *msg)

Variables

- REAL xmin [DIM]
- REAL xmax [DIM]
- REAL cellsize
- int ncells [DIM+1]
- int mcells = 0
- int mcells1 = 0
- Container< Molecule > * nodes
- Pool< Molecule > * pool

12.2.1 Detailed Description

Domain Segmentation for Interaction Acceleration.

Splits space into cubic cells to consider local interactions between ajacent cells only

12.2.2 Function Documentation

12.2.2.1 bool GridContainer::checkPool (int *icell*, char * *msg*)

12.2.2.2 int * GridContainer::dimensions ()

Definition at line 181 of file grid.cc.

References ncells.

12.2.2.3 Container< Molecule > * GridContainer::get (int *ind*[ ])

Definition at line 178 of file grid.cc.

References index(), and nodes.

12.2.2.4 void GridContainer::index (int *n*, int *ind*[ ])

Definition at line 68 of file grid.cc.

References DIM, mcells1, and ncells.

Referenced by Domain::interaction().

12.2.2.5 int GridContainer::index (int *ind*[ ])

Definition at line 61 of file grid.cc.

References DIM, and ncells.

Referenced by get(), and put().

12.2.2.6 void GridContainer::init (REAL *ymin*[ ], REAL *ymax*[ ], REAL *radius*, Pool< Molecule > * *newpool*)

Definition at line 25 of file grid.cc.

References cellsize, DIM, mcells, mcells1, ncells, nodes, Run::option, pool, REAL, xmax, and xmin.

12.2.2.7 void GridContainer::put (Molecule * *node*, int *icounter*)

DDD

DDD

Definition at line 128 of file grid.cc.

References cellsize, Molecule::Coordinates(), DIM, index(), ncells, nodes, REAL, Molecule::Type(), VOIDSPECIE, and xmin.

Referenced by Domain::Domain(), Boundary::Inject(), and Domain::run().

12.2.2.8 void GridContainer::put (Molecule * *node*)

Definition at line 81 of file grid.cc.

References cellsize, Molecule::Coordinates(), DIM, index(), ncells, nodes, REAL, Species::species, Run::time, Molecule::Type(), Molecule::Velocity(), VOIDSPECIE, and xmin.

12.2.3 Variable Documentation

12.2.3.1 REAL GridContainer::cellsize

Definition at line 20 of file grid.cc.

Referenced by Domain::Domain(), init(), put(), and Domain::run().

12.2.3.2 int GridContainer::mcells = 0

Definition at line 22 of file grid.cc.

Referenced by init().

12.2.3.3 int GridContainer::mcells1 = 0

Definition at line 22 of file grid.cc.

Referenced by index(), and init().

12.2.3.4 int GridContainer::ncells

Definition at line 21 of file grid.cc.

Referenced by dimensions(), index(), init(), Domain::interaction(), and put().

12.2.3.5 Container< Molecule > * GridContainer::nodes

Definition at line 23 of file grid.cc.

Referenced by get(), init(), put(), and Domain::run().

12.2.3.6 Pool< Molecule > * GridContainer::pool

Definition at line 24 of file grid.cc.

Referenced by Container< Element >::append0(), init(), Container< Element >::insert0(), and Container< Element >::remove0().

12.2.3.7 REAL GridContainer::xmax[DIM]

Definition at line 19 of file grid.cc.

Referenced by init().

12.2.3.8 REAL GridContainer::xmin[DIM]

Definition at line 19 of file grid.cc.

Referenced by init(), and put().

12.3 Gui Namespace Reference

OpenGL window output routines.

Classes

- struct ElementDisp
- struct ColorScale
- struct Scene
- struct WindowGeom

Enumerations

- enum Elements {
  points = 0, nodes, edges, faces,
  cells, frame, mesh, boundary_nodes,
  boundary_edges, boundary_faces, boundary_cells, maxelements }
- enum Color {
  red = 0, green, blue, skyblue,
  brown, magenta, yellow, color6,
  color7, color8, color9, color10,
  color11, color12, color13, color14,
  color15, maxcolor }
- enum ColorSchemes {
  colorByType = 0, colorByBoundary, colorByTime, colorByMass,
  maxColorSchemes }
- enum PointParameters {
  variable = maxcolor, vmin, vmax, size,
  sizevar, massvar, maxpointprm }
- enum LineParameters { thickness = maxcolor, length, maxlineprm }
- enum AxesParameters {
  axeswidth = 0, xaxislength, yaxislength, zaxislength,
  arrowheight, arrowidth, maxaxesprm }
- enum SurfDispType { gridlines = 0, solidsurface, maxsurfdisptypes }
- enum Movement { stay = 0, rotate, moveuv, movew }
- enum ShowPars {
  showRun = 0, showAxes, showSpheres, showBonds,
  showGrid, showNodes, showVariables, showBoundaryVertexes,
  showBoundaryVectors, showToolVertexes, showBoundaryFaceCenters, showBoundaryFaces,
  showBoundaryGrid, showToolGrid, showFrame, showCellCenters,
  showFaceCenters, showIsoSurfaces, dumpWindow, maxshowpars }

Functions

- int query_extension (char *extName)
- void init (int argc, char *argv[ ], Domain *newdomain)
- void helpDisplay ()
- int readparam (char *s, char *param[ ], int maxparam, char *filename, int val[ ])
- int readparam (char *s, char *param[ ], int maxparam, char *filename, REAL val[ ])
- void readconf ()
- void refresh ()
- void initdisp ()
- void Materials (int argc, char *argv[ ])
- void showVector (double *x, double *v)
- void showParticle (double vmn, double vmx, double val, double *x)
- void showSphere (double vmn, double vmx, double val, double rad, double *x)
- void displayAxes ()
- void getScaling (double &l0, double &l1)
- void getXLimits (double *x0, double *x1)
- void Exit ()
- void Quit ()
- void menu (int value)
- void displayMenu ()
- void consoleMenu ()
- void setBackgroundRun ()
- void setForegroundRun ()
- void toggleSpheres ()
- void switchColorScheme ()
- void runmany ()
- void toggleWindowDump ()
- void dumpwindow ()
- void commandMode ()
- void display ()
- void animate ()
- void helpCommand ()
- void reshape (int w, int h)
- void mouse (int button, int state, int x, int y)
- void motion (int x, int y)
- void keyboard (unsigned int key)
- void run ()
- void displaymessage (char *msg)
- void setElementColor (int element_type, REAL rgbcolor[ ])
- void getElementColor (int element_type, REAL rgbcolor[ ])
- void writeData ()
- void printGridXLimits ()
- void printGridVecLimits ()
- void getXLimits (REAL *xmin, REAL *xmax)
- void getScaling (REAL &lmin, REAL &lmax)
- void printPartVelLimits ()
- void printParticleVariables ()
- void showGridElements (int ne, double *X, REAL color[ ])
- void showVectorComponent (int ivar, int icomp, double *X, double vmn, double vmx)

- void showVector (int ivar, double *X)
- void printVariables (int n)
- void finish ()
- void InitMaterials (void)
- void selectVariable ()
- void keyboard (unsigned char key, int x, int y)
- void drawSegment (REAL *x, REAL *y)

Variables

- Domain * domain
- ElementDisp disp [maxelements]
- char * configfile = (char*)"gui.cfg"
- char windowname [MAXLINLEN]
- int showpar [maxshowpars]
- int finished
- int animation
- int nwdump
- int iwdump
- int attributeList [ ]
- REAL step
- REAL vecval [maxlineprm]
- REAL axes [maxaxesprm]
- REAL rgbcolor [maxcolor][3]
- REAL wdtime
- REAL xo [3]
- REAL dx
- REAL dy
- REAL dz
- REAL lastx
- REAL lasty
- REAL lastz
- int mouseButtons [3]
- REAL zoom
- REAL rotx
- REAL roty
- REAL tx
- REAL ty
- REAL xmin [DIM]
- REAL xmax [DIM]
- REAL lx
- REAL ly
- REAL lz
- REAL lmin
- REAL lmax
- enum Movement movement
- struct ColorScale colorscale
- struct Scene scene
- struct WindowGeom window
- struct BFaceList * bface_root

- Display * dpy
- Window win
- int firstR = 1
- int * vars
- int * coms

12.3.1 Detailed Description

OpenGL window output routines.

12.3.2 Enumeration Type Documentation

12.3.2.1 enum Gui::AxesParameters

Enumerator:

axeswidth

xaxislength

yaxislength

zaxislength

arrowheight

arrowidth

maxaxesprm

Definition at line 71 of file gui.h.

12.3.2.2 enum Gui::Color

Enumerator:

red

green

blue

skyblue

brown

magenta

yellow

color6

color7

color8

color9

color10

color11

color12

color13

color14

color15

maxcolor

Definition at line 31 of file gui.h.

12.3.2.3 enum Gui::ColorSchemes

Enumerator:

colorByType

colorByBoundary

colorByTime

colorByMass

maxColorSchemes

Definition at line 51 of file gui.h.

12.3.2.4 enum Gui::Elements

Enumerator:

points

nodes

edges

faces

cells

frame

mesh

boundary_nodes

boundary_edges

boundary_faces

boundary_cells

maxelements

Definition at line 17 of file gui.h.

12.3.2.5 enum Gui::LineParameters

Enumerator:

thickness

length

maxlineprm

Definition at line 65 of file gui.h.

12.3.2.6 enum Gui::Movement

Enumerator:

stay

rotate

moveuv

movew

Definition at line 123 of file gui.h.

12.3.2.7 enum Gui::PointParameters

Enumerator:

variable

vmin

vmax

size

sizevar

massvar

maxpointprm

Definition at line 58 of file gui.h.

12.3.2.8 enum Gui::ShowPars

Enumerator:

showRun

showAxes

showSpheres

showBonds

showGrid

showNodes

showVariables

showBoundaryVertexes

showBoundaryVectors

showToolVertexes

showBoundaryFaceCenters

showBoundaryFaces

showBoundaryGrid

showToolGrid

showFrame

showCellCenters

showFaceCenters

showIsoSurfaces

dumpWindow

maxshowpars

Definition at line 129 of file gui.h.

12.3.2.9 enum Gui::SurfDispType

Enumerator:

gridlines

solidsurface

maxsurfdisptypes

Definition at line 81 of file gui.h.

12.3.3 Function Documentation

12.3.3.1 void Gui::animate ()

Definition at line 1851 of file gui.cc.

References animation, display(), domain, dumpwindow(), dumpWindow, ESC, finished, iwdump, nwdump, Run::option, Domain::run(), showpar, showRun, and Run::time.

Referenced by menu().

12.3.3.2 void Gui::commandMode ()

Definition at line 1465 of file gui.cc.

References consoleMenu(), dumpwindow(), Exit(), helpCommand(), MAXLINLEN, Quit(), runmany(), setBackgroundRun(), setForegroundRun(), switchColorScheme(), toggleSpheres(), and toggleWindow-Dump().

Referenced by keyboard().

12.3.3.3 void Gui::consoleMenu ()

Definition at line 1360 of file gui.cc.

References displayMenu(), MAXLINLEN, and menu().

Referenced by commandMode(), and keyboard().

12.3.3.4 void Gui::display ()

Definition at line 1530 of file gui.cc.

References blue, Gui::Scene::color, colorByBoundary, colorByMass, colorByTime, colorByType, Molecule::Coordinates(), Collection< Element >::Current(), displayAxes(), domain, dpy, faces, Gui::Scene::frame, frame, getElementColor(), Collection< Element >::goFirst(), Collection<

Element >::goNext(), green, init(), Collection< Element >::isFirst(), Potential::lengthscale(), Gui::Scene::Frame::line, Species::Specie::Mass(), Gui::Scene::Color::maxvalue, Gui::Scene::mesh, Gui::Scene::Color::minvalue, Domain::Molecules(), Gui::Scene::Mesh::node, nodes, Collection< Element >::number(), Run::option, Palette::pickcolor(), REAL, red, refresh(), rotx, roty, scene, Gui::Scene::Color::scheme, showBoundaryGrid, showBoundaryVertexes, showFrame, showGrid, showNodes, showpar, showSpheres, Species::Specie::Size(), size, Species::species, thickness, Run::time, tx, ty, Molecule::Type(), win, xmax, xmin, and zoom.

Referenced by animate().

12.3.3.5 void Gui::displayAxes ()

Definition at line 1181 of file gui.cc.

References arrowheight, arrowidth, axes, axeswidth, lx, ly, lz, showAxes, showpar, xaxislength, xo, yaxislength, and zaxislength.

Referenced by display().

12.3.3.6 void Gui::displayMenu ()

Definition at line 1334 of file gui.cc.

Referenced by consoleMenu().

12.3.3.7 void Gui::displaymessage (char * *msg*)

Definition at line 2162 of file gui.cc.

12.3.3.8 void Gui::drawSegment (REAL * *x*, REAL * *y*)

12.3.3.9 void Gui::dumpwindow ()

Definition at line 1461 of file gui.cc.

References windowname, and IO::xwd().

Referenced by animate(), and commandMode().

12.3.3.10 void Gui::Exit ()

Definition at line 1229 of file gui.cc.

References animation, and MAXLINLEN.

Referenced by commandMode(), and keyboard().

12.3.3.11 void Gui::finish ()

12.3.3.12 void Gui::getElementColor (int *element_type*, REAL *rgbcolor*[ ])

Definition at line 2172 of file gui.cc.

References disp, and maxelements.

Referenced by display().

12.3.3.13 void Gui::getScaling (REAL & *lmin*, REAL & *lmax*)

12.3.3.14 void Gui::getScaling (double & *l0*, double & *l1*)

Definition at line 1212 of file gui.cc.

References lmax, and lmin.

Referenced by reshape().

12.3.3.15 void Gui::getXLimits (REAL * *xmin*, REAL * *xmax*)

12.3.3.16 void Gui::getXLimits (double * *x0*, double * *x1*)

Definition at line 1220 of file gui.cc.

References xmax, and xmin.

12.3.3.17 void Gui::helpCommand ()

Definition at line 1871 of file gui.cc.

References Run::outputname.

Referenced by commandMode().

12.3.3.18 void Gui::helpDisplay ()

Definition at line 175 of file gui.cc.

References configfile, and Run::outputname.

Referenced by init(), keyboard(), and menu().

12.3.3.19 void Gui::init (int *argc*, char * *argv*[ ], Domain * *newdomain*)

Definition at line 91 of file gui.cc.

References animation, attributeList, Gui::Scene::color, colorByMass, domain, dpy, dumpWindow, ERROR, finished, Gui::WindowGeom::height, helpDisplay(), initdisp(), lastx, lasty, lastz, Materials(), mouseButtons, Run::option, query_extension(), rotx, roty, scene, Gui::Scene::Color::scheme, showAxes, showBonds, showBoundaryFaceCenters, showBoundaryFaces, showBoundaryGrid, showBoundaryVectors, showBoundaryVertexes, showCellCenters, showFaceCenters, showFrame, showGrid, showNodes, showpar, showRun, showSpheres, showToolGrid, showToolVertexes, showVariables, tx, ty, wdtime, Gui::WindowGeom::width, win, window, windowname, and zoom.

Referenced by display(), and main().

12.3.3.20 void Gui::initdisp ()

Definition at line 701 of file gui.cc.

References arrowheight, arrowidth, axes, axeswidth, blue, brown, cells, colorscale, DIM, domain, dx, dy, dz, edges, faces, frame, Gui::Scene::frame, green, Gui::WindowGeom::height, LARGE, length, Gui::Scene::Mesh::line, Gui::Scene::Frame::line, lmax, lmin, lx, ly, lz, magenta, MAX_WINDOW_HEIGHT, MAX_WINDOW_WIDTH, maxcolor, maxelements, mesh, Gui::Scene::mesh, Domain::Molecules(), Gui::Scene::Mesh::node, nodes, Collection< Element >::number(), Run::option, readconf(), REAL, red, Gui::ColorScale::relative, rgbcolor, scene, setElementColor(), Domain::setMaxBound(), Domain::setMinBound(), size, skyblue, step, thickness, vecval, Gui::WindowGeom::width, window, WINDOW_SIZE, xaxislength, xmax, xmin, xo, yaxislength, yellow, zaxislength, and zoom.

Referenced by init().

12.3.3.21 void Gui::InitMaterials (void)

12.3.3.22 void Gui::keyboard (unsigned char *key*, int *x*, int *y*)

12.3.3.23 void Gui::keyboard (unsigned int *key*)

refresh();

Definition at line 1978 of file gui.cc.

References animation, commandMode(), consoleMenu(), domain, ESC, Exit(), finished, helpDisplay(), MAXLINLEN, Run::option, Run::outputname, readconf(), Domain::run(), Domain::save(), showAxes, showBoundaryFaces, showBoundaryGrid, showBoundaryVectors, showBoundaryVertexes, showFrame, showGrid, showNodes, showpar, switchColorScheme(), Run::time, and zoom.

12.3.3.24 void Gui::Materials (int *argc*, char * *argv*[ ])

Definition at line 818 of file gui.cc.

References lz, Run::option, and xo.

Referenced by init().

12.3.3.25 void Gui::menu (int *value*)

Definition at line 1253 of file gui.cc.

References ABOUT, animate(), animation, finished, helpDisplay(), showAxes, showBonds, showBoundaryFaceCenters, showBoundaryGrid, showBoundaryVectors, showBoundaryVertexes, showCellCenters, showFaceCenters, showGrid, showNodes, showpar, and showVariables.

Referenced by consoleMenu().

12.3.3.26 void Gui::motion (int *x*, int *y*)

Definition at line 1954 of file gui.cc.

References lastx, lasty, mouseButtons, REAL, rotx, roty, tx, ty, and zoom.

12.3.3.27 void Gui::mouse (int *button*, int *state*, int *x*, int *y*)

Definition at line 1927 of file gui.cc.

References lastx, lasty, LEFT_BUTTON, MIDDLE_BUTTON, mouseButtons, and RIGHT_BUTTON.

12.3.3.28 void Gui::printGridVecLimits ()

12.3.3.29 void Gui::printGridXLimits ()

12.3.3.30 void Gui::printParticleVariables ()

12.3.3.31 void Gui::printPartVelLimits ()

12.3.3.32 void Gui::printVariables (int *n*)

12.3.3.33 int Gui::query_extension (char * *extName*)

Definition at line 78 of file gui.cc.

Referenced by init().

12.3.3.34 void Gui::Quit ()

Definition at line 1241 of file gui.cc.

References animation, and MAXLINLEN.

Referenced by commandMode().

12.3.3.35 void Gui::readconf ()

Definition at line 259 of file gui.cc.

References arrowheight, arrowidth, axeswidth, blue, brown, Gui::Scene::color, colorByMass, colorByType, Run::configfile, configfile, DIM, DOCTYPE, domain, dx, dy, dz, frame, Gui::Scene::frame, green, length, Gui::Scene::Frame::line, Gui::Scene::Mesh::line, lx, ly, lz, magenta, massvar, maxaxesprm, Domain::maxBound(), maxcolor, maxlineprm, MAXLINLEN, maxpointprm, maxshowpars, Gui::Scene::Color::maxvalue, mesh, Gui::Scene::mesh, Domain::minBound(), Gui::Scene::Color::minvalue, Gui::Scene::Mesh::node, nodes, Run::option, IO::parseWord(), REAL, red, rgbcolor, scene, Gui::Scene::Color::scheme, setElementColor(), showpar, showSpheres, size, sizevar, skyblue, step, thickness, variable, vecval, vmax, vmin, xaxislength, xmax, xmin, yaxislength, and zaxislength.

Referenced by initdisp(), and keyboard().

12.3.3.36 int Gui::readparam (char * *s*, char * *param*[ ], int *maxparam*, char * *filename*, REAL *val*[ ])

Definition at line 230 of file gui.cc.

12.3.3.37 int Gui::readparam (char * *s*, char * *param*[ ], int *maxparam*, char * *filename*, int *val*[ ])

Definition at line 198 of file gui.cc.

12.3.3.38 void Gui::refresh ()

Definition at line 689 of file gui.cc.

Referenced by display().

12.3.3.39 void Gui::reshape (int *w*, int *h*)

Definition at line 1890 of file gui.cc.

References getScaling(), lmax, and lmin.

12.3.3.40 void Gui::run ()

Definition at line 2159 of file gui.cc.

Referenced by main().

12.3.3.41 void Gui::runmany ()

Definition at line 1392 of file gui.cc.

References domain, and Domain::run().

Referenced by commandMode().

12.3.3.42 void Gui::selectVariable ()

12.3.3.43 void Gui::setBackgroundRun ()

Definition at line 1376 of file gui.cc.

References showpar, and showRun.

Referenced by commandMode().

12.3.3.44 void Gui::setElementColor (int *element_type*, REAL *rgbcolor*[ ])

Definition at line 2166 of file gui.cc.

References disp, and maxelements.

Referenced by initdisp(), and readconf().

12.3.3.45 void Gui::setForegroundRun ()

Definition at line 1380 of file gui.cc.

References showpar, and showRun.

Referenced by commandMode().

12.3.3.46 void Gui::showGridElements (int *ne*, double * *X*, REAL *color*[ ])

12.3.3.47 void Gui::showParticle (double *vmn*, double *vmx*, double *val*, double * *x*)

Definition at line 952 of file gui.cc.

References PI, REAL, and Palette::vav.

12.3.3.48 void Gui::showSphere (double *vmn*, double *vmx*, double *val*, double *rad*, double * *x*)

= { 0.6, 0.8, 0.3, 1.0 },

Definition at line 982 of file gui.cc.

References PI, REAL, and Palette::vav.

12.3.3.49 void Gui::showVector (int *ivar*, double * *X*)

12.3.3.50 void Gui::showVector (double * *x*, double * *v*)

Definition at line 874 of file gui.cc.

References length, and vecval.

12.3.3.51 void Gui::showVectorComponent (int *ivar*, int *icomp*, double * *X*, double *vmn*, double *vmx*)

12.3.3.52 void Gui::switchColorScheme ()

Definition at line 1388 of file gui.cc.

References Gui::Scene::color, maxColorSchemes, scene, and Gui::Scene::Color::scheme.

Referenced by commandMode(), and keyboard().

12.3.3.53 void Gui::toggleSpheres ()

Definition at line 1384 of file gui.cc.

References showpar, and showSpheres.

Referenced by commandMode().

12.3.3.54 void Gui::toggleWindowDump ()

Definition at line 1448 of file gui.cc.

References dumpWindow, iwdump, nwdump, showpar, step, Run::time, and wdtime.

Referenced by commandMode().

12.3.3.55 void Gui::writeData ()

12.3.4 Variable Documentation

12.3.4.1 int Gui::animation

Definition at line 29 of file gui.cc.

Referenced by animate(), Exit(), init(), keyboard(), menu(), and Quit().

12.3.4.2 int Gui::attributeList[ ]

Initial value:

```
{       GLX_RGBA,
        GLX_RED_SIZE, 1,
        GLX_GREEN_SIZE, 1,
        GLX_BLUE_SIZE, 1,
        GLX_DOUBLEBUFFER,
        GLX_DEPTH_SIZE, 1,
        None
}
```

Definition at line 33 of file gui.cc.

Referenced by init().

12.3.4.3 REAL Gui::axes ()

Definition at line 43 of file gui.cc.

Referenced by displayAxes(), and initdisp().

12.3.4.4 struct BFaceList* Gui::bface_root

Definition at line 70 of file gui.cc.

12.3.4.5 struct ColorScale Gui::colorscale

Definition at line 66 of file gui.cc.

Referenced by initdisp().

12.3.4.6 int * Gui::coms

Definition at line 76 of file gui.cc.

12.3.4.7 char * Gui::configfile = (char*)"gui.cfg"

Definition at line 26 of file gui.cc.

Referenced by helpDisplay(), and readconf().

12.3.4.8 ElementDisp Gui::disp

Definition at line 25 of file gui.cc.

Referenced by getElementColor(), and setElementColor().

12.3.4.9 Domain* Gui::domain

Definition at line 24 of file gui.cc.

Referenced by animate(), display(), init(), initdisp(), keyboard(), main(), readconf(), and runmany().

12.3.4.10 Display* Gui::dpy

Definition at line 72 of file gui.cc.

Referenced by display(), and init().

12.3.4.11 REAL Gui::dx

Definition at line 43 of file gui.cc.

Referenced by Domain::boundary(), initdisp(), Boundary::Inject(), Domain::interact(), Domain::interaction(), and readconf().

12.3.4.12 REAL Gui::dy

Definition at line 43 of file gui.cc.

Referenced by initdisp(), and readconf().

12.3.4.13 REAL Gui::dz

Definition at line 43 of file gui.cc.

Referenced by initdisp(), and readconf().

12.3.4.14 int Gui::finished

Definition at line 29 of file gui.cc.

Referenced by animate(), init(), keyboard(), and menu().

12.3.4.15 int Gui::firstR = 1

Definition at line 75 of file gui.cc.

12.3.4.16 int Gui::iwdump

Definition at line 29 of file gui.cc.

Referenced by animate(), and toggleWindowDump().

12.3.4.17 REAL Gui::lastx

Definition at line 43 of file gui.cc.

Referenced by init(), motion(), and mouse().

12.3.4.18 REAL Gui::lasty

Definition at line 43 of file gui.cc.

Referenced by init(), motion(), and mouse().

12.3.4.19 REAL Gui::lastz

Definition at line 43 of file gui.cc.

Referenced by init().

12.3.4.20 REAL Gui::lmax

Definition at line 61 of file gui.cc.

Referenced by getScaling(), initdisp(), and reshape().

12.3.4.21 REAL Gui::lmin

Definition at line 61 of file gui.cc.

Referenced by getScaling(), initdisp(), and reshape().

12.3.4.22 REAL Gui::lx

Definition at line 61 of file gui.cc.

Referenced by displayAxes(), initdisp(), and readconf().

12.3.4.23 REAL Gui::ly

Definition at line 61 of file gui.cc.

Referenced by displayAxes(), initdisp(), and readconf().

12.3.4.24 REAL Gui::lz

Definition at line 61 of file gui.cc.

Referenced by displayAxes(), initdisp(), Materials(), and readconf().

12.3.4.25 int Gui::mouseButtons

Definition at line 53 of file gui.cc.

Referenced by init(), motion(), and mouse().

12.3.4.26 enum Movement Gui::movement

Definition at line 64 of file gui.cc.

12.3.4.27 int Gui::nwdump

Definition at line 29 of file gui.cc.

Referenced by animate(), and toggleWindowDump().

12.3.4.28 REAL Gui::rgbcolor

Definition at line 43 of file gui.cc.

Referenced by initdisp(), and readconf().

12.3.4.29 REAL Gui::rotx

Definition at line 55 of file gui.cc.

Referenced by display(), init(), and motion().

12.3.4.30 REAL Gui::roty

Definition at line 56 of file gui.cc.

Referenced by display(), init(), and motion().

12.3.4.31 struct Scene Gui::scene

Definition at line 67 of file gui.cc.

Referenced by display(), init(), initdisp(), readconf(), and switchColorScheme().

12.3.4.32 int Gui::showpar

Definition at line 29 of file gui.cc.

Referenced by animate(), display(), displayAxes(), init(), keyboard(), menu(), readconf(), setBackgroundRun(), setForegroundRun(), toggleSpheres(), and toggleWindowDump().

12.3.4.33 REAL Gui::step

Definition at line 43 of file gui.cc.

Referenced by initdisp(), readconf(), and toggleWindowDump().

12.3.4.34 REAL Gui::tx

Definition at line 57 of file gui.cc.

Referenced by display(), init(), and motion().

12.3.4.35 REAL Gui::ty

Definition at line 58 of file gui.cc.

Referenced by display(), init(), and motion().

12.3.4.36 int* Gui::vars

Definition at line 76 of file gui.cc.

12.3.4.37 REAL Gui::vecval ()

Definition at line 43 of file gui.cc.

Referenced by initdisp(), readconf(), and showVector().

12.3.4.38 REAL Gui::wdtime

Definition at line 43 of file gui.cc.

Referenced by init(), and toggleWindowDump().

12.3.4.39 Window Gui::win

Definition at line 73 of file gui.cc.

Referenced by display(), and init().

12.3.4.40 struct WindowGeom Gui::window

Definition at line 68 of file gui.cc.

Referenced by init(), and initdisp().

12.3.4.41 char Gui::windowname[MAXLINLEN]

Definition at line 26 of file gui.cc.

Referenced by dumpwindow(), and init().

12.3.4.42 REAL Gui::xmax ()

Definition at line 61 of file gui.cc.

Referenced by display(), Domain::Domain(), getXLimits(), initdisp(), and readconf().

12.3.4.43 REAL Gui::xmin

Definition at line 61 of file gui.cc.

Referenced by display(), Domain::Domain(), getXLimits(), initdisp(), and readconf().

12.3.4.44 REAL Gui::xo

Definition at line 43 of file gui.cc.

Referenced by displayAxes(), initdisp(), and Materials().

12.3.4.45 REAL Gui::zoom

Definition at line 54 of file gui.cc.

Referenced by display(), init(), initdisp(), keyboard(), and motion().

12.4 IO Namespace Reference

Some IO routines.

Functions

- void initxwd (int i)
- void xwd (char ∗windowname)
- int getCharAttr (xmlNodePtr cur, char ∗attr, char ∗result)
- int getIntAttr (xmlNodePtr cur, char ∗attr)
- int getIntAttr (xmlDocPtr doc, char ∗tag, char ∗keyname, char ∗key, char ∗attr)
- int parseWord (xmlDocPtr doc, xmlNodePtr cur, char ∗keyword, char ∗result)
- int parseInt (xmlDocPtr doc, xmlNodePtr cur, char ∗keyword)
- int parseFloat (xmlDocPtr doc, xmlNodePtr cur, char ∗keyword, REAL &result)
- double parseFloat (xmlDocPtr doc, xmlNodePtr cur, char ∗keyword)
- void getTimeXML (char inpfilename[ ])
- void getTime (char inpfilename[ ])
- int getIter (char inpfilename[ ])

Variables

- int ioutput = 0
- int nxwdump = 0

12.4.1 Detailed Description

Some IO routines.

12.4.2 Function Documentation

12.4.2.1 int IO::getCharAttr (xmlNodePtr *cur*, char ∗ *attr*, char ∗ *result*)

Definition at line 40 of file io.cc.

References MAXLINLEN, and Run::option.

Referenced by Domain::Domain(), and getIntAttr().

12.4.2.2 int IO::getIntAttr (xmlDocPtr *doc*, char ∗ *tag*, char ∗ *keyname*, char ∗ *key*, char ∗ *attr*)

Definition at line 77 of file io.cc.

References getCharAttr(), MAXLINLEN, Run::option, parseInt(), and Potential::value().

12.4.2.3 int IO::getIntAttr (xmlNodePtr *cur*, char ∗ *attr*)

Definition at line 57 of file io.cc.

References Run::option.

12.4.2.4 int IO::getIter (char *inpfilename*[ ])

Definition at line 249 of file io.cc.

References DOCTYPE, MAXLINLEN, and Run::option.

Referenced by main().

12.4.2.5 void IO::getTime (char *inpfilename*[ ])

Definition at line 239 of file io.cc.

References getTimeXML(), Run::option, and Run::time.

Referenced by Run::init().

12.4.2.6 void IO::getTimeXML (char *inpfilename*[ ])

Definition at line 198 of file io.cc.

References DOCTYPE, MAXLINLEN, parseFloat(), and Run::time.

Referenced by getTime().

12.4.2.7 void IO::initxwd (int *i*)

Definition at line 15 of file io.cc.

References nxwdump.

12.4.2.8 double IO::parseFloat (xmlDocPtr *doc*, xmlNodePtr *cur*, char * *keyword*)

Definition at line 178 of file io.cc.

References Run::option.

Referenced by Domain::Domain().

12.4.2.9 int IO::parseFloat (xmlDocPtr *doc*, xmlNodePtr *cur*, char * *keyword*, REAL & *result*)

Definition at line 158 of file io.cc.

References Run::option, and REAL.

Referenced by getTimeXML().

12.4.2.10 int IO::parseInt (xmlDocPtr *doc*, xmlNodePtr *cur*, char * *keyword*)

Definition at line 138 of file io.cc.

References Run::option.

Referenced by getIntAttr().

12.4.2.11 int IO::parseWord (xmlDocPtr *doc*, xmlNodePtr *cur*, char * *keyword*, char * *result*)

Definition at line 117 of file io.cc.

References MAXLINLEN, and Run::option.

Referenced by Domain::Domain(), and Gui::readconf().

12.4.2.12 void IO::xwd (char * *windowname*)

Definition at line 19 of file io.cc.

References MAXLINLEN, nxwdump, and Run::option.

Referenced by Gui::dumpwindow().

12.4.3 Variable Documentation

12.4.3.1 int IO::ioutput = 0

Definition at line 13 of file io.cc.

Referenced by Domain::load(), Domain::run(), and Domain::save().

12.4.3.2 int IO::nxwdump = 0

Definition at line 14 of file io.cc.

Referenced by initxwd(), and xwd().

12.5 Palette Namespace Reference

Defines color palette.

Functions

- void init (REAL vmin, REAL vmax)
- void pickcolor (REAL var, REAL color[ ])

Variables

- REAL vmn
- REAL vmx
- REAL vav
- REAL dvi

12.5.1 Detailed Description

Defines color palette.

12.5.2 Function Documentation

12.5.2.1 void Palette::init (REAL *vmin*, REAL *vmax*)

Definition at line 2189 of file gui.cc.

References dvi, vav, vmn, and vmx.

12.5.2.2 void Palette::pickcolor (REAL *var*, REAL *color*[ ])

Definition at line 2197 of file gui.cc.

References dvi, REAL, vav, vmn, and vmx.

Referenced by Gui::display().

12.5.3 Variable Documentation

12.5.3.1 REAL Palette::dvi

Definition at line 2185 of file gui.cc.

Referenced by init(), Domain::interact(), and pickcolor().

12.5.3.2 REAL Palette::vav

Definition at line 2185 of file gui.cc.

Referenced by init(), pickcolor(), Gui::showParticle(), and Gui::showSphere().

12.5.3.3 REAL Palette::vmn

Definition at line 2185 of file gui.cc.

Referenced by init(), and pickcolor().

12.5.3.4 REAL Palette::vmx

Definition at line 2185 of file gui.cc.

Referenced by init(), and pickcolor().

12.6 Potential Namespace Reference

Interaction-potential functions, such as LJ.

Functions

- REAL invdist (REAL x)
- void strength (REAL strength)
- REAL strength ()
- void lengthscale (REAL lengthscale)
- REAL lengthscale ()
- void Cutoff (REAL newcutoff)
- REAL Cutoff ()
- REAL value (REAL r)
- REAL force (REAL r)
- REAL derivative (REAL r)

Variables

- REAL sigma = 1.0
- REAL eta = 1.0
- REAL cutoff = 2.0
- const REAL small = 1.0e-20
- const REAL large = 1.0e20

12.6.1 Detailed Description

Interaction-potential functions, such as LJ.

12.6.2 Function Documentation

12.6.2.1 REAL Potential::Cutoff () `[inline]`

Definition at line 154 of file model.h.

References cutoff.

Referenced by Domain::load().

12.6.2.2 void Potential::Cutoff (REAL *newcutoff*) `[inline]`

Definition at line 153 of file model.h.

References cutoff.

12.6.2.3 REAL Potential::derivative (REAL *r*)

12.6.2.4 REAL Potential::force (REAL *r*) [inline]

Definition at line 166 of file model.h.

References eta, and sigma.

12.6.2.5 REAL Potential::invdist (REAL *x*)

Definition at line 102 of file model.cc.

12.6.2.6 REAL Potential::lengthscale () [inline]

Definition at line 152 of file model.h.

References sigma.

Referenced by Gui::display(), and Domain::Domain().

12.6.2.7 void Potential::lengthscale (REAL *lengthscale*) [inline]

Definition at line 149 of file model.h.

References sigma.

Referenced by Domain::load().

12.6.2.8 REAL Potential::strength () [inline]

Definition at line 148 of file model.h.

References eta.

Referenced by Domain::Domain().

12.6.2.9 void Potential::strength (REAL *strength*) [inline]

Definition at line 145 of file model.h.

References eta.

12.6.2.10 REAL Potential::value (REAL *r*) [inline]

Definition at line 155 of file model.h.

References cutoff, eta, large, REAL, sigma, and small.

Referenced by IO::getIntAttr().

12.6.3 Variable Documentation

12.6.3.1 REAL Potential::cutoff = 2.0

Definition at line 85 of file model.cc.

Referenced by Cutoff(), and value().

12.6.3.2 REAL Potential::eta = 1.0

Definition at line 85 of file model.cc.

Referenced by force(), strength(), and value().

12.6.3.3 const REAL Potential::large = 1.0e20

Definition at line 142 of file model.h.

Referenced by value().

12.6.3.4 REAL Potential::sigma = 1.0

Definition at line 85 of file model.cc.

Referenced by force(), lengthscale(), and value().

12.6.3.5 const REAL Potential::small = 1.0e-20

Definition at line 142 of file model.h.

Referenced by value().

12.7 Run Namespace Reference

Processing command-line and execution control parameters.

Classes

- struct Time
  Execution time-control structure.

Functions

- void testrnd ()
  Test random numer generator.
- REAL rnd ()
  Seeds random number.
- REAL gauss ()
  normal random number generator
- void init (int argc, char ∗argv[ ])
  Initialize all variables, and execution options.
- void readcmdline (int argc, char ∗argv[ ])
  Parses command-line options.
- int elapsed ()
  time (sec) elapsed since the start of the run
- void seed ()
  seed random number generator
- void(∗) usage ()

Variables

- struct Option option = {0,0,0,0}
  command-line options
- void(∗ usage)()
- char programname [MAXLINLEN]
- char configfile [MAXLINLEN]
- char outputfile [MAXLINLEN]
- char inputfile [MAXLINLEN]
- char outputname [MAXLINLEN]
- int nthreads
- struct timeb worldtime
- struct Time time

12.7.1 Detailed Description

Processing command-line and execution control parameters.

12.7.2 Function Documentation

12.7.2.1 int Run::elapsed ()

time (sec) elapsed since the start of the run

Definition at line 138 of file run.cc.

References worldtime.

Referenced by Domain::save().

12.7.2.2 REAL Run::gauss ()

normal random number generator

From Numerical Recepes in C, Ch.7.2 Zero mean and unit variance

Definition at line 57 of file run.cc.

References REAL, and rnd().

12.7.2.3 void Run::init (int *argc*, char * *argv*[ ])

Initialize all variables, and execution options.

Definition at line 79 of file run.cc.

References configfile, Option::debug, IO::getTime(), Option::mesh, option, readcmdline(), Option::restart, Option::verbose, worldtime, and Option::xterm.

Referenced by main().

12.7.2.4 void Run::readcmdline (int *argc*, char * *argv*[ ])

Parses command-line options.

Definition at line 93 of file run.cc.

References configfile, Option::debug, inputfile, Option::mesh, option, outputfile, outputname, programname, Option::restart, and Option::verbose.

Referenced by init().

12.7.2.5 REAL Run::rnd ()

Seeds random number.

random number generator

Generates random number between 0 and 1

Definition at line 51 of file run.cc.

References RAND_MAX, and REAL.

Referenced by gauss(), and testrnd().

12.7.2.6 void Run::seed ()

seed random number generator

12.7.2.7 void Run::testrnd ()

Test random numer generator.

Definition at line 31 of file run.cc.

References RAND_MAX, REAL, and rnd().

12.7.2.8 void(∗) Run::usage ()

Definition at line 23 of file job.cc.

References programname.

12.7.3 Variable Documentation

12.7.3.1 char Run::configfile

Definition at line 20 of file run.cc.

Referenced by Domain::Domain(), init(), main(), readcmdline(), and Gui::readconf().

12.7.3.2 char Run::inputfile

Definition at line 20 of file run.cc.

Referenced by main(), and readcmdline().

12.7.3.3 int Run::nthreads

Definition at line 26 of file run.cc.

Referenced by Domain::interaction(), and Domain::run().

12.7.3.4 struct Option Run::option = {0,0,0,0} [read]

command-line options

Definition at line 17 of file run.cc.

Referenced by Gui::animate(), Gui::display(), Domain::Domain(), IO::getCharAttr(), IO::getIntAttr(), IO::getIter(), IO::getTime(), init(), Gui::init(), GridContainer::init(), Domain::init(), Gui::initdisp(), Gui::keyboard(), Domain::load(), main(), Gui::Materials(), IO::parseFloat(), IO::parseInt(), IO::parseWord(), Pool< Element >::Pool(), readcmdline(), Gui::readconf(), Domain::run(), Domain::save(), IO::xwd(), and Domain::∼Domain().

12.7.3.5 char Run::outputfile

Definition at line 20 of file run.cc.

Referenced by readcmdline().

12.7.3.6 char Run::outputname

Definition at line 20 of file run.cc.

Referenced by Gui::helpCommand(), Gui::helpDisplay(), Gui::keyboard(), readcmdline(), and Domain::run().

12.7.3.7 char Run::programname

Definition at line 20 of file run.cc.

Referenced by main(), readcmdline(), usage(), and usage().

12.7.3.8 struct Time Run::time [read]

Definition at line 29 of file run.cc.

Referenced by Gui::animate(), Domain::boundary(), Gui::display(), IO::getTime(), IO::getTimeXML(), Bulk::inject(), Boundary::Inject(), Domain::injection(), Domain::interaction(), Gui::keyboard(), Domain::load(), Molecule::Molecule(), Molecule::Move(), GridContainer::put(), Domain::run(), Domain::save(), and Gui::toggleWindowDump().

12.7.3.9 void(∗ Run::usage)() ()

12.7.3.10 struct timeb Run::worldtime

Definition at line 28 of file run.cc.

Referenced by elapsed(), and init().

12.8 Species Namespace Reference

Description of Specie and Reaction classes.

Classes

- class Specie
- struct Gas

  Gas is a specie with some additional parameters.

- struct Reaction

  Reaction determines the two products only.

Enumerations

- enum Interaction { missed = 0, collided, reacted, annihalated }

Variables

- int nspecies
- Specie * species
- Reaction * reactions

12.8.1 Detailed Description

Description of Specie and Reaction classes.

12.8.2 Enumeration Type Documentation

12.8.2.1 enum Species::Interaction

Enumerator:

missed

collided

reacted two reactants -> two products

annihalated two reactants -> one product

Definition at line 164 of file species.h.

12.8.3 Variable Documentation

12.8.3.1 int Species::nspecies

Definition at line 8 of file species.cc.

Referenced by Domain::Domain(), Domain::interact(), Domain::load(), Molecule::Move(), Species::Reaction::Outcome::Outcome(), and Domain::run().

12.8.3.2 Reaction * Species::reactions

Definition at line 10 of file species.cc.

Referenced by Domain::Domain(), and Domain::interact().

12.8.3.3 Specie * Species::species

Definition at line 9 of file species.cc.

Referenced by Domain::boundary(), Gui::display(), Domain::Domain(), Domain::init(), Bulk::inject(), Boundary::Inject(), Domain::injection(), Domain::interact(), Molecule::KineticEnergy(), Domain::load(), Molecule::Move(), GridContainer::put(), Domain::run(), Domain::save(), and Molecule::Temperature().

Chapter 13

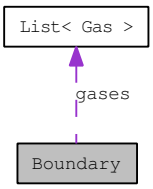
Class Documentation

13.1 Boundary Class Reference

Domain Boundary Definition.

`#include <domain.h>`

Collaboration diagram for Boundary:



Public Member Functions

- Boundary ()

  Boundary constructor: sets defaults.

- ~Boundary ()

  Boundary destructor.

- REAL Area ()
- void Area (REAL a)
- REAL Temperature ()
- void Temperature (REAL t)
- void init (int i, int j, REAL ymin[ ], REAL ymax[ ], int nspecies)
- void Inject (int specietype, REAL vavx, REAL temperature, Collection< Molecule > *molecules)

  Injecting a specie from accross the boundary with a specified velocity.

Public Attributes

- int idir

boundary orientation in 3D space: 0,1,2

- int iside

  side of the boundary: 0,1

- REAL * xmin
- REAL * xmax

  min/max bounds

- BoundaryTypes type

  defines boundary type

- bool adiabatic

  flag for adiabatic boundary

- REAL area

  boundary surface area

- REAL temperature

  boundary temperature

- List< Gas > gases

  list of gases across the boundary

- Reaction * reactions

13.1.1 Detailed Description

Domain Boundary Definition.

Definition at line 18 of file domain.h.

13.1.2 Constructor & Destructor Documentation

13.1.2.1 Boundary::Boundary () [inline]

Boundary constructor: sets defaults.

Definition at line 30 of file domain.h.

References adiabatic, area, elasticBoundary, idir, iside, reactions, temperature, type, xmax, and xmin.

13.1.2.2 Boundary::~Boundary () [inline]

Boundary destructor.

Definition at line 40 of file domain.h.

13.1.3 Member Function Documentation

13.1.3.1 void Boundary::Area (REAL *a*) [inline]

Definition at line 44 of file domain.h.

References area.

13.1.3.2 REAL Boundary::Area () [inline]

Definition at line 43 of file domain.h.

References area.

13.1.3.3 void Boundary::init (int *i*, int *j*, REAL *ymin*[ ], REAL *ymax*[ ], int *nspecies*)

Definition at line 27 of file domain.cc.

References idir, iside, reactions, xmax, and xmin.

Referenced by Domain::Domain().

13.1.3.4 void Boundary::Inject (int *specietype*, REAL *vavx*, REAL *temperature*, Collection< Molecule > * *molecules*)

Injecting a specie from accross the boundary with a specified velocity.

Parameters:

specietype injected specie type

vavx average velocity in on direction

temperature temperature

molecules collection of molecules

Definition at line 32 of file domain.cc.

References Collection< Element >::append(), Molecule::Coordinate(), DIM, Gui::dx, GAUSS, idir, iside, GridContainer::put(), REAL, RND, Species::Specie::Size(), SMALL, Species::species, Molecule::Temperature(), Run::time, Molecule::Type(), Molecule::Velocity(), xmax, and xmin.

Referenced by Domain::injection().

13.1.3.5 void Boundary::Temperature (REAL *t*) [inline]

Definition at line 46 of file domain.h.

References temperature.

13.1.3.6 REAL Boundary::Temperature () [inline]

Definition at line 45 of file domain.h.

References temperature.

13.1.4 Member Data Documentation

13.1.4.1 bool Boundary::adiabatic

flag for adiabatic boundary

Definition at line 23 of file domain.h.

Referenced by Boundary(), and Domain::Domain().

13.1.4.2 REAL Boundary::area

boundary surface area

Definition at line 25 of file domain.h.

Referenced by Area(), Boundary(), Domain::Domain(), and Domain::injection().

13.1.4.3 List<Gas> Boundary::gases

list of gases across the boundary

Definition at line 27 of file domain.h.

Referenced by Domain::Domain(), and Domain::injection().

13.1.4.4 int Boundary::idir

boundary orientation in 3D space: 0,1,2

Definition at line 19 of file domain.h.

Referenced by Boundary(), init(), and Inject().

13.1.4.5 int Boundary::iside

side of the boundary: 0,1

Definition at line 19 of file domain.h.

Referenced by Boundary(), init(), and Inject().

13.1.4.6 Reaction* Boundary::reactions

boundary reactions with all species

Definition at line 28 of file domain.h.

Referenced by Boundary(), Domain::boundary(), Domain::Domain(), and init().

13.1.4.7 REAL Boundary::temperature

boundary temperature

Definition at line 25 of file domain.h.

Referenced by Boundary(), Domain::Domain(), Domain::injection(), and Temperature().

13.1.4.8 BoundaryTypes Boundary::type

defines boundary type

Definition at line 22 of file domain.h.

Referenced by Boundary(), Domain::boundary(), Domain::BoundaryType(), and Domain::Domain().

13.1.4.9 REAL * Boundary::xmax

min/max bounds

Definition at line 21 of file domain.h.

Referenced by Boundary(), init(), and Inject().

13.1.4.10 REAL* Boundary::xmin

Definition at line 21 of file domain.h.

Referenced by Boundary(), init(), and Inject().

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

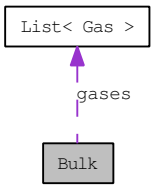
- domain.h
- domain.cc

13.2 Bulk Class Reference

Domain Bulk Properties.

`#include <domain.h>`

Collaboration diagram for Bulk:



Public Member Functions

- REAL Temperature ()
- void Temperature (REAL temp)
- REAL Volume ()
- void Volume (REAL vol)
- void init (REAL xmin[ ], REAL xmax[ ])

  Initializing bulk: setting volume.

- Molecule * inject (int specie, REAL velocity, Collection< Molecule > *molecules)

  Adding a molecule to the pool with not registering on the grid.

Public Attributes

- List< Gas > gases

  list of gases initially present in the bulk

Private Attributes

- REAL temperature
- REAL volume
- REAL xmin [DIM]
- REAL xmax [DIM]

  box-dimensions

13.2.1 Detailed Description

Domain Bulk Properties.

Holds thermodynamics properties and the list of species in the bulk of the domain. Initialized only when the new run. If Run::option.restart=1, it is ingored and the bulk properties and species are retrieved from the input file.

Definition at line 63 of file domain.h.

13.2.2 Member Function Documentation

13.2.2.1 void Bulk::init (REAL *xmin*[ ], REAL *xmax*[ ])

Initializing bulk: setting volume.

Definition at line 657 of file domain.cc.

References DIM, volume, xmax, and xmin.

Referenced by Domain::Domain().

13.2.2.2 Molecule * Bulk::inject (int *specie*, REAL *velocity*, Collection< Molecule > * *molecules*)

Adding a molecule to the pool with not registering on the grid.

Injecting a specie into the bulk with a specified velocity (no registering in the grid).

Definition at line 665 of file domain.cc.

References Collection< Element >::append(), Molecule::Coordinate(), DIM, GAUSS, REAL, RND, Species::Specie::Size(), SMALL, Species::species, Run::time, Molecule::Type(), Molecule::Velocity(), xmax, and xmin.

Referenced by Domain::init().

13.2.2.3 void Bulk::Temperature (REAL *temp*) [inline]

Definition at line 69 of file domain.h.

References temperature.

13.2.2.4 REAL Bulk::Temperature () [inline]

Definition at line 68 of file domain.h.

References temperature.

Referenced by Domain::Domain(), and Domain::init().

13.2.2.5 void Bulk::Volume (REAL *vol*) [inline]

Definition at line 71 of file domain.h.

References volume.

13.2.2.6 REAL Bulk::Volume () [inline]

Definition at line 70 of file domain.h.

References volume.

Referenced by Domain::init().

13.2.3 Member Data Documentation

13.2.3.1 List<Gas> Bulk::gases

list of gases initially present in the bulk

Definition at line 67 of file domain.h.

Referenced by Domain::Domain(), and Domain::init().

13.2.3.2 REAL Bulk::temperature [private]

Definition at line 64 of file domain.h.

Referenced by Temperature().

13.2.3.3 REAL Bulk::volume [private]

Definition at line 64 of file domain.h.

Referenced by init(), and Volume().

13.2.3.4 REAL Bulk::xmax[DIM] [private]

box-dimensions

Definition at line 64 of file domain.h.

Referenced by init(), and inject().

13.2.3.5 REAL Bulk::xmin[DIM] [private]

Definition at line 64 of file domain.h.

Referenced by init(), and inject().

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

- domain.h
- domain.cc

13.3 Collection< Element > Class Template Reference

`#include <collection.h>`

Public Member Functions

- Collection ()
- ~Collection ()
- int maxCounters ()
- int number ()
- int maxnumber ()
- void setFirst ()
- void setFirstLast ()
- void goFirst ()
- void goFirst (int i)
- void goFirstNext ()
- void goFirstNext (int i)
- void FirstNext ()
- void FirstPrev ()
- bool isFirstLast ()
- void goLastNext ()
- void goLastNext (int i)
- void goLast ()
- void goLast (int i)
- void goNext ()
- void goNext (int i)
- void goPrev ()
- void goPrev (int i)
- bool isFirst ()
- bool isFirst (int i)
- bool isLast ()
- bool isLast (int i)
- void LastNext ()
- void LastPrev ()
- void go (Item< Element > *p)
- Element * First ()
- Element * Last ()
- Element * Next ()
- Element * Next (int i)
- Element * getNext ()
- Element * getNext (int i)
- Element * Prev ()
- Element * Prev (int i)
- Element * getPrev ()
- Element * getPrev (int i)
- Element * Current ()
- Element * Current (int i)
- Item< Element > * getItem ()
- Item< Element > * getItem (int i)

- Item< Element > * getFirstItem ()
- Item< Element > * getLastItem ()
- bool init (int n)
- Element * insertAfter ()
- Element * insert0 ()
- Element * insert ()
- Element * insert (int icounter)
- bool insert0 (Element *element)
- bool insert (Element *element)
- bool insert (Element *element, int icounter)
- Element * append0 ()
- Element * append ()
- Element * append (int icounter)
- bool append0 (Element *element)
- bool append (Element *element)
- bool append (Element *element, int icounter)
- bool remove0 ()
- bool remove ()
- bool remove (int icounter)

Private Attributes

- int mitems
- int nitems
- bool locked
- struct Item< Element > * items
- struct Item< Element > * dead
- struct Item< Element > * first
- struct Item< Element > * last
- struct Item< Element > * current
- struct Item< Element > * current1 [maxcounters]

13.3.1 Detailed Description

template<class Element> class Collection< Element >

Definition at line 25 of file collection.h.

13.3.2 Constructor & Destructor Documentation

13.3.2.1 template<class Element > Collection< Element >::Collection () [inline]

Definition at line 103 of file collection.h.

References Collection< Element >::current, Collection< Element >::current1, Collection< Element >::dead, Collection< Element >::first, Collection< Element >::last, Collection< Element >::locked, maxcounters, Collection< Element >::mitems, and Collection< Element >::nitems.

13.3.2.2 template<class Element > Collection< Element >::~Collection () [inline]

Definition at line 110 of file collection.h.

References Collection< Element >::current, Collection< Element >::current1, Collection< Element >::dead, Collection< Element >::first, Collection< Element >::last, maxcounters, Collection< Element >::mitems, and Collection< Element >::nitems.

13.3.3 Member Function Documentation

13.3.3.1 template<class Element > bool Collection< Element >::append (Element * *element*, int *icounter*) [inline]

Definition at line 329 of file collection.h.

References Collection< Element >::append0(), Collection< Element >::current, Collection< Element >::current1, Collection< Element >::locked, maxcounters, and WAIT.

13.3.3.2 template<class Element > bool Collection< Element >::append (Element * *element*) [inline]

Definition at line 322 of file collection.h.

References Collection< Element >::append().

13.3.3.3 template<class Element > Element * Collection< Element >::append (int *icounter*) [inline]

Definition at line 308 of file collection.h.

References Collection< Element >::append0(), Collection< Element >::current, Collection< Element >::current1, Item< Element >::element, Collection< Element >::locked, maxcounters, and WAIT.

13.3.3.4 template<class Element > Element * Collection< Element >::append () [inline]

Definition at line 297 of file collection.h.

References Collection< Element >::append0(), Item< Element >::element, Collection< Element >::locked, and WAIT.

Referenced by Collection< Element >::append(), Bulk::inject(), Boundary::Inject(), and Domain::load().

13.3.3.5 template<class Element > bool Collection< Element >::append0 (Element * *element*)

13.3.3.6 template<class Element > Element * Collection< Element >::append0 () [inline]

Definition at line 263 of file collection.h.

References Collection< Element >::current, Collection< Element >::current1, Collection< Element >::dead, Collection< Element >::first, Collection< Element >::last, maxcounters, Item< Element >::next, Collection< Element >::nitems, and Item< Element >::prev.

Referenced by Collection< Element >::append().

13.3.3.7 template<class Element > Element* Collection< Element >::Current (int *i*) [inline]

Definition at line 79 of file collection.h.

13.3.3.8 template<class Element > Element* Collection< Element >::Current () [inline]

Definition at line 78 of file collection.h.

Referenced by Domain::computeBounds(), Gui::display(), Domain::Domain(), Domain::run(), and Domain::save().

13.3.3.9 template<class Element > Element* Collection< Element >::First () [inline]

Definition at line 68 of file collection.h.

13.3.3.10 template<class Element > void Collection< Element >::FirstNext () [inline]

Definition at line 50 of file collection.h.

13.3.3.11 template<class Element > void Collection< Element >::FirstPrev () [inline]

Definition at line 51 of file collection.h.

13.3.3.12 template<class Element > Item<Element>* Collection< Element >::getFirstItem () [inline]

Definition at line 82 of file collection.h.

13.3.3.13 template<class Element > Item<Element>* Collection< Element >::getItem (int *i*) [inline]

Definition at line 81 of file collection.h.

13.3.3.14 template<class Element > Item<Element>* Collection< Element >::getItem () [inline]

Definition at line 80 of file collection.h.

13.3.3.15 template<class Element > Item<Element>* Collection< Element >::getLastItem () [inline]

Definition at line 83 of file collection.h.

13.3.3.16 template<class Element > Element* Collection< Element >::getNext (int *i*) [inline]

Definition at line 73 of file collection.h.

13.3.3.17 template<class Element > Element* Collection< Element >::getNext () [inline]

Definition at line 72 of file collection.h.

13.3.3.18 template<class Element > Element* Collection< Element >::getPrev (int *i*) [inline]

Definition at line 77 of file collection.h.

13.3.3.19 template<class Element > Element* Collection< Element >::getPrev () [inline]

Definition at line 76 of file collection.h.

13.3.3.20 template<class Element > void Collection< Element >::go (Item< Element > * *p*) [inline]

Definition at line 67 of file collection.h.

13.3.3.21 template<class Element > void Collection< Element >::goFirst (int *i*) [inline]

Definition at line 47 of file collection.h.

13.3.3.22 template<class Element > void Collection< Element >::goFirst () [inline]

Definition at line 41 of file collection.h.

Referenced by Domain::computeBounds(), Gui::display(), Domain::Domain(), Domain::run(), and Domain::save().

13.3.3.23 template<class Element > void Collection< Element >::goFirstNext (int *i*) [inline]

Definition at line 49 of file collection.h.

13.3.3.24 template<class Element > void Collection< Element >::goFirstNext () [inline]

Definition at line 48 of file collection.h.

13.3.3.25 template<class Element > void Collection< Element >::goLast (int *i*) [inline]

Definition at line 56 of file collection.h.

13.3.3.26 template<class Element > void Collection< Element >::goLast () [inline]

Definition at line 55 of file collection.h.

13.3.3.27 template<class Element > void Collection< Element >::goLastNext (int *i*) [inline]

Definition at line 54 of file collection.h.

13.3.3.28 template<class Element > void Collection< Element >::goLastNext () [inline]

Definition at line 53 of file collection.h.

13.3.3.29 template<class Element > void Collection< Element >::goNext (int *i*) [inline]

Definition at line 58 of file collection.h.

13.3.3.30 template<class Element > void Collection< Element >::goNext () [inline]

Definition at line 57 of file collection.h.

Referenced by Domain::computeBounds(), Gui::display(), Domain::Domain(), Domain::run(), and Domain::save().

13.3.3.31 template<class Element > void Collection< Element >::goPrev (int *i*) [inline]

Definition at line 60 of file collection.h.

13.3.3.32 template<class Element > void Collection< Element >::goPrev () [inline]

Definition at line 59 of file collection.h.

13.3.3.33 template<class Element > bool Collection< Element >::init (int *n*) [inline]

Definition at line 117 of file collection.h.

References Collection< Element >::current, Collection< Element >::current1, Collection< Element >::dead, Collection< Element >::first, Collection< Element >::last, maxcounters, Collection< Element >::mitems, and Collection< Element >::nitems.

Referenced by Domain::Domain().

13.3.3.34 template<class Element > bool Collection< Element >::insert (Element * *element*, int *icounter*) [inline]

Definition at line 247 of file collection.h.

References Collection< Element >::current, Collection< Element >::current1, Collection< Element >::insert0(), Collection< Element >::locked, maxcounters, and WAIT.

13.3.3.35 template<class Element > bool Collection< Element >::insert (Element * *element*) [inline]

Definition at line 240 of file collection.h.

References Collection< Element >::insert().

13.3.3.36 template<class Element > Element * Collection< Element >::insert (int *icounter*) [inline]

Definition at line 226 of file collection.h.

References Collection< Element >::current, Collection< Element >::current1, Item< Element >::element, Collection< Element >::insert0(), Collection< Element >::locked, maxcounters, and WAIT.

13.3.3.37 template<class Element > Element * Collection< Element >::insert () [inline]

Definition at line 214 of file collection.h.

References Collection< Element >::insert0(), Collection< Element >::locked, Collection< Element >::number(), and WAIT.

Referenced by Collection< Element >::insert().

13.3.3.38 template<class Element > bool Collection< Element >::insert0 (Element * *element*)

13.3.3.39 template<class Element > Element * Collection< Element >::insert0 () [inline]

Definition at line 179 of file collection.h.

References Collection< Element >::current, Collection< Element >::current1, Collection< Element >::dead, Item< Element >::element, Collection< Element >::first, Collection< Element >::last, maxcounters, Item< Element >::next, Collection< Element >::nitems, and Item< Element >::prev.

Referenced by Collection< Element >::insert().

13.3.3.40 template<class Element > Element * Collection< Element >::insertAfter () [inline]

Definition at line 144 of file collection.h.

References Collection< Element >::current, Collection< Element >::current1, Collection< Element >::dead, Item< Element >::element, Collection< Element >::first, Collection< Element >::last, maxcounters, Item< Element >::next, Collection< Element >::nitems, and Item< Element >::prev.

Referenced by Domain::boundary().

13.3.3.41 template<class Element > bool Collection< Element >::isFirst (int *i*) [inline]

Definition at line 62 of file collection.h.

13.3.3.42 template<class Element > bool Collection< Element >::isFirst () [inline]

Definition at line 61 of file collection.h.

Referenced by Domain::computeBounds(), Gui::display(), Domain::Domain(), Domain::run(), and Domain::save().

13.3.3.43 template<class Element > bool Collection< Element >::isFirstLast () [inline]

Definition at line 52 of file collection.h.

13.3.3.44 template<class Element > bool Collection< Element >::isLast (int *i*) [inline]

Definition at line 64 of file collection.h.

13.3.3.45 template<class Element > bool Collection< Element >::isLast () [inline]

Definition at line 63 of file collection.h.

13.3.3.46 template<class Element > Element* Collection< Element >::Last () [inline]

Definition at line 69 of file collection.h.

13.3.3.47 template<class Element > void Collection< Element >::LastNext () [inline]

Definition at line 65 of file collection.h.

13.3.3.48 template<class Element > void Collection< Element >::LastPrev () [inline]

Definition at line 66 of file collection.h.

13.3.3.49 template<class Element > int Collection< Element >::maxCounters () [inline]

Definition at line 36 of file collection.h.

Referenced by Domain::run().

13.3.3.50 template<class Element > int Collection< Element >::maxnumber () [inline]

Definition at line 38 of file collection.h.

Referenced by Domain::run().

13.3.3.51 template<class Element > Element* Collection< Element >::Next (int *i*) [inline]

Definition at line 71 of file collection.h.

13.3.3.52 template<class Element > Element* Collection< Element >::Next () [inline]

Definition at line 70 of file collection.h.

13.3.3.53 template<class Element > int Collection< Element >::number () [inline]

Definition at line 37 of file collection.h.

Referenced by Gui::display(), Domain::Domain(), Gui::initdisp(), Collection< Element >::insert(), Domain::load(), Domain::run(), and Domain::save().

13.3.3.54 template<class Element > Element* Collection< Element >::Prev (int *i*) [inline]

Definition at line 75 of file collection.h.

13.3.3.55 template<class Element > Element* Collection< Element >::Prev () [inline]

Definition at line 74 of file collection.h.

13.3.3.56 template<class Element > bool Collection< Element >::remove (int *icounter*) [inline]

Definition at line 393 of file collection.h.

References Collection< Element >::current, Collection< Element >::current1, Collection< Element >::locked, maxcounters, Collection< Element >::remove0(), and WAIT.

13.3.3.57 template<class Element > bool Collection< Element >::remove () [inline]

Definition at line 379 of file collection.h.

References Collection< Element >::current, Collection< Element >::current1, Collection< Element >::locked, maxcounters, Collection< Element >::remove0(), and WAIT.

13.3.3.58 template<class Element > bool Collection< Element >::remove0 () [inline]

Definition at line 344 of file collection.h.

References Collection< Element >::current, Collection< Element >::current1, Collection< Element >::dead, Collection< Element >::first, Collection< Element >::last, maxcounters, Item< Element >::next, and Collection< Element >::nitems.

Referenced by Collection< Element >::remove(), and Domain::run().

13.3.3.59 template<class Element > void Collection< Element >::setFirst () [inline]

Definition at line 39 of file collection.h.

13.3.3.60 template<class Element > void Collection< Element >::setFirstLast () [inline]

Definition at line 40 of file collection.h.

13.3.4 Member Data Documentation

13.3.4.1 template<class Element > struct Item< Element > * Collection< Element >::current [read, private]

Definition at line 28 of file collection.h.

Referenced by Collection< Element >::append(), Collection< Element >::append0(), Collection< Element >::Collection(), Collection< Molecule >::Current(), Collection< Molecule >::getItem(), Collection< Molecule >::getNext(), Collection< Molecule >::getPrev(), Collection< Molecule >::go(),

Collection< Molecule >::goFirst(), Collection< Molecule >::goFirstNext(), Collection< Molecule >::goLast(), Collection< Molecule >::goLastNext(), Collection< Molecule >::goNext(), Collection< Molecule >::goPrev(), Collection< Element >::init(), Collection< Element >::insert(), Collection< Element >::insert0(), Collection< Element >::insertAfter(), Collection< Molecule >::isFirst(), Collection< Molecule >::isLast(), Collection< Molecule >::Next(), Collection< Molecule >::Prev(), Collection< Element >::remove(), Collection< Element >::remove0(), and Collection< Element >::∼Collection().

13.3.4.2 template<class Element > struct Item< Element > * Collection< Element >::current1[maxcounters] [read, private]

Definition at line 28 of file collection.h.

Referenced by Collection< Element >::append(), Collection< Element >::append0(), Collection< Element >::Collection(), Collection< Molecule >::Current(), Collection< Molecule >::getItem(), Collection< Molecule >::getNext(), Collection< Molecule >::getPrev(), Collection< Molecule >::goFirst(), Collection< Molecule >::goFirstNext(), Collection< Molecule >::goLast(), Collection< Molecule >::goLastNext(), Collection< Molecule >::goNext(), Collection< Molecule >::goPrev(), Collection< Element >::init(), Collection< Element >::insert(), Collection< Element >::insert0(), Collection< Element >::insertAfter(), Collection< Molecule >::isFirst(), Collection< Molecule >::isLast(), Collection< Molecule >::Next(), Collection< Molecule >::Prev(), Collection< Element >::remove(), Collection< Element >::remove0(), and Collection< Element >::∼Collection().

13.3.4.3 template<class Element > struct Item< Element > * Collection< Element >::dead [read, private]

Definition at line 28 of file collection.h.

Referenced by Collection< Element >::append0(), Collection< Element >::Collection(), Collection< Element >::init(), Collection< Element >::insert0(), Collection< Element >::insertAfter(), Collection< Element >::remove0(), and Collection< Element >::∼Collection().

13.3.4.4 template<class Element > struct Item< Element > * Collection< Element >::first [read, private]

Definition at line 28 of file collection.h.

Referenced by Collection< Element >::append0(), Collection< Element >::Collection(), Collection< Molecule >::First(), Collection< Molecule >::FirstNext(), Collection< Molecule >::FirstPrev(), Collection< Molecule >::getFirstItem(), Collection< Molecule >::goFirst(), Collection< Molecule >::goFirstNext(), Collection< Element >::init(), Collection< Element >::insert0(), Collection< Element >::insertAfter(), Collection< Molecule >::isFirst(), Collection< Molecule >::isFirstLast(), Collection< Element >::remove0(), Collection< Molecule >::setFirst(), Collection< Molecule >::setFirstLast(), and Collection< Element >::∼Collection().

13.3.4.5 template<class Element > struct Item< Element >* Collection< Element >::items [read, private]

Definition at line 28 of file collection.h.

13.3.4.6 template<class Element > struct Item< Element > * Collection< Element >::last [read, private]

Definition at line 28 of file collection.h.

Referenced by Collection< Element >::append0(), Collection< Element >::Collection(), Collection< Molecule >::getLastItem(), Collection< Molecule >::goLast(), Collection< Molecule >::goLastNext(), Collection< Element >::init(), Collection< Element >::insert0(), Collection< Element >::insertAfter(), Collection< Molecule >::isFirstLast(), Collection< Molecule >::isLast(), Collection< Molecule >::Last(), Collection< Molecule >::LastNext(), Collection< Molecule >::LastPrev(), Collection< Element >::remove0(), Collection< Molecule >::setFirst(), Collection< Molecule >::setFirstLast(), and Collection< Element >::~Collection().

13.3.4.7 template<class Element > bool Collection< Element >::locked [private]

Definition at line 27 of file collection.h.

Referenced by Collection< Element >::append(), Collection< Element >::Collection(), Collection< Element >::insert(), and Collection< Element >::remove().

13.3.4.8 template<class Element > int Collection< Element >::mitems [private]

Definition at line 26 of file collection.h.

Referenced by Collection< Element >::Collection(), Collection< Element >::init(), Collection< Molecule >::maxnumber(), and Collection< Element >::~Collection().

13.3.4.9 template<class Element > int Collection< Element >::nitems [private]

Definition at line 26 of file collection.h.

Referenced by Collection< Element >::append0(), Collection< Element >::Collection(), Collection< Element >::init(), Collection< Element >::insert0(), Collection< Element >::insertAfter(), Collection< Molecule >::number(), Collection< Element >::remove0(), and Collection< Element >::~Collection().

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

- collection.h

13.4 Gui::ColorScale Struct Reference

`#include <gui.h>`

Public Attributes

- int relative:1

13.4.1 Detailed Description

Definition at line 104 of file gui.h.

13.4.2 Member Data Documentation

13.4.2.1 int Gui::ColorScale::relative

Definition at line 105 of file gui.h.

Referenced by Gui::initdisp().

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

- gui.h

13.5 Container< Element > Class Template Reference

`#include <collection.h>`

Public Member Functions

- Container ()
- ~Container ()
- bool islocked ()
- void lock ()
- void unlock ()
- int number ()
- void setFirst ()
- void setFirst (int i)
- void setFirstLast ()
- void setFirstLast (int i)
- void goFirst ()
- void goFirst (int i)
- void goFirstNext ()
- void goFirstNext (int i)
- void FirstNext ()
- void FirstNext (int i)
- void FirstPrev ()
- void FirstPrev (int i)
- bool isFirstLast ()
- bool isFirstLast (int i)
- void goLastNext ()
- void goLastNext (int i)
- void goLast ()
- void goLast (int i)
- void goNext ()
- void goNext (int i)
- void goPrev ()
- void goPrev (int i)
- bool isFirst ()
- bool isFirst (int i)
- bool isLast ()
- bool isLast (int i)
- void LastNext ()
- void LastPrev ()
- void go (Ptr< Element > *p)
- void go (Ptr< Element > *p, int i)
- Element * First ()
- Element * First (int i)
- Element * Last ()
- Element * Next ()
- Element * Next (int i)
- Element * getNext ()
- Element * getNext (int i)

- Element * Prev ()
- Element * Prev (int i)
- Element * getPrev ()
- Element * getPrev (int i)
- Element * Current ()
- Element * Current (int i)
- Ptr< Element > * getPtr ()
- Ptr< Element > * getPtr (int i)
- Ptr< Element > * getFirstPtr ()
- Ptr< Element > * getFirstPtr (int i)
- Ptr< Element > * getLastPtr ()
- bool insert0 (Element *element)
- bool insert (Element *element)
- bool insert (Element *element, int i)
- Ptr< Element > * insert1 (Element *element, int i)
- bool insert0 ()
- bool insert ()
- bool insert (int i)
- bool append0 (Element *element)
- bool append (Element *element)
- bool append (Element *element, int i)
- bool append0 ()
- bool append ()
- bool append (int i)
- Ptr< Element > * append1 (Element *element, int i)
- bool link0 (Ptr< Element > *&ptr)
- bool link (Ptr< Element > *&ptr)
- bool unlink0 (Ptr< Element > *&ptr)
- bool unlink (Ptr< Element > *&ptr)
- bool remove0 ()
- bool remove ()
- bool remove (int i)
- bool remove0 (Ptr< Element > *&ptr)
- bool remove (Ptr< Element > *ptr)
- bool remove (Ptr< Element > *ptr, int i)
- bool checkPool (char *msg, Pool< Element > *pool)

Private Attributes

- int nptrs
- bool locked
- Ptr< Element > * first
- Ptr< Element > * last
- Ptr< Element > * current
- Ptr< Element > * first1 [maxcounters]
- Ptr< Element > * current1 [maxcounters]

13.5.1 Detailed Description

template<class Element> class Container< Element >

Definition at line 512 of file collection.h.

13.5.2 Constructor & Destructor Documentation

13.5.2.1 template<class Element > Container< Element >::Container () [inline]

Definition at line 2 of file container.h.

References Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, Container< Element >::last, Container< Element >::locked, maxcounters, and Container< Element >::nptrs.

13.5.2.2 template<class Element > Container< Element >::~Container () [inline]

Definition at line 11 of file container.h.

References Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, Container< Element >::last, maxcounters, and Container< Element >::nptrs.

13.5.3 Member Function Documentation

13.5.3.1 template<class Element > bool Container< Element >::append (int *i*) [inline]

Definition at line 82 of file container.h.

References Container< Element >::append0(), Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, Container< Element >::locked, maxcounters, and WAIT.

13.5.3.2 template<class Element > bool Container< Element >::append () [inline]

Definition at line 66 of file container.h.

References Container< Element >::append0(), Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, Container< Element >::locked, maxcounters, and WAIT.

13.5.3.3 template<class Element > bool Container< Element >::append (Element * *element*, int *i*) [inline]

Definition at line 119 of file container.h.

References Container< Element >::append0(), Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, Container< Element >::last, Container< Element >::locked, maxcounters, and WAIT.

13.5.3.4 template<class Element > bool Container< Element >::append (Element * *element*) [inline]

Definition at line 101 of file container.h.

References Container< Element >::append0(), Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, Container< Element >::last, Container< Element >::locked, maxcounters, and WAIT.

13.5.3.5 template<class Element > bool Container< Element >::append0 () [inline]

Definition at line 30 of file container.h.

References Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, Pool< Element >::get(), Container< Element >::last, maxcounters, Container< Element >::nptrs, GridContainer::pool, and Ptr< Element >::prev.

Referenced by Container< Element >::append(), and Container< Element >::append1().

13.5.3.6 template<class Element > bool Container< Element >::append0 (Element * *element*)

13.5.3.7 template<class Element > Ptr< Element > * Container< Element >::append1 (Element * *element*, int *i*) [inline]

Definition at line 141 of file container.h.

References Container< Element >::append0(), Container< Element >::last, Container< Element >::locked, and WAIT.

13.5.3.8 template<class Element > bool Container< Element >::checkPool (char * *msg*, Pool< Element > * *pool*) [inline]

Definition at line 19 of file container.h.

References Pool< Element >::check(), Container< Element >::current, Container< Element >::first, Pool< Element >::hook, and Container< Element >::nptrs.

13.5.3.9 template<class Element > Element* Container< Element >::Current (int *i*) [inline]

Definition at line 573 of file collection.h.

References Container< Element >::current1.

13.5.3.10 template<class Element > Element* Container< Element >::Current () [inline]

Definition at line 572 of file collection.h.

References Container< Element >::current.

Referenced by Domain::interaction().

13.5.3.11 template<class Element > Element* Container< Element >::First (int *i*) [inline]

Definition at line 562 of file collection.h.

References Container< Element >::first1.

13.5.3.12 template<class Element > Element* Container< Element >::First () [inline]

Definition at line 561 of file collection.h.

References Container< Element >::first.

Referenced by Domain::interaction().

13.5.3.13 template<class Element > void Container< Element >::FirstNext (int *i*) [inline]

Definition at line 540 of file collection.h.

References Container< Element >::first1.

13.5.3.14 template<class Element > void Container< Element >::FirstNext () [inline]

Definition at line 539 of file collection.h.

References Container< Element >::first.

Referenced by Domain::interaction().

13.5.3.15 template<class Element > void Container< Element >::FirstPrev (int *i*) [inline]

Definition at line 542 of file collection.h.

References Container< Element >::first1.

13.5.3.16 template<class Element > void Container< Element >::FirstPrev () [inline]

Definition at line 541 of file collection.h.

References Container< Element >::first.

13.5.3.17 template<class Element > Ptr<Element>* Container< Element >::getFirstPtr (int *i*) [inline]

Definition at line 577 of file collection.h.

References Container< Element >::first1.

13.5.3.18 template<class Element > Ptr<Element>* Container< Element >::getFirstPtr () [inline]

Definition at line 576 of file collection.h.

References Container< Element >::first.

13.5.3.19 template<class Element > Ptr<Element>* Container< Element >::getLastPtr () [inline]

Definition at line 578 of file collection.h.

References Container< Element >::last.

13.5.3.20 template<class Element > Element* Container< Element >::getNext (int *i*) [inline]

Definition at line 567 of file collection.h.

References Container< Element >::current1.

13.5.3.21 template<class Element > Element* Container< Element >::getNext () [inline]

Definition at line 566 of file collection.h.

References Container< Element >::current.

13.5.3.22 template<class Element > Element* Container< Element >::getPrev (int *i*) [inline]

Definition at line 571 of file collection.h.

References Container< Element >::current1.

13.5.3.23 template<class Element > Element* Container< Element >::getPrev () [inline]

Definition at line 570 of file collection.h.

References Container< Element >::current.

13.5.3.24 template<class Element > Ptr<Element>* Container< Element >::getPtr (int *i*) [inline]

Definition at line 575 of file collection.h.

References Container< Element >::current1.

13.5.3.25 template<class Element > Ptr<Element>* Container< Element >::getPtr () [inline]

Definition at line 574 of file collection.h.

References Container< Element >::current.

13.5.3.26 template<class Element > void Container< Element >::go (Ptr< Element > * *p*, int *i*) [inline]

Definition at line 560 of file collection.h.

References Container< Element >::current1.

13.5.3.27 template<class Element > void Container< Element >::go (Ptr< Element > * p) [inline]

Definition at line 559 of file collection.h.

References Container< Element >::current.

13.5.3.28 template<class Element > void Container< Element >::goFirst (int i) [inline]

Definition at line 536 of file collection.h.

References Container< Element >::current1, and Container< Element >::first1.

13.5.3.29 template<class Element > void Container< Element >::goFirst () [inline]

Definition at line 530 of file collection.h.

References Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, and maxcounters.

Referenced by Domain::interaction().

13.5.3.30 template<class Element > void Container< Element >::goFirstNext (int i) [inline]

Definition at line 538 of file collection.h.

References Container< Element >::current1, and Container< Element >::first1.

13.5.3.31 template<class Element > void Container< Element >::goFirstNext () [inline]

Definition at line 537 of file collection.h.

References Container< Element >::current, and Container< Element >::first.

13.5.3.32 template<class Element > void Container< Element >::goLast (int i) [inline]

Definition at line 548 of file collection.h.

References Container< Element >::current1, and Container< Element >::last.

13.5.3.33 template<class Element > void Container< Element >::goLast () [inline]

Definition at line 547 of file collection.h.

References Container< Element >::current, and Container< Element >::last.

13.5.3.34 template<class Element > void Container< Element >::goLastNext (int i) [inline]

Definition at line 546 of file collection.h.

References Container< Element >::current1, and Container< Element >::last.

13.5.3.35 template<class Element > void Container< Element >::goLastNext () [inline]

Definition at line 545 of file collection.h.

References Container< Element >::current, and Container< Element >::last.

13.5.3.36 template<class Element > void Container< Element >::goNext (int *i*) [inline]

Definition at line 550 of file collection.h.

References Container< Element >::current1.

13.5.3.37 template<class Element > void Container< Element >::goNext () [inline]

Definition at line 549 of file collection.h.

References Container< Element >::current.

Referenced by Domain::interaction().

13.5.3.38 template<class Element > void Container< Element >::goPrev (int *i*) [inline]

Definition at line 552 of file collection.h.

References Container< Element >::current1.

13.5.3.39 template<class Element > void Container< Element >::goPrev () [inline]

Definition at line 551 of file collection.h.

References Container< Element >::current.

13.5.3.40 template<class Element > bool Container< Element >::insert (int *i*) [inline]

Definition at line 326 of file container.h.

References Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, Container< Element >::insert0(), Container< Element >::locked, maxcounters, and WAIT.

13.5.3.41 template<class Element > bool Container< Element >::insert () [inline]

Definition at line 309 of file container.h.

References Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, Container< Element >::insert0(), Container< Element >::locked, maxcounters, and WAIT.

13.5.3.42 template<class Element > bool Container< Element >::insert (Element * *element*, int *i*) [inline]

Definition at line 365 of file container.h.

References Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, Container< Element >::insert0(), Container< Element >::locked, maxcounters, and WAIT.

13.5.3.43 template<class Element > bool Container< Element >::insert (Element * *element*) [inline]

Definition at line 347 of file container.h.

References Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, Container< Element >::insert0(), Container< Element >::locked, maxcounters, and WAIT.

13.5.3.44 template<class Element > bool Container< Element >::insert0 () [inline]

Definition at line 276 of file container.h.

References Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, Pool< Element >::get(), Container< Element >::last, maxcounters, Ptr< Element >::next, Container< Element >::nptrs, GridContainer::pool, and Ptr< Element >::prev.

Referenced by Container< Element >::insert(), and Container< Element >::insert1().

13.5.3.45 template<class Element > bool Container< Element >::insert0 (Element * *element*)

13.5.3.46 template<class Element > Ptr< Element > * Container< Element >::insert1 (Element * *element*, int *i*) [inline]

Definition at line 387 of file container.h.

References Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, Container< Element >::insert0(), Container< Element >::locked, maxcounters, and WAIT.

13.5.3.47 template<class Element > bool Container< Element >::isFirst (int *i*) [inline]

Definition at line 554 of file collection.h.

References Container< Element >::current1, and Container< Element >::first1.

13.5.3.48 template<class Element > bool Container< Element >::isFirst () [inline]

Definition at line 553 of file collection.h.

References Container< Element >::current, and Container< Element >::first.

Referenced by Domain::interaction().

13.5.3.49 template<class Element > bool Container< Element >::isFirstLast (int *i*) [inline]

Definition at line 544 of file collection.h.

References Container< Element >::first1, and Container< Element >::last.

13.5.3.50 template<class Element > bool Container< Element >::isFirstLast () [inline]

Definition at line 543 of file collection.h.

References Container< Element >::first, and Container< Element >::last.

Referenced by Domain::interaction().

13.5.3.51 template<class Element > bool Container< Element >::isLast (int *i*) [inline]

Definition at line 556 of file collection.h.

References Container< Element >::current1, and Container< Element >::last.

13.5.3.52 template<class Element > bool Container< Element >::isLast () [inline]

Definition at line 555 of file collection.h.

References Container< Element >::current, and Container< Element >::last.

Referenced by Domain::interaction().

13.5.3.53 template<class Element > bool Container< Element >::islocked () [inline]

Definition at line 522 of file collection.h.

References Container< Element >::locked.

13.5.3.54 template<class Element > Element* Container< Element >::Last () [inline]

Definition at line 563 of file collection.h.

References Container< Element >::last.

13.5.3.55 template<class Element > void Container< Element >::LastNext () [inline]

Definition at line 557 of file collection.h.

References Container< Element >::last.

13.5.3.56 template<class Element > void Container< Element >::LastPrev () [inline]

Definition at line 558 of file collection.h.

References Container< Element >::last.

13.5.3.57 template<class Element > bool Container< Element >::link (Ptr< Element > *&* *ptr*) [inline]

Definition at line 194 of file container.h.

References Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, Container< Element >::link0(), Container< Element >::locked, maxcounters, and WAIT.

13.5.3.58 template<class Element > bool Container< Element >::link0 (Ptr< Element > *&* *ptr*) [inline]

Definition at line 163 of file container.h.

References Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, Container< Element >::last, maxcounters, Ptr< Element >::next, Container< Element >::nptrs, and Ptr< Element >::prev.

Referenced by Container< Element >::link().

13.5.3.59 template<class Element > void Container< Element >::lock () [inline]

Definition at line 523 of file collection.h.

References Container< Element >::locked.

13.5.3.60 template<class Element > Element* Container< Element >::Next (int *i*) [inline]

Definition at line 565 of file collection.h.

References Container< Element >::current1.

13.5.3.61 template<class Element > Element* Container< Element >::Next () [inline]

Definition at line 564 of file collection.h.

References Container< Element >::current.

13.5.3.62 template<class Element > int Container< Element >::number () [inline]

Definition at line 525 of file collection.h.

References Container< Element >::nptrs.

Referenced by Domain::interaction().

13.5.3.63 template<class Element > Element* Container< Element >::Prev (int *i*) [inline]

Definition at line 569 of file collection.h.

References Container< Element >::current1.

13.5.3.64 template<class Element > Element* Container< Element >::Prev () [inline]

Definition at line 568 of file collection.h.

References Container< Element >::current.

13.5.3.65 template<class Element > bool Container< Element >::remove (Ptr< Element > * *ptr*, int *i*) [inline]

Definition at line 524 of file container.h.

References Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, Container< Element >::locked, maxcounters, Container< Element >::remove0(), and WAIT.

13.5.3.66 template<class Element > bool Container< Element >::remove (Ptr< Element > * *ptr*) [inline]

Definition at line 512 of file container.h.

References Container< Element >::locked, Container< Element >::remove0(), and WAIT.

13.5.3.67 template<class Element > bool Container< Element >::remove (int *i*) [inline]

Definition at line 451 of file container.h.

References Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, Container< Element >::locked, maxcounters, Container< Element >::remove0(), and WAIT.

13.5.3.68 template<class Element > bool Container< Element >::remove () [inline]

Definition at line 431 of file container.h.

References Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, Container< Element >::locked, maxcounters, Container< Element >::remove0(), and WAIT.

Referenced by Domain::interaction(), and Domain::run().

13.5.3.69 template<class Element > bool Container< Element >::remove0 (Ptr< Element > *& *ptr*) [inline]

Definition at line 473 of file container.h.

References Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, Container< Element >::last, maxcounters, Container< Element >::nptrs, GridContainer::pool, and Pool< Element >::put().

13.5.3.70 template<class Element > bool Container< Element >::remove0 () [inline]

Definition at line 409 of file container.h.

References Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, Container< Element >::last, maxcounters, Container< Element >::nptrs, GridContainer::pool, and Pool< Element >::put().

Referenced by Container< Element >::remove().

13.5.3.71 template<class Element > void Container< Element >::setFirst (int *i*) [inline]

Definition at line 527 of file collection.h.

References Container< Element >::first1, and Container< Element >::last.

13.5.3.72 template<class Element > void Container< Element >::setFirst () [inline]

Definition at line 526 of file collection.h.

References Container< Element >::first, and Container< Element >::last.

Referenced by Domain::interaction().

13.5.3.73 template<class Element > void Container< Element >::setFirstLast (int *i*) [inline]

Definition at line 529 of file collection.h.

References Container< Element >::first1, and Container< Element >::last.

13.5.3.74 template<class Element > void Container< Element >::setFirstLast () [inline]

Definition at line 528 of file collection.h.

References Container< Element >::first, and Container< Element >::last.

Referenced by Domain::interaction().

13.5.3.75 template<class Element > bool Container< Element >::unlink (Ptr< Element > *& *ptr*) [inline]

Definition at line 261 of file container.h.

References Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, Container< Element >::locked, maxcounters, Container< Element >::unlink0(), and WAIT.

13.5.3.76 template<class Element > bool Container< Element >::unlink0 (Ptr< Element > *& *ptr*) [inline]

Definition at line 211 of file container.h.

References Container< Element >::current, Container< Element >::current1, Container< Element >::first, Container< Element >::first1, Container< Element >::last, maxcounters, Ptr< Element >::next, Container< Element >::nptrs, and Ptr< Element >::prev.

Referenced by Container< Element >::unlink().

13.5.3.77 template<class Element > void Container< Element >::unlock () [inline]

Definition at line 524 of file collection.h.

References Container< Element >::locked.

13.5.4 Member Data Documentation

13.5.4.1 template<class Element > Ptr<Element> * Container< Element >::current [private]

Definition at line 517 of file collection.h.

Referenced by Container< Element >::append(), Container< Element >::append0(), Container< Element >::checkPool(), Container< Element >::Container(), Container< Element >::Current(), Container< Element >::getNext(), Container< Element >::getPrev(), Container< Element >::getPtr(), Container< Element >::go(), Container< Element >::goFirst(), Container< Element >::goFirstNext(), Container< Element >::goLast(), Container< Element >::goLastNext(), Container< Element >::goNext(), Container< Element >::goPrev(), Container< Element >::insert(), Container< Element >::insert0(), Container< Element >::insert1(), Container< Element >::isFirst(), Container< Element >::isLast(), Container< Element >::link(), Container< Element >::link0(), Container< Element >::Next(), Container< Element >::Prev(), Container< Element >::remove(), Container< Element >::remove0(), Container< Element >::unlink(), Container< Element >::unlink0(), and Container< Element >::~Container().

13.5.4.2 template<class Element > Ptr<Element> * Container< Element >::current1[maxcounters] [private]

Definition at line 517 of file collection.h.

Referenced by Container< Element >::append(), Container< Element >::append0(), Container< Element >::Container(), Container< Element >::Current(), Container< Element >::getNext(), Container< Element >::getPrev(), Container< Element >::getPtr(), Container< Element >::go(), Container< Element >::goFirst(), Container< Element >::goFirstNext(), Container< Element >::goLast(), Container< Element >::goLastNext(), Container< Element >::goNext(), Container< Element >::goPrev(), Container< Element >::insert(), Container< Element >::insert0(), Container< Element >::insert1(), Container< Element >::isFirst(), Container< Element >::isLast(), Container< Element >::link(), Container< Element >::link0(), Container< Element >::Next(), Container< Element >::Prev(), Container< Element >::remove(), Container< Element >::remove0(), Container< Element >::unlink(), Container< Element >::unlink0(), and Container< Element >::~Container().

13.5.4.3 template<class Element > Ptr<Element>* Container< Element >::first [private]

Definition at line 517 of file collection.h.

Referenced by Container< Element >::append(), Container< Element >::append0(), Container< Element >::checkPool(), Container< Element >::Container(), Container< Element >::First(), Container< Element >::FirstNext(), Container< Element >::FirstPrev(), Container< Element >::getFirstPtr(), Container< Element >::goFirst(), Container< Element >::goFirstNext(), Container< Element >::insert(), Container< Element >::insert0(), Container< Element >::insert1(), Container< Element >::isFirst(), Container< Element >::isFirstLast(), Container< Element >::link(), Container< Element >::link0(), Container< Element >::remove(), Container< Element >::remove0(), Container< Element >::setFirst(), Container< Element >::setFirstLast(), Container< Element >::unlink(), Container< Element >::unlink0(), and Container< Element >::~Container().

13.5.4.4 template<class Element > Ptr<Element> * Container< Element >::first1[maxcounters] [private]

Definition at line 517 of file collection.h.

Referenced by Container< Element >::append(), Container< Element >::append0(), Container< Element >::Container(), Container< Element >::First(), Container< Element >::FirstNext(), Container< Element >::FirstPrev(), Container< Element >::getFirstPtr(), Container< Element >::goFirst(), Container< Element >::goFirstNext(), Container< Element >::insert(), Container< Element >::insert0(), Container< Element >::insert1(), Container< Element >::isFirst(), Container< Element >::isFirstLast(), Container< Element >::link(), Container< Element >::link0(), Container< Element >::remove(), Container< Element >::remove0(), Container< Element >::setFirst(), Container< Element >::setFirstLast(), Container<

Element >::unlink(), Container< Element >::unlink0(), and Container< Element >::~Container().

13.5.4.5 template<class Element > Ptr<Element> * Container< Element >::last [private]

Definition at line 517 of file collection.h.

Referenced by Container< Element >::append(), Container< Element >::append0(), Container< Element >::append1(), Container< Element >::Container(), Container< Element >::getLastPtr(), Container< Element >::goLast(), Container< Element >::goLastNext(), Container< Element >::insert0(), Container< Element >::isFirstLast(), Container< Element >::isLast(), Container< Element >::Last(), Container< Element >::LastNext(), Container< Element >::LastPrev(), Container< Element >::link0(), Container< Element >::remove0(), Container< Element >::setFirst(), Container< Element >::setFirstLast(), Container< Element >::unlink0(), and Container< Element >::~Container().

13.5.4.6 template<class Element > bool Container< Element >::locked [private]

Definition at line 514 of file collection.h.

Referenced by Container< Element >::append(), Container< Element >::append1(), Container< Element >::Container(), Container< Element >::insert(), Container< Element >::insert1(), Container< Element >::islocked(), Container< Element >::link(), Container< Element >::lock(), Container< Element >::remove(), Container< Element >::unlink(), and Container< Element >::unlock().

13.5.4.7 template<class Element > int Container< Element >::nptrs [private]

Definition at line 513 of file collection.h.

Referenced by Container< Element >::append0(), Container< Element >::checkPool(), Container< Element >::Container(), Container< Element >::insert0(), Container< Element >::link0(), Container< Element >::number(), Container< Element >::remove0(), Container< Element >::unlink0(), and Container< Element >::~Container().

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

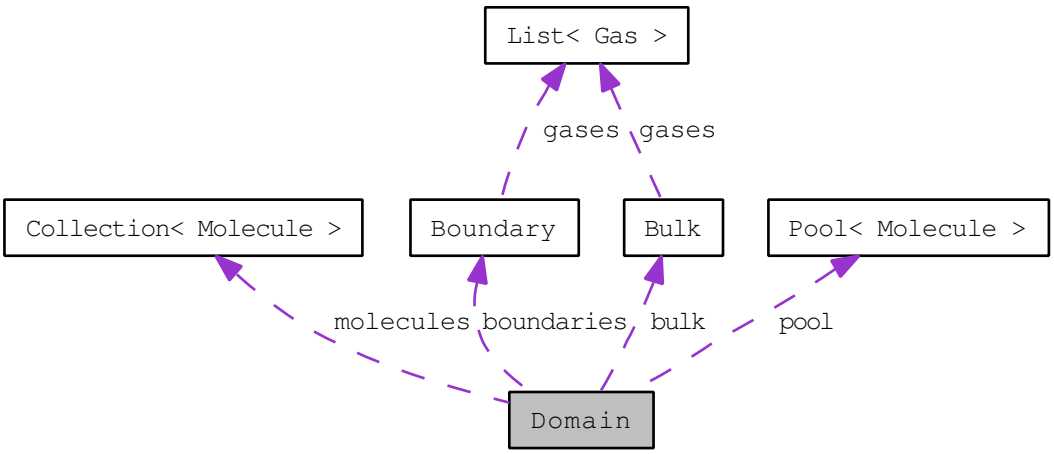
- collection.h
- container.h

13.6 Domain Class Reference

Computational Domain.

`#include <domain.h>`

Collaboration diagram for Domain:



Public Member Functions

- Domain (char *filename)

  Domain constructor creates an instance of a domain.

- ~Domain ()
- void BoundaryType (enum BoundaryTypes b, int idir, int inside)
- enum BoundaryTypes BoundaryType (int idir, int inside)
- void setMinBound (int i, REAL x)
- void setMaxBound (int i, REAL x)
- REAL minBound (int i)
- REAL maxBound (int i)
- int computeBounds (REAL x0[ ], REAL x1[ ])
- Collection< Molecule > * Molecules ()
- int run (int niter)

  The Domain solver: running **niter** *iterations.*

- void step (int iter)
- int boundary (Molecule *molecule)
- void injection ()

  Inject cross-boundary species:.

- void interaction ()
- void interaction (int icounter)
- Interaction interact (Molecule *a, Molecule *b)
- void init ()
- void load (char *filename)

Initializing molecules according to bulk properties (restart=0).

- void save (char *taskname)

Private Attributes

- int * distribution
  molecule counts for all species
- REAL bounds [2][DIM]
- char boundaryName [maxBoundaryTypes][WORDLENGTH]
  to be depricated
- Bulk bulk
  bulk of the domain: initialized only if Run::option.restart=0
- Boundary boundaries [DIM][2]
  six boundaries of a hexahedral domain
- Collection< Molecule > molecules
  Collection of molecules.
- Pool< Molecule > * pool
  Molecule pointer pool.

13.6.1 Detailed Description

Computational Domain.

Implements main data types inside a computational domain

Definition at line 83 of file domain.h.

13.6.2 Constructor & Destructor Documentation

13.6.2.1 Domain::Domain (char * *filename*)

Domain constructor creates an instance of a domain.

get domain specs from XML configfile

read XML input file

Loop over file records

set xterm output mode:

Read the number of molecules:

Read species:

load reactions

Read domain specs:

Read domain bounds

Read initial bulk properties

Read boundary specs

Read boundary reactions:

< probability for the formation of these products as opposed to different products If only one pair of products exists the probability = 1

Definition at line 72 of file domain.cc.

References Species::Reaction::Add(), Boundary::adiabatic, List< Element >::append(), Boundary::area, Geom::area(), AtomicMassUnit, AvogadroNumber, BoltzmannConstant, boundaries, boundary(), boundaryName, bounds, bulk, GridContainer::cellsize, Run::configfile, Species::Specie::Cp(), Collection< Element >::Current(), Species::Gas::density, DIM, distribution, DOCTYPE, elasticBoundary, Species::Reaction::Outcome::Enthalpy(), Species::Reaction::First(), GasConstant, Boundary::gases, Bulk::gases, IO::getCharAttr(), Collection< Element >::goFirst(), Collection< Element >::goNext(), Species::Specie::Id(), init(), Bulk::init(), Boundary::init(), Collection< Element >::init(), insideBoundary, Collection< Element >::isFirst(), Potential::lengthscale(), load(), Species::Specie::Mass(), maxBound(), maxBoundaryTypes, MAXLINLEN, minBound(), molecules, Species::Reaction::Next(), Species::nspecies, Collection< Element >::number(), openBoundary, Run::option, IO::parseFloat(), IO::parseWord(), periodicBoundary, pool, Species::Reaction::Outcome::Probability(), Species::Reaction::Outcome::Product(), GridContainer::put(), Boundary::reactions, Species::reactions, REAL, setMaxBound(), setMinBound(), Species::Specie::Size(), Gui::size, Species::species, Potential::strength(), Boundary::temperature, Bulk::Temperature(), TINY, Boundary::type, VOIDSPECIE, WORDLENGTH, XMAX, Gui::xmax, XMIN, Gui::xmin, and Option::xterm.

13.6.2.2 Domain::~Domain ()

Definition at line 617 of file domain.cc.

References Run::option.

13.6.3 Member Function Documentation

13.6.3.1 int Domain::boundary (Molecule * *molecule*)

< do reaction: A + B =

< new molecule A type

< new molecule B type

Definition at line 1076 of file domain.cc.

References boundaries, bounds, Molecule::Coordinates(), Species::Specie::Cp(), DIM, DOF, DOFI, DOFK, Gui::dx, elasticBoundary, Species::Reaction::Outcome::Enthalpy(), Species::Reaction::First(), Collection< Element >::insertAfter(), insideBoundary, Molecule::InternalEnergy(), Molecule::KineticEnergy(), LENGTH, Species::Specie::Mass(), molecules, MULC, Species::Reaction::Next(), openBoundary, periodicBoundary, Species::Reaction::Outcome::Probability(), Species::Reaction::Outcome::Product(), Species::reacted, Boundary::reactions, REAL, RND, Species::Specie::Size(), SMALL, Species::species, Run::time, Species::Reaction::Outcome::Time(), Molecule::Type(), Boundary::type, Molecule::Velocity(), VOIDSPECIE, XMAX, and XMIN.

Referenced by Domain(), injection(), and run().

13.6.3.2 enum BoundaryTypes Domain::BoundaryType (int *idir*, int *inside*) [inline]

Definition at line 101 of file domain.h.

References boundaries, DIM, and Boundary::type.

13.6.3.3 void Domain::BoundaryType (enum BoundaryTypes *b*, int *idir*, int *inside*) [inline]

Definition at line 94 of file domain.h.

References boundaries, DIM, and Boundary::type.

13.6.3.4 int Domain::computeBounds (REAL *x0*[ ], REAL *x1*[ ])

Definition at line 829 of file domain.cc.

References Molecule::Coordinates(), Collection< Element >::Current(), DIM, Collection< Element >::goFirst(), Collection< Element >::goNext(), Collection< Element >::isFirst(), LARGE, molecules, and REAL.

13.6.3.5 void Domain::init ()

create local gas-array

Go over all gases

point to current gas

select current gas-specie

Estimate the average velocity and the number of molecules of each specie to be injected into the bulk

get molecule's mass in atomic units

convert molecule's mass to kg

average velocity in one direction

get density in kg/m^3

get the number of molecules in the bulk

Inject all molecules:

Definition at line 621 of file domain.cc.

References AtomicMassUnit, BoltzmannConstant, bulk, List< Element >::Current(), Species::Gas::density, Bulk::gases, List< Element >::goFirst(), List< Element >::goNext(), Species::Specie::Id(), Bulk::inject(), List< Element >::isFirst(), Species::Specie::Mass(), molecules, List< Element >::number(), Run::option, Species::Gas::specie, Species::species, Molecule::Temperature(), Bulk::Temperature(), and Bulk::Volume().

Referenced by Domain().

13.6.3.6 void Domain::injection ()

Inject cross-boundary species:.

Inject cross-boundary species. The algorithm uses the density and temperature to caclulate the frequency of injection of molecules of specie, s at the boundary. The injection frequency, f_s per unit area, A is

computed as

$$f_s = \frac{N}{\Delta t}$$

where Δt_s is the time interval at which a molecule hits the boundary area A, and N is the number of molecules in a volume with the base A and length Δx as shown in the figure: The time inteval, Δt, between the collisions can be related to the component of velocity of the molecule of species s, in direction x, v_{sx}, as follows:

$$\Delta t = \frac{2\Delta x}{v_{sx}}$$

The number of molecules, N can be related to density, ρ, as:

$$N = \frac{\rho}{\mu}\Delta x A$$

where μ is the mass of one molecule and $A = \Delta y \Delta z$. Thus, the frequency is:

$$f_s = \frac{\rho}{\mu}\Delta x A \frac{v_{sx}}{2\Delta x} = \frac{\rho v_{sx}}{2\mu}A$$

get time-step in sec

Go over all 6 boundaries:

select a boundary

get boundry area in m^2

get boundary temperature in K

create local gas-array

Go over all gases

point to current gas

select current gas-specie

Use kinetic theory of gases to estimate collision frequency with the wall and the number of molecules injected. This number can be fractional, so split it into integer and fractional part and inject the fractional part using probability.

get molecule's mass in atomic units

convert molecule's mass to kg

get density in kg/m^3

estimate collision frequency per unit area

calculate the number of collisions with the boundary during the past time step

get the whole integer number of molecules injected

calculate the fractional part of a molecule injected

Inject all whole molecules:

Probabilistically inject the fractional molecules:

Definition at line 1260 of file domain.cc.

References Boundary::area, Geom::area(), AtomicMassUnit, BoltzmannConstant, boundaries, boundary(), Species::Gas::density, DIM, Boundary::gases, List< Element >::goFirst(), Boundary::Inject(), Species::Specie::Mass(), molecules, REAL, RND, Species::Gas::specie, Species::species, step(), Boundary::temperature, and Run::time.

Referenced by run().

13.6.3.7 Interaction Domain::interact (Molecule * *a*, Molecule * *b*)

Computes interaction between two molecules with the exchange of energy and momentum according to hard-ball collisions, and the possibility of chemical reactions. Also estimates time to the next collision. Initializing molecules according to bulk properties (restart=0) The velocity of each molecule is set from given temperature according to:

$$\frac{3}{2}kT = \frac{mV_{av}^2}{2}$$

Since the average velocity relates to the average velocity in one direction, x, as:

$$V_{av}^2 = 3V_{x,av}^2$$

we obtain for $V_{av,x} = kT$

Definition at line 1486 of file domain.cc.

References Species::Reaction::Outcome::ActivationEnergy(), Species::annihalated, Species::collided, Molecule::Coordinates(), Species::Specie::Cp(), DIM, DOF, DOFI, DOFK, Palette::dvi, Gui::dx, Species::Reaction::Outcome::Enthalpy(), Species::Reaction::First(), Species::Specie::Id(), Molecule::InternalEnergy(), Species::Specie::Mass(), Species::missed, Species::Reaction::Next(), Species::nspecies, Species::Reaction::Outcome::Probability(), Species::Reaction::Outcome::Product(), Species::reacted, Species::reactions, REAL, RND, SCLP, Species::Specie::Size(), SMALL, Species::species, Molecule::Type(), Molecule::Velocity(), and VOIDSPECIE.

Referenced by interaction().

13.6.3.8 void Domain::interaction (int *icounter*)

DDD: dirty fix, should be as below, but did not work

DDD: end dirty fix

DDD: dirty fix, should be as below, but did not work

DDD

DDD: dirty fix: some interactions may go unaccounted

DDD

Definition at line 1383 of file domain.cc.

References Species::annihalated, Container< Element >::Current(), DIM, Gui::dx, Container< Element >::First(), Container< Element >::FirstNext(), Container< Element >::goFirst(), Container< Element >::goNext(), GridContainer::index(), interact(), Container< Element >::isFirst(), Container< Element >::isFirstLast(), Container< Element >::isLast(), Species::missed, GridContainer::ncells, Gui::nodes, Run::nthreads, Container< Element >::number(), REAL, Container< Element >::setFirst(), Container< Element >::setFirstLast(), Run::time, Molecule::Type(), VOIDSPECIE, XMAX, and XMIN.

13.6.3.9 void Domain::interaction ()

Definition at line 1306 of file domain.cc.

References Species::annihalated, Container< Element >::Current(), DIM, Gui::dx, Container< Element >::First(), Container< Element >::FirstNext(), Container< Element >::goFirst(), Container< Element >::goNext(), GridContainer::index(), interact(), Container< Element >::isFirst(), Container< Element >::isFirstLast(), Container< Element >::isLast(), Species::missed, GridContainer::ncells, Gui::nodes, Container< Element >::number(), REAL, Container< Element >::remove(), Container< Element

>::setFirst(), Container< Element >::setFirstLast(), Molecule::Type(), VOIDSPECIE, XMAX, and XMIN.

Referenced by run().

13.6.3.10 void Domain::load (char * *filename*)

Initializing molecules according to bulk properties (restart=0).

Definition at line 687 of file domain.cc.

References Collection< Element >::append(), Molecule::Coordinate(), Potential::Cutoff(), DIM, Molecule::InternalEnergy(), IO::ioutput, LARGE, Potential::lengthscale(), MAXLINLEN, molecules, Species::nspecies, Collection< Element >::number(), Run::option, REAL, Species::Specie::Size(), Gui::size, Species::species, Run::time, Molecule::Type(), Molecule::Velocity(), and WORDLENGTH.

Referenced by Domain().

13.6.3.11 REAL Domain::maxBound (int *i*) [inline]

Definition at line 111 of file domain.h.

References bounds.

Referenced by Domain(), and Gui::readconf().

13.6.3.12 REAL Domain::minBound (int *i*) [inline]

Definition at line 110 of file domain.h.

References bounds.

Referenced by Domain(), and Gui::readconf().

13.6.3.13 Collection<Molecule>* Domain::Molecules () [inline]

Definition at line 115 of file domain.h.

References molecules.

Referenced by Gui::display(), and Gui::initdisp().

13.6.3.14 int Domain::run (int *niter*)

The Domain solver: running **niter** iterations.

The main loop over niter iterations or till the end of time:

Definition at line 849 of file domain.cc.

References AtomicMassUnit, BoltzmannConstant, boundary(), GridContainer::cellsize, Species::Specie::Cp(), Collection< Element >::Current(), DIM, distribution, DOF, DOFI, ESC, Collection< Element >::goFirst(), Collection< Element >::goNext(), injection(), interaction(), Molecule::InternalEnergy(), IO::ioutput, Collection< Element >::isFirst(), Molecule::KineticEnergy(), LARGE, Collection< Element >::maxCounters(), maxcounters, Collection< Element >::maxnumber(), molecules, Molecule::Move(), GridContainer::nodes, Species::nspecies, Run::nthreads, Collection< Element >::number(), onethird, Run::option, Run::outputname, GridContainer::put(), REAL, Container<

Element >::remove(), Collection< Element >::remove0(), save(), SMALL, Species::species, step(), Run::time, twothirds, Molecule::Type(), Molecule::Velocity(), and VOIDSPECIE.

Referenced by Gui::animate(), Gui::keyboard(), main(), and Gui::runmany().

13.6.3.15 void Domain::save (char * *taskname*)

Definition at line 1935 of file domain.cc.

References Molecule::Coordinate(), Collection< Element >::Current(), Run::elapsed(), Collection< Element >::goFirst(), Collection< Element >::goNext(), Species::Specie::Id(), Molecule::InternalEnergy(), IO::ioutput, Collection< Element >::isFirst(), MAXLINLEN, molecules, Collection< Element >::number(), Run::option, Species::species, Run::time, Molecule::Type(), Molecule::Velocity(), and VOIDSPECIE.

Referenced by Gui::keyboard(), main(), and run().

13.6.3.16 void Domain::setMaxBound (int *i*, REAL *x*) [inline]

Definition at line 109 of file domain.h.

References bounds.

Referenced by Domain(), and Gui::initdisp().

13.6.3.17 void Domain::setMinBound (int *i*, REAL *x*) [inline]

Definition at line 108 of file domain.h.

References bounds.

Referenced by Domain(), and Gui::initdisp().

13.6.3.18 void Domain::step (int *iter*)

Referenced by injection(), and run().

13.6.4 Member Data Documentation

13.6.4.1 Boundary Domain::boundaries[DIM][2] [private]

six boundaries of a hexahedral domain

Definition at line 88 of file domain.h.

Referenced by boundary(), BoundaryType(), Domain(), and injection().

13.6.4.2 char Domain::boundaryName[maxBoundaryTypes][WORDLENGTH] [private]

to be depricated

Definition at line 86 of file domain.h.

Referenced by Domain().

13.6.4.3 REAL Domain::bounds[2][DIM] [private]

Definition at line 85 of file domain.h.

Referenced by boundary(), Domain(), maxBound(), minBound(), setMaxBound(), and setMinBound().

13.6.4.4 Bulk Domain::bulk [private]

bulk of the domain: initialized only if Run::option.restart=0

Definition at line 87 of file domain.h.

Referenced by Domain(), and init().

13.6.4.5 int* Domain::distribution [private]

molecule counts for all species

Definition at line 84 of file domain.h.

Referenced by Domain(), and run().

13.6.4.6 Collection<Molecule> Domain::molecules [private]

Collection of molecules.

Definition at line 89 of file domain.h.

Referenced by boundary(), computeBounds(), Domain(), init(), injection(), load(), Molecules(), run(), and save().

13.6.4.7 Pool<Molecule>* Domain::pool [private]

Molecule pointer pool.

Definition at line 90 of file domain.h.

Referenced by Domain().

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

- domain.h
- domain.cc

13.7 Gui::ElementDisp Struct Reference

`#include <gui.h>`

Public Attributes

- int lighting
- REAL rgbcolor [3]

13.7.1 Detailed Description

Definition at line 97 of file gui.h.

13.7.2 Member Data Documentation

13.7.2.1 int Gui::ElementDisp::lighting

Definition at line 99 of file gui.h.

13.7.2.2 REAL Gui::ElementDisp::rgbcolor[3]

Definition at line 101 of file gui.h.

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

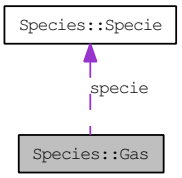
- gui.h

13.8 Species::Gas Struct Reference

Gas is a specie with some additional parameters.

`#include <species.h>`

Collaboration diagram for Species::Gas:



Public Member Functions

- Gas (Specie *s)

Public Attributes

- REAL density

  density in kg/m^3

- Specie * specie

13.8.1 Detailed Description

Gas is a specie with some additional parameters.

Definition at line 29 of file species.h.

13.8.2 Constructor & Destructor Documentation

13.8.2.1 Species::Gas::Gas (Specie * *s*) [inline]

Definition at line 32 of file species.h.

References specie.

13.8.3 Member Data Documentation

13.8.3.1 REAL Species::Gas::density

density in kg/m^3

Definition at line 30 of file species.h.

Referenced by Domain::Domain(), Domain::init(), and Domain::injection().

13.8.3.2 Specie* Species::Gas::specie

Definition at line 31 of file species.h.

Referenced by Gas(), Domain::init(), and Domain::injection().

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

- species.h

13.9 Item< Element > Struct Template Reference

`#include <collection.h>`

Collaboration diagram for Item< Element >:

Public Attributes

- Element element
- Item * next
- Item * prev

13.9.1 Detailed Description

template<class Element> struct Item< Element >

Definition at line 20 of file collection.h.

13.9.2 Member Data Documentation

13.9.2.1 template<class Element > Element Item< Element >::element

Definition at line 21 of file collection.h.

Referenced by Collection< Element >::append(), Collection< Element >::insert(), Collection< Element >::insert0(), and Collection< Element >::insertAfter().

13.9.2.2 template<class Element > Item* Item< Element >::next

Definition at line 22 of file collection.h.

Referenced by Collection< Element >::append0(), Collection< Element >::insert0(), Collection< Element >::insertAfter(), and Collection< Element >::remove0().

13.9.2.3 template<class Element > Item * Item< Element >::prev

Definition at line 22 of file collection.h.

Referenced by Collection< Element >::append0(), Collection< Element >::insert0(), and Collection< Element >::insertAfter().

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

- collection.h

13.10 List< Element > Class Template Reference

`#include <list.h>`

Public Member Functions

- List ()
- List (int n)
- ~List ()
- int number ()
- void setFirst ()
- void setFirstLast ()
- void goFirst ()
- void goFirstNext ()
- void FirstNext ()
- void FirstPrev ()
- bool isFirstLast ()
- void goLastNext ()
- void goLast ()
- void goNext ()
- void goPrev ()
- bool isFirst ()
- bool isLast ()
- void LastNext ()
- void LastPrev ()
- void go (Pointer< Element > *p)
- Element * First ()
- Element * Last ()
- Element * Next ()
- Element * getNext ()
- Element * Prev ()
- Element * getPrev ()
- Element * Current ()
- Pointer< Element > * getPointer ()
- Pointer< Element > * getFirstPointer ()
- Pointer< Element > * getLastPointer ()
- int init (int n)
- int insert (Element *element)
- int insert ()
- int append (Element *element)
- int append ()
- int link (Pointer< Element > *p)
- void unlink (Pointer< Element > *p)
- int prepend (Element *element)
- bool locate (Element *element)
- bool locate (Pointer< Element > *pointer)
- void moveAfterFirst ()
- void swapAfterFirst ()
- void moveBehindFirst ()

- int erase ()
- bool erase (Element *element)
- void eraseall ()
- bool remove ()
- void cleanup ()
- void remove (Pointer< Element > *pointer)

Private Attributes

- int nelements
- struct Pointer< Element > * first
- struct Pointer< Element > * last
- struct Pointer< Element > * current

13.10.1 Detailed Description

template<class Element> class List< Element >

Definition at line 24 of file list.h.

13.10.2 Constructor & Destructor Documentation

13.10.2.1 template<class Element > List< Element >::List () [inline]

Definition at line 80 of file list.h.

References List< Element >::current, List< Element >::first, List< Element >::last, and List< Element >::nelements.

13.10.2.2 template<class Element > List< Element >::List (int *n*)

13.10.2.3 template<class Element > List< Element >::~List () [inline]

Definition at line 90 of file list.h.

References List< Element >::cleanup().

13.10.3 Member Function Documentation

13.10.3.1 template<class Element > int List< Element >::append () [inline]

Definition at line 159 of file list.h.

References Pointer< Element >::element.

Referenced by List< Element >::init().

13.10.3.2 template<class Element > int List< Element >::append (Element * *element*) [inline]

Definition at line 136 of file list.h.

References List< Element >::current, List< Element >::first, List< Element >::last, List< Element >::nelements, and Pointer< Element >::prev.

Referenced by Domain::Domain().

13.10.3.3 template<class Element > void List< Element >::cleanup () [inline]

Definition at line 100 of file list.h.

References List< Element >::current, List< Element >::first, List< Element >::last, and List< Element >::nelements.

Referenced by List< Element >::~List().

13.10.3.4 template<class Element > Element* List< Element >::Current () [inline]

Definition at line 54 of file list.h.

Referenced by Domain::init().

13.10.3.5 template<class Element > bool List< Element >::erase (Element * *element*) [inline]

Definition at line 287 of file list.h.

References List< Element >::erase(), and List< Element >::locate().

13.10.3.6 template<class Element > int List< Element >::erase () [inline]

Definition at line 235 of file list.h.

References List< Element >::current, Pointer< Element >::element, List< Element >::first, List< Element >::last, and List< Element >::nelements.

Referenced by List< Element >::erase(), and List< Element >::eraseall().

13.10.3.7 template<class Element > void List< Element >::eraseall () [inline]

Definition at line 94 of file list.h.

References List< Element >::current, List< Element >::erase(), List< Element >::first, List< Element >::last, and List< Element >::nelements.

13.10.3.8 template<class Element > Element* List< Element >::First () [inline]

Definition at line 48 of file list.h.

13.10.3.9 template<class Element > void List< Element >::FirstNext () [inline]

Definition at line 36 of file list.h.

13.10.3.10 template<class Element > void List< Element >::FirstPrev () [inline]

Definition at line 37 of file list.h.

13.10.3.11 template<class Element > Pointer<Element>* List< Element >::getFirstPointer () [inline]

Definition at line 56 of file list.h.

13.10.3.12 template<class Element > Pointer<Element>* List< Element >::getLastPointer () [inline]

Definition at line 57 of file list.h.

13.10.3.13 template<class Element > Element* List< Element >::getNext () [inline]

Definition at line 51 of file list.h.

13.10.3.14 template<class Element > Pointer<Element>* List< Element >::getPointer () [inline]

Definition at line 55 of file list.h.

13.10.3.15 template<class Element > Element* List< Element >::getPrev () [inline]

Definition at line 53 of file list.h.

13.10.3.16 template<class Element > void List< Element >::go (Pointer< Element > * *p*) [inline]

Definition at line 47 of file list.h.

13.10.3.17 template<class Element > void List< Element >::goFirst () [inline]

Definition at line 34 of file list.h.

Referenced by Domain::init(), and Domain::injection().

13.10.3.18 template<class Element > void List< Element >::goFirstNext () [inline]

Definition at line 35 of file list.h.

13.10.3.19 template<class Element > void List< Element >::goLast () [inline]

Definition at line 40 of file list.h.

13.10.3.20 template<class Element > void List< Element >::goLastNext () [inline]

Definition at line 39 of file list.h.

13.10.3.21 template<class Element > void List< Element >::goNext () [inline]

Definition at line 41 of file list.h.

Referenced by Domain::init().

13.10.3.22 template<class Element > void List< Element >::goPrev () [inline]

Definition at line 42 of file list.h.

13.10.3.23 template<class Element > int List< Element >::init (int *n*) [inline]

Definition at line 106 of file list.h.

References List< Element >::append(), and List< Element >::nelements.

13.10.3.24 template<class Element > int List< Element >::insert () [inline]

Definition at line 209 of file list.h.

References Pointer< Element >::element.

13.10.3.25 template<class Element > int List< Element >::insert (Element * *element*) [inline]

Definition at line 186 of file list.h.

References List< Element >::current, List< Element >::first, List< Element >::last, List< Element >::nelements, and Pointer< Element >::prev.

13.10.3.26 template<class Element > bool List< Element >::isFirst () [inline]

Definition at line 43 of file list.h.

Referenced by Domain::init().

13.10.3.27 template<class Element > bool List< Element >::isFirstLast () [inline]

Definition at line 38 of file list.h.

13.10.3.28 template<class Element > bool List< Element >::isLast () [inline]

Definition at line 44 of file list.h.

13.10.3.29 template<class Element > Element* List< Element >::Last () [inline]

Definition at line 49 of file list.h.

13.10.3.30 template<class Element > void List< Element >::LastNext () [inline]

Definition at line 45 of file list.h.

13.10.3.31 template<class Element > void List< Element >::LastPrev () [inline]

Definition at line 46 of file list.h.

13.10.3.32 template<class Element > int List< Element >::link (Pointer< Element > * *p*) [inline]

Definition at line 165 of file list.h.

References List< Element >::current, List< Element >::first, List< Element >::last, List< Element >::nelements, and Pointer< Element >::prev.

13.10.3.33 template<class Element > bool List< Element >::locate (Pointer< Element > * *pointer*) [inline]

Definition at line 303 of file list.h.

References List< Element >::current, and List< Element >::first.

13.10.3.34 template<class Element > bool List< Element >::locate (Element * *element*) [inline]

Definition at line 293 of file list.h.

References List< Element >::current, and List< Element >::first.

Referenced by List< Element >::erase(), and List< Element >::remove().

13.10.3.35 template<class Element > void List< Element >::moveAfterFirst () [inline]

Definition at line 320 of file list.h.

References List< Element >::current, List< Element >::first, and Pointer< Element >::prev.

13.10.3.36 template<class Element > void List< Element >::moveBehindFirst () [inline]

Definition at line 331 of file list.h.

References List< Element >::current, List< Element >::first, and Pointer< Element >::next.

13.10.3.37 template<class Element > Element* List< Element >::Next () [inline]

Definition at line 50 of file list.h.

13.10.3.38 template<class Element > int List< Element >::number () [inline]

Definition at line 31 of file list.h.

Referenced by Domain::init().

13.10.3.39 template<class Element > int List< Element >::prepend (Element * *element*) [inline]

Definition at line 113 of file list.h.

References List< Element >::current, List< Element >::first, List< Element >::last, List< Element >::nelements, and Pointer< Element >::next.

13.10.3.40 template<class Element > Element* List< Element >::Prev () [inline]

Definition at line 52 of file list.h.

13.10.3.41 template<class Element > void List< Element >::remove (Pointer< Element > * *pointer*) [inline]

DDD: slow but safe

DDD

Definition at line 272 of file list.h.

References List< Element >::current, and List< Element >::locate().

13.10.3.42 template<class Element > bool List< Element >::remove () [inline]

Definition at line 215 of file list.h.

References List< Element >::current, List< Element >::first, List< Element >::last, and List< Element >::nelements.

13.10.3.43 template<class Element > void List< Element >::setFirst () [inline]

Definition at line 32 of file list.h.

13.10.3.44 template<class Element > void List< Element >::setFirstLast () [inline]

Definition at line 33 of file list.h.

13.10.3.45 template<class Element > void List< Element >::swapAfterFirst () [inline]

Definition at line 313 of file list.h.

References List< Element >::current, and List< Element >::first.

13.10.3.46 template<class Element > void List< Element >::unlink (Pointer< Element > * *p*) [inline]

Definition at line 257 of file list.h.

References List< Element >::current, List< Element >::first, List< Element >::last, List< Element >::nelements, Pointer< Element >::next, and Pointer< Element >::prev.

13.10.4 Member Data Documentation

13.10.4.1 template<class Element > struct Pointer< Element > * List< Element >::current [read, private]

Definition at line 26 of file list.h.

Referenced by List< Element >::append(), List< Element >::cleanup(), List< Gas >::Current(), List< Element >::erase(), List< Element >::eraseall(), List< Gas >::getNext(), List< Gas >::getPointer(), List< Gas >::getPrev(), List< Gas >::go(), List< Gas >::goFirst(), List< Gas >::goFirstNext(), List< Gas >::goLast(), List< Gas >::goLastNext(), List< Gas >::goNext(), List< Gas >::goPrev(), List< Element >::insert(), List< Gas >::isFirst(), List< Gas >::isLast(), List< Element >::link(), List< Element >::List(), List< Element >::locate(), List< Element >::moveAfterFirst(), List< Element >::moveBehindFirst(), List< Gas >::Next(), List< Element >::prepend(), List< Gas >::Prev(), List< Element >::remove(), List< Element >::swapAfterFirst(), and List< Element >::unlink().

13.10.4.2 template<class Element > struct Pointer< Element >* List< Element >::first [read, private]

Definition at line 26 of file list.h.

Referenced by List< Element >::append(), List< Element >::cleanup(), List< Element >::erase(), List< Element >::eraseall(), List< Gas >::First(), List< Gas >::FirstNext(), List< Gas >::FirstPrev(), List< Gas >::getFirstPointer(), List< Gas >::goFirst(), List< Gas >::goFirstNext(), List< Element >::insert(), List< Gas >::isFirst(), List< Gas >::isFirstLast(), List< Element >::link(), List< Element >::List(), List< Element >::locate(), List< Element >::moveAfterFirst(), List< Element >::moveBehindFirst(), List< Element >::prepend(), List< Element >::remove(), List< Gas >::setFirst(), List< Gas >::setFirstLast(), List< Element >::swapAfterFirst(), and List< Element >::unlink().

13.10.4.3 template<class Element > struct Pointer< Element > * List< Element >::last [read, private]

Definition at line 26 of file list.h.

Referenced by List< Element >::append(), List< Element >::cleanup(), List< Element >::erase(), List< Element >::eraseall(), List< Gas >::getLastPointer(), List< Gas >::goLast(), List< Gas >::goLastNext(), List< Element >::insert(), List< Gas >::isFirstLast(), List< Gas >::isLast(), List< Gas >::Last(), List< Gas >::LastNext(), List< Gas >::LastPrev(), List< Element >::link(), List< Element >::List(), List< Element >::prepend(), List< Element >::remove(), List< Gas >::setFirst(), List< Gas >::setFirstLast(), and List< Element >::unlink().

13.10.4.4 template<class Element > int List< Element >::nelements [private]

Definition at line 25 of file list.h.

Referenced by List< Element >::append(), List< Element >::cleanup(), List< Element >::erase(), List< Element >::eraseall(), List< Element >::init(), List< Element >::insert(), List< Element >::link(), List< Element >::List(), List< Gas >::number(), List< Element >::prepend(), List< Element >::remove(), and List< Element >::unlink().

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

- list.h

13.11 Molecule Class Reference

`#include <model.h>`

Public Member Functions

- Molecule ()
- void Type (int t)
- int Type ()
- void InternalEnergy (REAL e)
- REAL InternalEnergy ()
- REAL Coordinate (int i)
- void Coordinate (int i, REAL y)
- REAL * Coordinates ()
- void Coordinates (REAL y[ ])
- void setCoordinates (REAL y[ ])
- REAL Velocity (int i)
- void Velocity (int i, REAL u)
- REAL * Velocity ()
- void Velocity (REAL u[ ])
- void setVelocity (REAL u[ ])
- REAL KineticEnergy ()

  Retrieve kinetic energy.

- void Temperature (REAL temperature)

  Set internal energy according to temperature:.

- void Move ()

  Moving a molecule by one time step.

- void copy (Molecule *molecule)

Private Attributes

- int type

  points to the species[type];

- REAL energy

  internal energy

- REAL x [DIM]

  position of center of mass

- REAL v [DIM]

  velocity of center of mass

13.11.1 Detailed Description

Definition at line 23 of file model.h.

13.11.2 Constructor & Destructor Documentation

13.11.2.1 Molecule::Molecule ()

Definition at line 20 of file model.cc.

References energy, Run::time, and type.

13.11.3 Member Function Documentation

13.11.3.1 void Molecule::Coordinate (int *i*, REAL *y*) [inline]

Definition at line 103 of file model.h.

References DIM, and x.

13.11.3.2 REAL Molecule::Coordinate (int *i*) [inline]

Definition at line 95 of file model.h.

References DIM, and x.

Referenced by copy(), Bulk::inject(), Boundary::Inject(), Domain::load(), and Domain::save().

13.11.3.3 void Molecule::Coordinates (REAL *y*[ ]) [inline]

Definition at line 111 of file model.h.

References DIM, and x.

13.11.3.4 REAL* Molecule::Coordinates () [inline]

Definition at line 110 of file model.h.

References x.

Referenced by Domain::boundary(), Domain::computeBounds(), Gui::display(), Domain::interact(), and GridContainer::put().

13.11.3.5 void Molecule::copy (Molecule * *molecule*)

Definition at line 36 of file model.cc.

References Coordinate(), DIM, Type(), type, v, Velocity(), and x.

13.11.3.6 REAL Molecule::InternalEnergy () [inline]

Definition at line 86 of file model.h.

References energy.

Referenced by Temperature().

13.11.3.7 void Molecule::InternalEnergy (REAL *e*) [inline]

Definition at line 85 of file model.h.

References energy.

Referenced by Domain::boundary(), Domain::interact(), Domain::load(), Domain::run(), and Domain::save().

13.11.3.8 REAL Molecule::KineticEnergy ()

Retrieve kinetic energy.

Definition at line 46 of file model.cc.

References DIM, Species::Specie::Mass(), REAL, Species::species, type, and v.

Referenced by Domain::boundary(), and Domain::run().

13.11.3.9 void Molecule::Move ()

Moving a molecule by one time step.

Definition at line 68 of file model.cc.

References DIM, Species::Specie::Mass(), Species::nspecies, REAL, SMALL, Species::species, Run::time, type, v, and x.

Referenced by Domain::run().

13.11.3.10 void Molecule::setCoordinates (REAL *y*[ ]) [inline]

Definition at line 112 of file model.h.

References DIM, and x.

13.11.3.11 void Molecule::setVelocity (REAL *u*[ ]) [inline]

Definition at line 130 of file model.h.

References DIM, and v.

13.11.3.12 void Molecule::Temperature (REAL *temperature*)

Set internal energy according to temperature:.

Set internal energy according to the temperature.

Parameters:

temperature temperature in K

Definition at line 57 of file model.cc.

References AtomicMassUnit, BoltzmannConstant, Species::Specie::Cp(), DOF, DOFI, energy, InternalEnergy(), REAL, Species::species, and Type().

Referenced by Domain::init(), and Boundary::Inject().

13.11.3.13 int Molecule::Type () [inline]

Definition at line 50 of file model.h.

References type.

Referenced by Temperature().

13.11.3.14 void Molecule::Type (int *t*) [inline]

Definition at line 49 of file model.h.

References type.

Referenced by Domain::boundary(), copy(), Gui::display(), Bulk::inject(), Boundary::Inject(), Domain::interact(), Domain::interaction(), Domain::load(), GridContainer::put(), Domain::run(), and Domain::save().

13.11.3.15 void Molecule::Velocity (REAL *u*[ ]) [inline]

Definition at line 129 of file model.h.

References DIM, and v.

13.11.3.16 REAL* Molecule::Velocity () [inline]

Definition at line 128 of file model.h.

References v.

13.11.3.17 void Molecule::Velocity (int *i*, REAL *u*) [inline]

Definition at line 121 of file model.h.

References DIM, and v.

13.11.3.18 REAL Molecule::Velocity (int *i*) [inline]

Definition at line 113 of file model.h.

References DIM, and v.

Referenced by Domain::boundary(), copy(), Bulk::inject(), Boundary::Inject(), Domain::interact(), Domain::load(), GridContainer::put(), Domain::run(), and Domain::save().

13.11.4 Member Data Documentation

13.11.4.1 REAL Molecule::energy [private]

internal energy

Definition at line 40 of file model.h.

Referenced by InternalEnergy(), Molecule(), and Temperature().

13.11.4.2 int Molecule::type [private]

points to the species[type];

Definition at line 24 of file model.h.

Referenced by copy(), KineticEnergy(), Molecule(), Move(), and Type().

13.11.4.3 REAL Molecule::v[DIM] [private]

velocity of center of mass

Definition at line 40 of file model.h.

Referenced by copy(), KineticEnergy(), Move(), setVelocity(), and Velocity().

13.11.4.4 REAL Molecule::x[DIM] [private]

position of center of mass

Definition at line 40 of file model.h.

Referenced by Coordinate(), Coordinates(), copy(), Move(), and setCoordinates().

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

- model.h
- model.cc

13.12 Option Struct Reference

Execution options.

`#include <run.h>`

Public Attributes

- unsigned int restart:1
- unsigned int verbose:1
- unsigned int debug:1

  run in debugging mode

- unsigned int mesh:1

  used to start the mesh generator

- unsigned int tags:1

  used in the trim module to trigger tag assignement

- unsigned int xterm:1

  used in the trim module to trigger tag assignement

13.12.1 Detailed Description

Execution options.

Definition at line 3 of file run.h.

13.12.2 Member Data Documentation

13.12.2.1 unsigned int Option::debug

run in debugging mode

Definition at line 6 of file run.h.

Referenced by Run::init(), and Run::readcmdline().

13.12.2.2 unsigned int Option::mesh

used to start the mesh generator

Definition at line 7 of file run.h.

Referenced by Run::init(), and Run::readcmdline().

13.12.2.3 unsigned int Option::restart

Definition at line 4 of file run.h.

Referenced by Run::init(), and Run::readcmdline().

13.12.2.4 unsigned int Option::tags

used in the trim module to trigger tag assignement

Definition at line 8 of file run.h.

13.12.2.5 unsigned int Option::verbose

Definition at line 5 of file run.h.

Referenced by Run::init(), and Run::readcmdline().

13.12.2.6 unsigned int Option::xterm

used in the trim module to trigger tag assignement

Definition at line 9 of file run.h.

Referenced by Domain::Domain(), and Run::init().

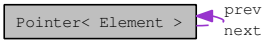
The documentation for this struct was generated from the following file:

- run.h

13.13 Pointer< Element > Struct Template Reference

`#include <list.h>`

Collaboration diagram for Pointer< Element >:



Public Attributes

- Element * element
- Pointer * next
- Pointer * prev

13.13.1 Detailed Description

template<class Element> struct Pointer< Element >

Definition at line 19 of file list.h.

13.13.2 Member Data Documentation

13.13.2.1 template<class Element > Element* Pointer< Element >::element

Definition at line 20 of file list.h.

Referenced by List< Element >::append(), List< Element >::erase(), and List< Element >::insert().

13.13.2.2 template<class Element > Pointer* Pointer< Element >::next

Definition at line 21 of file list.h.

Referenced by List< Element >::moveBehindFirst(), List< Element >::prepend(), and List< Element >::unlink().

13.13.2.3 template<class Element > Pointer * Pointer< Element >::prev

Definition at line 21 of file list.h.

Referenced by List< Element >::append(), List< Element >::insert(), List< Element >::link(), List< Element >::moveAfterFirst(), and List< Element >::unlink().

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

- list.h

13.14 Pool< Element > Struct Template Reference

`#include <collection.h>`

Public Member Functions

- Pool (int nptrs)
- ~Pool ()
- int size ()
- Ptr< Element > * get ()
- bool put (Ptr< Element > *ptr)
- bool check (char *msg)

Public Attributes

- int mptrs
- int nptrs
- Ptr< Element > * hook

13.14.1 Detailed Description

template<class Element> struct Pool< Element >

Definition at line 414 of file collection.h.

13.14.2 Constructor & Destructor Documentation

13.14.2.1 template<class Element > Pool< Element >::Pool (int *nptrs*) [inline]

Definition at line 425 of file collection.h.

References Ptr< Element >::element, Pool< Element >::hook, Pool< Element >::mptrs, Ptr< Element >::next, Pool< Element >::nptrs, Run::option, and Ptr< Element >::prev.

13.14.2.2 template<class Element > Pool< Element >::~Pool () [inline]

Definition at line 451 of file collection.h.

References Pool< Element >::hook, Pool< Element >::mptrs, and Pool< Element >::nptrs.

13.14.3 Member Function Documentation

13.14.3.1 template<class Element > bool Pool< Element >::check (char * *msg*) [inline]

DDD

DDD

DDD

DDD

DDD

DDD

DDD

DDD

Definition at line 495 of file collection.h.

References Pool< Element >::hook, Pool< Element >::mptrs, Ptr< Element >::next, and Pool< Element >::nptrs.

Referenced by Container< Element >::checkPool().

13.14.3.2 template<class Element > Ptr< Element > * Pool< Element >::get () [inline]

DDD: probably not needed, but just to be on the safe side

Definition at line 457 of file collection.h.

References Pool< Element >::hook, Ptr< Element >::next, Pool< Element >::nptrs, and Ptr< Element >::prev.

Referenced by Container< Element >::append0(), and Container< Element >::insert0().

13.14.3.3 template<class Element > bool Pool< Element >::put (Ptr< Element > * *ptr*) [inline]

Definition at line 471 of file collection.h.

References Pool< Element >::hook, Pool< Element >::mptrs, Ptr< Element >::next, Pool< Element >::nptrs, and Ptr< Element >::prev.

Referenced by Container< Element >::remove0().

13.14.3.4 template<class Element > int Pool< Element >::size () [inline]

Definition at line 419 of file collection.h.

13.14.4 Member Data Documentation

13.14.4.1 template<class Element > Ptr<Element>* Pool< Element >::hook

Definition at line 416 of file collection.h.

Referenced by Pool< Element >::check(), Container< Element >::checkPool(), Pool< Element >::get(), Pool< Element >::Pool(), Pool< Element >::put(), and Pool< Element >::~Pool().

13.14.4.2 template<class Element > int Pool< Element >::mptrs

Definition at line 415 of file collection.h.

Referenced by Pool< Element >::check(), Pool< Element >::Pool(), Pool< Element >::put(), and Pool< Element >::~Pool().

13.14.4.3 template<class Element > int Pool< Element >::nptrs

Definition at line 415 of file collection.h.

Referenced by Pool< Element >::check(), Pool< Element >::get(), Pool< Element >::Pool(), Pool< Element >::put(), Pool< Molecule >::size(), and Pool< Element >::~Pool().

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

- collection.h

13.15 Ptr< Element > Struct Template Reference

`#include <collection.h>`

Collaboration diagram for Ptr< Element >:

Public Attributes

- Element * element
- Ptr * next
- Ptr * prev

13.15.1 Detailed Description

template<class Element> struct Ptr< Element >

Definition at line 409 of file collection.h.

13.15.2 Member Data Documentation

13.15.2.1 template<class Element > Element* Ptr< Element >::element

Definition at line 410 of file collection.h.

Referenced by Pool< Element >::Pool().

13.15.2.2 template<class Element > Ptr* Ptr< Element >::next

Definition at line 411 of file collection.h.

Referenced by Pool< Element >::check(), Pool< Element >::get(), Container< Element >::insert0(), Container< Element >::link0(), Pool< Element >::Pool(), Pool< Element >::put(), and Container< Element >::unlink0().

13.15.2.3 template<class Element > Ptr * Ptr< Element >::prev

Definition at line 411 of file collection.h.

Referenced by Container< Element >::append0(), Pool< Element >::get(), Container< Element >::insert0(), Container< Element >::link0(), Pool< Element >::Pool(), Pool< Element >::put(), and Container< Element >::unlink0().

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

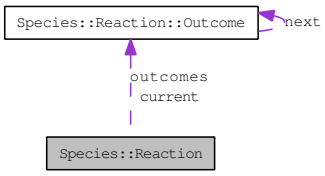
- collection.h

13.16 Species::Reaction Struct Reference

Reaction determines the two products only.

`#include <species.h>`

Collaboration diagram for Species::Reaction:



Classes

- struct Outcome

  Possible outcomes of a reaction.

Public Member Functions

- Reaction ()
- ~Reaction ()
- void Erase (Outcome *outcome)
- void Add (int ip0, int ip1, REAL a, REAL p, REAL h)
- Outcome * First ()
- Outcome * Next ()

Public Attributes

- struct Species::Reaction::Outcome * outcomes

  Possible outcomes of a reaction.

- struct Species::Reaction::Outcome * current

  all outcomes, and the current outcome

13.16.1 Detailed Description

Reaction determines the two products only.

Definition at line 35 of file species.h.

13.16.2 Constructor & Destructor Documentation

13.16.2.1 Species::Reaction::Reaction () `[inline]`

Definition at line 126 of file species.h.

References current, and outcomes.

13.16.2.2 Species::Reaction::∼Reaction () [inline]

Definition at line 127 of file species.h.

References Erase(), and outcomes.

13.16.3 Member Function Documentation

13.16.3.1 void Species::Reaction::Add (int *ip0*, int *ip1*, REAL *a*, REAL *p*, REAL *h*) [inline]

Add reaction products, probability, and enthalpy:

Definition at line 135 of file species.h.

References Species::Reaction::Outcome::next, and outcomes.

Referenced by Domain::Domain().

13.16.3.2 void Species::Reaction::Erase (Outcome ∗ *outcome*) [inline]

Definition at line 131 of file species.h.

References Species::Reaction::Outcome::next.

Referenced by ∼Reaction().

13.16.3.3 Outcome∗ Species::Reaction::First () [inline]

Definition at line 157 of file species.h.

References current, and outcomes.

Referenced by Domain::boundary(), Domain::Domain(), and Domain::interact().

13.16.3.4 Outcome∗ Species::Reaction::Next () [inline]

Definition at line 158 of file species.h.

References current, Species::Reaction::Outcome::next, and outcomes.

Referenced by Domain::boundary(), Domain::Domain(), and Domain::interact().

13.16.4 Member Data Documentation

13.16.4.1 struct Species::Reaction::Outcome∗ Species::Reaction::current

all outcomes, and the current outcome

Referenced by First(), Next(), and Reaction().

13.16.4.2 struct Species::Reaction::Outcome * Species::Reaction::outcomes

Possible outcomes of a reaction.

Referenced by Add(), First(), Next(), Reaction(), and ~Reaction().

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

- species.h

13.17 Species::Reaction::Outcome Struct Reference

Possible outcomes of a reaction.

`#include <species.h>`

Collaboration diagram for Species::Reaction::Outcome:

Public Member Functions

- Outcome ()
- Outcome (int ip0, int ip1, REAL a, REAL p, REAL h)
- void Products (int ip0, int ip1)
- int Product (int i)
- void Time (REAL t)
- REAL Time ()
- void ActivationEnergy (REAL a)
- REAL ActivationEnergy ()
- void Probability (REAL r)
- REAL Probability ()
- void Enthalpy (REAL h)
- REAL Enthalpy ()

Public Attributes

- int product [2]

  two indexes of the products of a reaction

- REAL activationEnergy
- REAL probability
- REAL enthalpy
- REAL time
- Outcome * next

  linked list of outcomes

13.17.1 Detailed Description

Possible outcomes of a reaction.

Definition at line 37 of file species.h.

13.17.2 Constructor & Destructor Documentation

13.17.2.1 Species::Reaction::Outcome::Outcome () [inline]

Definition at line 44 of file species.h.

References enthalpy, next, probability, product, time, and VOIDSPECIE.

13.17.2.2 Species::Reaction::Outcome::Outcome (int *ip0*, int *ip1*, REAL *a*, REAL *p*, REAL *h*) [inline]

Parameters:

ip0 index of the first reaction product

ip1 index of the second reaction product

a activation energy

p outcome probability

h enthalpy of reaction

Definition at line 49 of file species.h.

References activationEnergy, enthalpy, next, Species::nspecies, probability, product, and time.

13.17.3 Member Function Documentation

13.17.3.1 REAL Species::Reaction::Outcome::ActivationEnergy () [inline]

Definition at line 120 of file species.h.

References activationEnergy.

13.17.3.2 void Species::Reaction::Outcome::ActivationEnergy (REAL *a*) [inline]

Definition at line 119 of file species.h.

References activationEnergy.

Referenced by Domain::interact().

13.17.3.3 REAL Species::Reaction::Outcome::Enthalpy () [inline]

Definition at line 124 of file species.h.

References enthalpy.

13.17.3.4 void Species::Reaction::Outcome::Enthalpy (REAL *h*) [inline]

Definition at line 123 of file species.h.

References enthalpy.

Referenced by Domain::boundary(), Domain::Domain(), and Domain::interact().

13.17.3.5 REAL Species::Reaction::Outcome::Probability () [inline]

Definition at line 122 of file species.h.

References probability.

13.17.3.6 void Species::Reaction::Outcome::Probability (REAL *r*) [inline]

Definition at line 121 of file species.h.

References probability.

Referenced by Domain::boundary(), Domain::Domain(), and Domain::interact().

13.17.3.7 int Species::Reaction::Outcome::Product (int *i*) [inline]

Definition at line 110 of file species.h.

References product.

Referenced by Domain::boundary(), Domain::Domain(), and Domain::interact().

13.17.3.8 void Species::Reaction::Outcome::Products (int *ip0*, int *ip1*) [inline]

Definition at line 98 of file species.h.

References product.

13.17.3.9 REAL Species::Reaction::Outcome::Time () [inline]

Definition at line 118 of file species.h.

References time.

13.17.3.10 void Species::Reaction::Outcome::Time (REAL *t*) [inline]

Definition at line 117 of file species.h.

References time.

Referenced by Domain::boundary().

13.17.4 Member Data Documentation

13.17.4.1 REAL Species::Reaction::Outcome::activationEnergy

Definition at line 39 of file species.h.

Referenced by ActivationEnergy(), and Outcome().

13.17.4.2 REAL Species::Reaction::Outcome::enthalpy

Definition at line 39 of file species.h.

Referenced by Enthalpy(), and Outcome().

13.17.4.3 Outcome* Species::Reaction::Outcome::next

linked list of outcomes

Definition at line 43 of file species.h.

Referenced by Species::Reaction::Add(), Species::Reaction::Erase(), Species::Reaction::Next(), and Outcome().

13.17.4.4 REAL Species::Reaction::Outcome::probability

Definition at line 39 of file species.h.

Referenced by Outcome(), and Probability().

13.17.4.5 int Species::Reaction::Outcome::product[2]

two indexes of the products of a reaction

Definition at line 38 of file species.h.

Referenced by Outcome(), Product(), and Products().

13.17.4.6 REAL Species::Reaction::Outcome::time

time of reaction: used primarily for surface reactions, where there is a time delay between species adsorption on the surface and product formation.

Definition at line 39 of file species.h.

Referenced by Outcome(), and Time().

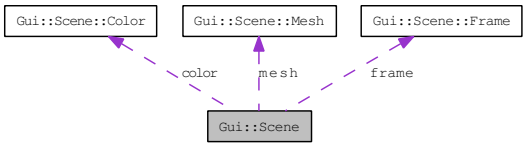
The documentation for this struct was generated from the following file:

- species.h

13.18 Gui::Scene Struct Reference

`#include <gui.h>`

Collaboration diagram for Gui::Scene:



Classes

- struct Color
- struct Frame
- struct Mesh

Public Attributes

- struct Gui::Scene::Color color
- struct Gui::Scene::Mesh mesh
- struct Gui::Scene::Frame frame

13.18.1 Detailed Description

Definition at line 107 of file gui.h.

13.18.2 Member Data Documentation

13.18.2.1 struct Gui::Scene::Color Gui::Scene::color

Referenced by Gui::display(), Gui::init(), Gui::readconf(), and Gui::switchColorScheme().

13.18.2.2 struct Gui::Scene::Frame Gui::Scene::frame

Referenced by Gui::display(), Gui::initdisp(), and Gui::readconf().

13.18.2.3 struct Gui::Scene::Mesh Gui::Scene::mesh

Referenced by Gui::display(), Gui::initdisp(), and Gui::readconf().

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

- gui.h

13.19 Gui::Scene::Color Struct Reference

`#include <gui.h>`

Public Attributes

- ColorSchemes scheme
- REAL minvalue
- REAL maxvalue

13.19.1 Detailed Description

Definition at line 108 of file gui.h.

13.19.2 Member Data Documentation

13.19.2.1 REAL Gui::Scene::Color::maxvalue

Definition at line 110 of file gui.h.

Referenced by Gui::display(), and Gui::readconf().

13.19.2.2 REAL Gui::Scene::Color::minvalue

Definition at line 110 of file gui.h.

Referenced by Gui::display(), and Gui::readconf().

13.19.2.3 ColorSchemes Gui::Scene::Color::scheme

Definition at line 109 of file gui.h.

Referenced by Gui::display(), Gui::init(), Gui::readconf(), and Gui::switchColorScheme().

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

- gui.h

13.20 Gui::Scene::Frame Struct Reference

`#include <gui.h>`

Public Attributes

- REAL line [maxlineprm]

13.20.1 Detailed Description

Definition at line 117 of file gui.h.

13.20.2 Member Data Documentation

13.20.2.1 REAL Gui::Scene::Frame::line[maxlineprm]

Definition at line 119 of file gui.h.

Referenced by Gui::display(), Gui::initdisp(), and Gui::readconf().

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

- gui.h

13.21 Gui::Scene::Mesh Struct Reference

`#include <gui.h>`

Public Attributes

- REAL node [maxpointprm]
- REAL line [maxlineprm]

13.21.1 Detailed Description

Definition at line 112 of file gui.h.

13.21.2 Member Data Documentation

13.21.2.1 REAL Gui::Scene::Mesh::line[maxlineprm]

Definition at line 114 of file gui.h.

Referenced by Gui::initdisp(), and Gui::readconf().

13.21.2.2 REAL Gui::Scene::Mesh::node[maxpointprm]

Definition at line 114 of file gui.h.

Referenced by Gui::display(), Gui::initdisp(), and Gui::readconf().

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

- gui.h

13.22 Species::Specie Class Reference

`#include <species.h>`

Public Member Functions

- Specie ()
- void Cp (REAL c)
- REAL Cp ()
- char * Id ()
- void Mass (REAL m)
- REAL Mass ()
- REAL Size ()
- void Size (REAL s)

Private Attributes

- char id [WORDLENGTH]
- REAL mass
- REAL size
- REAL cp
- REAL inertia [DIM]

13.22.1 Detailed Description

Definition at line 6 of file species.h.

13.22.2 Constructor & Destructor Documentation

13.22.2.1 Species::Specie::Specie () `[inline]`

Definition at line 13 of file species.h.

References cp, DIM, inertia, mass, and size.

13.22.3 Member Function Documentation

13.22.3.1 REAL Species::Specie::Cp () `[inline]`

Definition at line 21 of file species.h.

References cp.

13.22.3.2 void Species::Specie::Cp (REAL *c*) `[inline]`

Definition at line 20 of file species.h.

References cp.

Referenced by Domain::boundary(), Domain::Domain(), Domain::interact(), Domain::run(), and Molecule::Temperature().

13.22.3.3 char* Species::Specie::Id () [inline]

Definition at line 22 of file species.h.

References id.

Referenced by Domain::Domain(), Domain::init(), Domain::interact(), and Domain::save().

13.22.3.4 REAL Species::Specie::Mass () [inline]

Definition at line 24 of file species.h.

References mass.

13.22.3.5 void Species::Specie::Mass (REAL *m*) [inline]

Definition at line 23 of file species.h.

References mass.

Referenced by Domain::boundary(), Gui::display(), Domain::Domain(), Domain::init(), Domain::injection(), Domain::interact(), Molecule::KineticEnergy(), and Molecule::Move().

13.22.3.6 void Species::Specie::Size (REAL *s*) [inline]

Definition at line 26 of file species.h.

References size.

13.22.3.7 REAL Species::Specie::Size () [inline]

Definition at line 25 of file species.h.

References size.

Referenced by Domain::boundary(), Gui::display(), Domain::Domain(), Bulk::inject(), Boundary::Inject(), Domain::interact(), and Domain::load().

13.22.4 Member Data Documentation

13.22.4.1 REAL Species::Specie::cp [private]

Definition at line 8 of file species.h.

Referenced by Cp(), and Specie().

13.22.4.2 char Species::Specie::id[WORDLENGTH] [private]

Definition at line 7 of file species.h.

Referenced by Id().

13.22.4.3 REAL Species::Specie::inertia[DIM] [private]

Definition at line 8 of file species.h.

Referenced by Specie().

13.22.4.4 REAL Species::Specie::mass [private]

Definition at line 8 of file species.h.

Referenced by Mass(), and Specie().

13.22.4.5 REAL Species::Specie::size [private]

Definition at line 8 of file species.h.

Referenced by Size(), and Specie().

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

- species.h

13.23 State Union Reference

`#include <model.h>`

Public Attributes

- unsigned int locked: 1
- unsigned int done: 1

13.23.1 Detailed Description

Definition at line 16 of file model.h.

13.23.2 Member Data Documentation

13.23.2.1 unsigned int State::done

Definition at line 21 of file model.h.

13.23.2.2 unsigned int State::locked

Definition at line 20 of file model.h.

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

- model.h

13.24 Run::Time Struct Reference

Execution time-control structure.

`#include <run.h>`

Public Attributes

- double start
  start-time
- double end
  end-time
- double prev
  previous time
- double current
  current time
- double step
  time-step
- double nextstep
  next time-step
- double step0
  previous time-step
- double output
  data dump time inteval

13.24.1 Detailed Description

Execution time-control structure.

Definition at line 25 of file run.h.

13.24.2 Member Data Documentation

13.24.2.1 double Run::Time::current

current time

Definition at line 27 of file run.h.

13.24.2.2 double Run::Time::end

end-time

Definition at line 27 of file run.h.

13.24.2.3 double Run::Time::nextstep

next time-step

Definition at line 27 of file run.h.

13.24.2.4 double Run::Time::output

data dump time inteval

Definition at line 27 of file run.h.

13.24.2.5 double Run::Time::prev

previous time

Definition at line 27 of file run.h.

13.24.2.6 double Run::Time::start

start-time

Definition at line 27 of file run.h.

13.24.2.7 double Run::Time::step

time-step

Definition at line 27 of file run.h.

13.24.2.8 double Run::Time::step0

previous time-step

Definition at line 27 of file run.h.

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

- run.h

13.25 Gui::WindowGeom Struct Reference

`#include <gui.h>`

Public Attributes

- int width
- int height

13.25.1 Detailed Description

Definition at line 169 of file gui.h.

13.25.2 Member Data Documentation

13.25.2.1 int Gui::WindowGeom::height

Definition at line 172 of file gui.h.

Referenced by Gui::init(), and Gui::initdisp().

13.25.2.2 int Gui::WindowGeom::width

Definition at line 172 of file gui.h.

Referenced by Gui::init(), and Gui::initdisp().

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

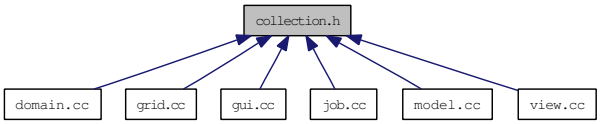
- gui.h

Chapter 14

File Documentation

14.1 collection.h File Reference

This graph shows which files directly or indirectly include this file:



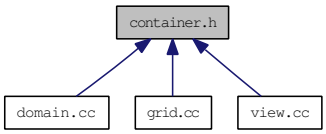
Classes

- struct Item< Element >
- class Collection< Element >
- struct Ptr< Element >
- struct Pool< Element >
- class Container< Element >

14.2 configfile.dox File Reference

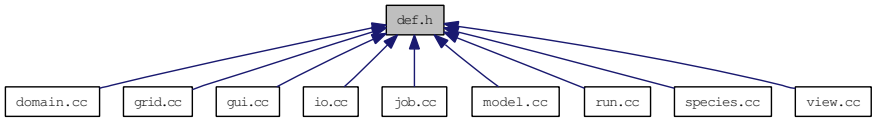
14.3 container.h File Reference

This graph shows which files directly or indirectly include this file:



14.4 def.h File Reference

This graph shows which files directly or indirectly include this file:



Defines

- #define ABOUT "MOLECULAR DYNAMICS SIMULATOR BY A.V.SMIRNOV\nandrei.v.smirnov@gmail.com\n"
- #define DOCTYPE "remody"
- #define REAL double
- #define TINY 1e-10
- #define SMALL 1e-30
- #define LARGE 1e30
- #define MAXLINLEN 510
- #define WORDLENGTH 64
- #define ESC 0x1B
- #define PI 3.14159265358979323846
- #define SQRTPIo8 0.62666
- #define ERROR(message) { fprintf(stderr,"\nERROR: %s\n",message);exit(1);}
- #define TRUE 1
- #define FALSE 0
- #define OMP
- #define WAIT for(int i=0;i<999999&&locked;i++)
- #define LOCAL
- #define COLLISIONTIME
- #define RND (REAL)((double)rand()/RAND_MAX)
- #define MAX(a, b) ((a)>(b)?a:b)
- #define ZERO(n, x) for (int i=0; i<(n); i++)x[i]=0.0
- #define ADD(n, x, y) for (int i=0; i<(n); i++) (x)[i] += (y)[i]
- #define SUB(n, x, y) for (int i=0; i<(n); i++) (x)[i] -= (y)[i]
- #define ADDC(n, x, y, d) for (int i=0; i<(n); i++) (x)[i] += (y)[i]*(d)
- #define SUBC(n, x, y, d) for (int i=0; i<(n); i++) (x)[i] -= (y)[i]*(d)
- #define MUL(n, x, y) for (int i=0; i<(n); i++) (x)[i] *= (y)[i]
- #define MULC(n, x, c) for (int i=0; i<(n); i++) (x)[i] *= (c)
- #define DIV(n, x, y) for (int i=0; i<(n); i++) (x)[i] /= (y)[i]
- #define MULVEC(x, s) for (int i=0; i<DIM; i++) (x)[i] *= (s)
- #define ADDVEC(x, y) for (int i=0; i<DIM; i++) (x)[i] += (y)[i]
- #define COPYVEC(x, y) for (int i=0; i<DIM; i++) (x)[i] = (y)[i]
- #define ZEROVEC(x) for (int i=0; i<DIM; i++) (x)[i] = 0.
- #define SCLP(A, B) (A[0]*B[0]+A[1]*B[1]+A[2]*B[2])
- #define VECP(A, B, C)
- #define LENGTH(A) sqrt(SCLP(A,A))
- #define VOIDSPECIE nspecies
- #define GAUSS Run::gauss()

- #define DIM 3
- #define BoltzmannConstant 1.38066e-23
- #define AtomicMassUnit 1.66053886e-27
- #define AvogadroNumber 6.02214179e23

  Avogadro Number in 1/mol.

- #define DOFK 3
- #define DOF(cp) MAX(2.0∗((cp)∗GasConstantInv-1.0),DOFK)
- #define DOFI(dof) (dof-DOFK)

Variables

- const int maxcounters = 4
- const REAL onethird = 1.0/3.0
- const REAL twothirds = 2.0/3.0
- const REAL Sqrt2 = sqrt(2.0)
- const REAL Sqrt2Over2 = 0.5∗Sqrt2
- const REAL sqrt1p5 = sqrt(1.5)
- const REAL sqrt1p25 = sqrt(1.25)
- const REAL Sqrt3 = sqrt(3.0)
- const REAL OneOverSqrt2 = 1.0/Sqrt2
- const REAL OneOverSqrt3 = 1.0/Sqrt3
- const REAL Sqrt3Over2 = 0.5∗Sqrt3
- const REAL GasConstant = BoltzmannConstant∗AvogadroNumber
- const REAL GasConstantInv = 1.0/GasConstant

14.4.1 Define Documentation

14.4.1.1 #define ABOUT "MOLECULAR DYNAMICS SIMULATOR BY A.V.SMIRNOV\nandrei.v.smirnov@gmail.com\n"

Definition at line 1 of file def.h.

Referenced by Gui::menu().

14.4.1.2 #define ADD(n, x, y) for (int i=0; i<(n); i++) (x)[i] += (y)[i]

Definition at line 46 of file def.h.

14.4.1.3 #define ADDC(n, x, y, d) for (int i=0; i<(n); i++) (x)[i] += (y)[i]∗(d)

Definition at line 48 of file def.h.

14.4.1.4 #define ADDVEC(x, y) for (int i=0; i<DIM; i++) (x)[i] += (y)[i]

Definition at line 54 of file def.h.

14.4.1.5 #define AtomicMassUnit 1.66053886e-27

Definition at line 68 of file def.h.

Referenced by Domain::Domain(), Domain::init(), Domain::injection(), Domain::run(), and Molecule::Temperature().

14.4.1.6 #define AvogadroNumber 6.02214179e23

Avogadro Number in 1/mol.

Definition at line 69 of file def.h.

Referenced by Domain::Domain().

14.4.1.7 #define BoltzmannConstant 1.38066e-23

Definition at line 67 of file def.h.

Referenced by Domain::Domain(), Domain::init(), Domain::injection(), Domain::run(), and Molecule::Temperature().

14.4.1.8 #define COLLISIONTIME

Definition at line 38 of file def.h.

14.4.1.9 #define COPYVEC(x, y) for (int i=0; i<DIM; i++) (x)[i] = (y)[i]

Definition at line 55 of file def.h.

14.4.1.10 #define DIM 3

Definition at line 66 of file def.h.

Referenced by Geom::area(), Domain::boundary(), Domain::BoundaryType(), Domain::computeBounds(), Molecule::Coordinate(), Molecule::Coordinates(), Molecule::copy(), Geom::distance(), Geom::distvec(), Domain::Domain(), GridContainer::index(), GridContainer::init(), Bulk::init(), Gui::initdisp(), Bulk::inject(), Boundary::Inject(), Domain::injection(), Domain::interact(), Domain::interaction(), Molecule::KineticEnergy(), Geom::length(), Domain::load(), Molecule::Move(), Geom::normalize(), GridContainer::put(), Gui::readconf(), Domain::run(), Geom::sclp(), Molecule::setCoordinates(), Molecule::setVelocity(), Species::Specie::Specie(), and Molecule::Velocity().

14.4.1.11 #define DIV(n, x, y) for (int i=0; i<(n); i++) (x)[i] /= (y)[i]

Definition at line 52 of file def.h.

14.4.1.12 #define DOCTYPE "remody"

Definition at line 3 of file def.h.

Referenced by Domain::Domain(), IO::getIter(), IO::getTimeXML(), and Gui::readconf().

14.4.1.13 #define DOF(cp) MAX(2.0∗((cp)∗GasConstantInv-1.0),DOFK)

Definition at line 77 of file def.h.

Referenced by Domain::boundary(), Domain::interact(), Domain::run(), and Molecule::Temperature().

14.4.1.14 #define DOFI(dof) (dof-DOFK)

Definition at line 78 of file def.h.

Referenced by Domain::boundary(), Domain::interact(), Domain::run(), and Molecule::Temperature().

14.4.1.15 #define DOFK 3

Definition at line 75 of file def.h.

Referenced by Domain::boundary(), and Domain::interact().

14.4.1.16 #define ERROR(message) { fprintf(stderr,"\nERROR: %s\n",message);exit(1);}

Definition at line 13 of file def.h.

Referenced by Gui::init().

14.4.1.17 #define ESC 0x1B

Definition at line 10 of file def.h.

Referenced by Gui::animate(), Gui::keyboard(), main(), and Domain::run().

14.4.1.18 #define FALSE 0

Definition at line 16 of file def.h.

14.4.1.19 #define GAUSS Run::gauss()

Definition at line 63 of file def.h.

Referenced by Bulk::inject(), and Boundary::Inject().

14.4.1.20 #define LARGE 1e30

Definition at line 7 of file def.h.

Referenced by Domain::computeBounds(), Gui::initdisp(), Domain::load(), and Domain::run().

14.4.1.21 #define LENGTH(A) sqrt(SCLP(A,A))

Definition at line 61 of file def.h.

Referenced by Geom::area(), and Domain::boundary().

14.4.1.22 #define LOCAL

Definition at line 37 of file def.h.

14.4.1.23 #define MAX(a, b) ((a)>(b)?a:b)

Definition at line 42 of file def.h.

14.4.1.24 #define MAXLINLEN 510

Definition at line 8 of file def.h.

Referenced by Gui::commandMode(), Gui::consoleMenu(), Domain::Domain(), Gui::Exit(), IO::getCharAttr(), IO::getIntAttr(), IO::getIter(), IO::getTimeXML(), Gui::keyboard(), Domain::load(), IO::parseWord(), Gui::Quit(), Gui::readconf(), Domain::save(), and IO::xwd().

14.4.1.25 #define MUL(n, x, y) for (int i=0; i<(n); i++) (x)[i] *= (y)[i]

Definition at line 50 of file def.h.

14.4.1.26 #define MULC(n, x, c) for (int i=0; i<(n); i++) (x)[i] *= (c)

Definition at line 51 of file def.h.

Referenced by Domain::boundary().

14.4.1.27 #define MULVEC(x, s) for (int i=0; i<DIM; i++) (x)[i] *= (s)

Definition at line 53 of file def.h.

14.4.1.28 #define OMP

Definition at line 19 of file def.h.

14.4.1.29 #define PI 3.14159265358979323846

Definition at line 11 of file def.h.

Referenced by Gui::showParticle(), and Gui::showSphere().

14.4.1.30 #define REAL double

Definition at line 4 of file def.h.

Referenced by Geom::area(), Domain::boundary(), Domain::computeBounds(), Gui::display(), Geom::distance(), Domain::Domain(), Run::gauss(), GridContainer::init(), Gui::initdisp(), Bulk::inject(), Boundary::Inject(), Domain::injection(), Domain::interact(), Domain::interaction(), Molecule::KineticEnergy(), Geom::length(), Domain::load(), Gui::motion(), Molecule::Move(), Geom::normalize(), IO::parseFloat(), Palette::pickcolor(), GridContainer::put(), Gui::readconf(),

Run::rnd(), Domain::run(), Geom::sclp(), Gui::showParticle(), Gui::showSphere(), Molecule::Temperature(), Run::testrnd(), and Potential::value().

14.4.1.31 #define RND (REAL)((double)rand()/RAND_MAX)

Definition at line 40 of file def.h.

Referenced by Domain::boundary(), Bulk::inject(), Boundary::Inject(), Domain::injection(), and Domain::interact().

14.4.1.32 #define SCLP(A, B) (A[0]*B[0]+A[1]*B[1]+A[2]*B[2])

Definition at line 57 of file def.h.

Referenced by Domain::interact().

14.4.1.33 #define SMALL 1e-30

Definition at line 6 of file def.h.

Referenced by Domain::boundary(), Bulk::inject(), Boundary::Inject(), Domain::interact(), Molecule::Move(), and Domain::run().

14.4.1.34 #define SQRTPIo8 0.62666

Definition at line 12 of file def.h.

14.4.1.35 #define SUB(n, x, y) for (int i=0; i<(n); i++) (x)[i] -= (y)[i]

Definition at line 47 of file def.h.

14.4.1.36 #define SUBC(n, x, y, d) for (int i=0; i<(n); i++) (x)[i] -= (y)[i]*(d)

Definition at line 49 of file def.h.

14.4.1.37 #define TINY 1e-10

Definition at line 5 of file def.h.

Referenced by Domain::Domain().

14.4.1.38 #define TRUE 1

Definition at line 15 of file def.h.

14.4.1.39 #define VECP(A, B, C)

Value:

```
A[0]=B[1]*C[2]-B[2]*C[1];\
                                                    A[1]=B[2]*C[0]-B[0]*C[2];\
                                                    A[2]=B[0]*C[1]-B[1]*C[0];
```

Definition at line 58 of file def.h.

Referenced by Geom::area().

14.4.1.40 #define VOIDSPECIE nspecies

Definition at line 62 of file def.h.

Referenced by Domain::boundary(), Domain::Domain(), Domain::interact(), Domain::interaction(), Species::Reaction::Outcome::Outcome(), GridContainer::put(), Domain::run(), and Domain::save().

14.4.1.41 #define WAIT for(int i=0;i<999999&&locked;i++)

Definition at line 20 of file def.h.

Referenced by Container< Element >::append(), Collection< Element >::append(), Container< Element >::append1(), Container< Element >::insert(), Collection< Element >::insert(), Container< Element >::insert1(), Container< Element >::link(), Container< Element >::remove(), Collection< Element >::remove(), and Container< Element >::unlink().

14.4.1.42 #define WORDLENGTH 64

Definition at line 9 of file def.h.

Referenced by Domain::Domain(), Domain::load(), and main().

14.4.1.43 #define ZERO(n, x) for (int i=0; i<(n); i++)x[i]=0.0

Definition at line 44 of file def.h.

14.4.1.44 #define ZEROVEC(x) for (int i=0; i<DIM; i++) (x)[i] = 0.

Definition at line 56 of file def.h.

14.4.2 Variable Documentation

14.4.2.1 const REAL GasConstant = BoltzmannConstant*AvogadroNumber

Definition at line 72 of file def.h.

Referenced by Domain::Domain().

14.4.2.2 const REAL GasConstantInv = 1.0/GasConstant

Definition at line 73 of file def.h.

14.4.2.3 const int maxcounters = 4

Definition at line 21 of file def.h.

Referenced by Container< Element >::append(), Collection< Element >::append(), Container< Element >::append0(), Collection< Element >::append0(), Collection< Element >::Collection(), Container< Element >::Container(), Container< Element >::goFirst(), Collection< Molecule >::goFirst(), Collection< Element >::init(), Container< Element >::insert(), Collection< Element >::insert(), Container< Element >::insert0(), Collection< Element >::insert0(), Container< Element >::insert1(), Collection< Element >::insertAfter(), Container< Element >::link(), Container< Element >::link0(), Collection< Molecule >::maxCounters(), Container< Element >::remove(), Collection< Element >::remove(), Container< Element >::remove0(), Collection< Element >::remove0(), Domain::run(), Container< Element >::unlink(), Container< Element >::unlink0(), Collection< Element >::∼Collection(), and Container< Element >::∼Container().

14.4.2.4 const REAL OneOverSqrt2 = 1.0/Sqrt2

Definition at line 32 of file def.h.

14.4.2.5 const REAL OneOverSqrt3 = 1.0/Sqrt3

Definition at line 33 of file def.h.

14.4.2.6 const REAL onethird = 1.0/3.0

Definition at line 25 of file def.h.

Referenced by Domain::run().

14.4.2.7 const REAL sqrt1p25 = sqrt(1.25)

Definition at line 30 of file def.h.

14.4.2.8 const REAL sqrt1p5 = sqrt(1.5)

Definition at line 29 of file def.h.

14.4.2.9 const REAL Sqrt2 = sqrt(2.0)

Definition at line 27 of file def.h.

14.4.2.10 const REAL Sqrt2Over2 = 0.5∗Sqrt2

Definition at line 28 of file def.h.

14.4.2.11 const REAL Sqrt3 = sqrt(3.0)

Definition at line 31 of file def.h.

14.4.2.12 const REAL Sqrt3Over2 = 0.5*Sqrt3

Definition at line 34 of file def.h.

14.4.2.13 const REAL twothirds = 2.0/3.0

Definition at line 26 of file def.h.

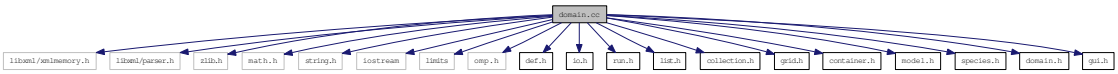
Referenced by Domain::run().

14.5 domain.cc File Reference

Implementation of Domain and Boundary classes.

```
#include <libxml/xmlmemory.h>
#include <libxml/parser.h>
#include <zlib.h>
#include <math.h>
#include <string.h>
#include <iostream>
#include <limits>
#include <omp.h>
#include "def.h"
#include "io.h"
#include "run.h"
#include "list.h"
#include "collection.h"
#include "grid.h"
#include "container.h"
#include "model.h"
#include "species.h"
#include "domain.h"
#include "gui.h"
```

Include dependency graph for domain.cc:



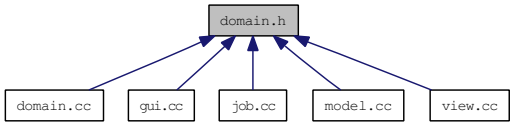
14.5.1 Detailed Description

Implementation of Domain and Boundary classes.

Definition in file domain.cc.

14.6 domain.h File Reference

This graph shows which files directly or indirectly include this file:



Classes

- class Boundary

  Domain Boundary Definition.

- class Bulk

  Domain Bulk Properties.

- class Domain

  Computational Domain.

Defines

- #define XMIN bounds[0]
- #define XMAX bounds[1]

Enumerations

- enum BoundaryTypes {
  insideBoundary = 0, periodicBoundary, elasticBoundary, openBoundary,
  maxBoundaryTypes }

14.6.1 Detailed Description

Main definitions of the Domain class and its associate class Boundary

Definition in file domain.h.

14.6.2 Define Documentation

14.6.2.1 #define XMAX bounds[1]

Definition at line 2 of file domain.h.

Referenced by Domain::boundary(), Domain::Domain(), and Domain::interaction().

14.6.2.2 #define XMIN bounds[0]

Definition at line 1 of file domain.h.

Referenced by Domain::boundary(), Domain::Domain(), and Domain::interaction().

14.6.3 Enumeration Type Documentation

14.6.3.1 enum BoundaryTypes

Enumerator:

insideBoundary

periodicBoundary

elasticBoundary

openBoundary

maxBoundaryTypes

Definition at line 7 of file domain.h.

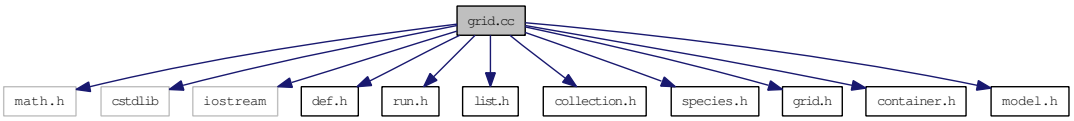
14.7 examples.dox File Reference

14.8 faq.dox File Reference

14.9 grid.cc File Reference

```
#include <math.h>
#include <cstdlib>
#include <iostream>
#include "def.h"
#include "run.h"
#include "list.h"
#include "collection.h"
#include "species.h"
#include "grid.h"
#include "container.h"
#include "model.h"
```

Include dependency graph for grid.cc:



Namespaces

- namespace GridContainer

  Domain Segmentation for Interaction Acceleration.

Functions

- void GridContainer::init (REAL ymin[ ], REAL ymax[ ], REAL radius, Pool< Molecule > *newpool)
- int GridContainer::index (int ind[ ])
- void GridContainer::index (int n, int ind[ ])
- void GridContainer::put (Molecule *node)
- void GridContainer::put (Molecule *node, int icounter)
- Container< Molecule > * GridContainer::get (int ind[ ])
- int * GridContainer::dimensions ()

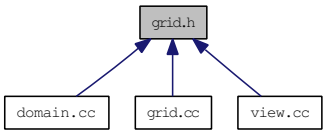
Variables

- REAL GridContainer::xmin [DIM]
- REAL GridContainer::xmax [DIM]
- REAL GridContainer::cellsize
- int GridContainer::ncells [DIM+1]
- int GridContainer::mcells = 0

- int GridContainer::mcells1 = 0
- Container< Molecule > * GridContainer::nodes
- Pool< Molecule > * GridContainer::pool

14.10 grid.h File Reference

This graph shows which files directly or indirectly include this file:



Namespaces

- namespace GridContainer

  Domain Segmentation for Interaction Acceleration.

Functions

- int * GridContainer::dimensions ()
- int GridContainer::index (int ind[ ])
- void GridContainer::index (int n, int ind[ ])
- void GridContainer::init (REAL ymin[ ], REAL ymax[ ], REAL radius, Pool< Molecule > *newpool)
- void GridContainer::put (Molecule *node)
- Container< Molecule > * GridContainer::get (int ind[ ])
- bool GridContainer::checkPool (int icell, char *msg)

14.11 gui.cc File Reference

```
#include <iostream>
#include <fstream>
#include <math.h>
#include <string.h>
#include <libxml/xmlmemory.h>
#include <GL/glut.h>
#include <GL/glx.h>
#include <GL/glu.h>
#include <X11/keysym.h>
#include "def.h"
#include "run.h"
#include "io.h"
#include "list.h"
#include "collection.h"
#include "model.h"
#include "species.h"
#include "domain.h"
#include "gui.h"
```

Include dependency graph for gui.cc:

Namespaces

- namespace Gui

  OpenGL window output routines.

- namespace Palette

  Defines color palette.

Functions

- int Gui::query_extension (char *extName)
- void Gui::init (int argc, char *argv[ ], Domain *newdomain)
- void Gui::helpDisplay ()
- int Gui::readparam (char *s, char *param[ ], int maxparam, char *filename, int val[ ])
- int Gui::readparam (char *s, char *param[ ], int maxparam, char *filename, REAL val[ ])

- void Gui::readconf ()
- void Gui::refresh ()
- void Gui::initdisp ()
- void Gui::Materials (int argc, char *argv[ ])
- void Gui::showVector (double *x, double *v)
- void Gui::showParticle (double vmn, double vmx, double val, double *x)
- void Gui::showSphere (double vmn, double vmx, double val, double rad, double *x)
- void Gui::displayAxes ()
- void Gui::getScaling (double &l0, double &l1)
- void Gui::getXLimits (double *x0, double *x1)
- void Gui::Exit ()
- void Gui::Quit ()
- void Gui::menu (int value)
- void Gui::displayMenu ()
- void Gui::consoleMenu ()
- void Gui::setBackgroundRun ()
- void Gui::setForegroundRun ()
- void Gui::toggleSpheres ()
- void Gui::switchColorScheme ()
- void Gui::runmany ()
- void Gui::toggleWindowDump ()
- void Gui::dumpwindow ()
- void Gui::commandMode ()
- void Gui::display ()
- void Gui::animate ()
- void Gui::helpCommand ()
- void Gui::reshape (int w, int h)
- void Gui::mouse (int button, int state, int x, int y)
- void Gui::motion (int x, int y)
- void Gui::keyboard (unsigned int key)
- void Gui::run ()
- void Gui::displaymessage (char *msg)
- void Gui::setElementColor (int element_type, REAL rgbcolor[ ])
- void Gui::getElementColor (int element_type, REAL rgbcolor[ ])
- void Palette::init (REAL vmin, REAL vmax)
- void Palette::pickcolor (REAL var, REAL color[ ])

Variables

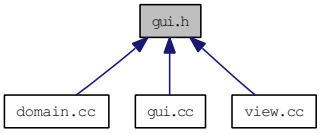
- Domain * Gui::domain
- ElementDisp Gui::disp [maxelements]
- char * Gui::configfile = (char*)"gui.cfg"
- char Gui::windowname [MAXLINLEN]
- int Gui::showpar [maxshowpars]
- int Gui::finished
- int Gui::animation
- int Gui::nwdump
- int Gui::iwdump
- int Gui::attributeList [ ]
- REAL Gui::step

- REAL Gui::vecval [maxlineprm]
- REAL Gui::axes [maxaxesprm]
- REAL Gui::rgbcolor [maxcolor][3]
- REAL Gui::wdtime
- REAL Gui::xo [3]
- REAL Gui::dx
- REAL Gui::dy
- REAL Gui::dz
- REAL Gui::lastx
- REAL Gui::lasty
- REAL Gui::lastz
- int Gui::mouseButtons [3]
- REAL Gui::zoom
- REAL Gui::rotx
- REAL Gui::roty
- REAL Gui::tx
- REAL Gui::ty
- REAL Gui::xmin [DIM]
- REAL Gui::xmax [DIM]
- REAL Gui::lx
- REAL Gui::ly
- REAL Gui::lz
- REAL Gui::lmin
- REAL Gui::lmax
- enum Movement Gui::movement
- struct ColorScale Gui::colorscale
- struct Scene Gui::scene
- struct WindowGeom Gui::window
- struct BFaceList * Gui::bface_root
- Display * Gui::dpy
- Window Gui::win
- int Gui::firstR = 1
- int * Gui::vars
- int * Gui::coms
- REAL Palette::vmn
- REAL Palette::vmx
- REAL Palette::vav
- REAL Palette::dvi

14.12 gui.dox File Reference

14.13 gui.h File Reference

This graph shows which files directly or indirectly include this file:



Classes

- struct Gui::ElementDisp
- struct Gui::ColorScale
- struct Gui::Scene
- struct Gui::Scene::Color
- struct Gui::Scene::Mesh
- struct Gui::Scene::Frame
- struct Gui::WindowGeom

Namespaces

- namespace Gui

  OpenGL window output routines.

- namespace Palette

  Defines color palette.

Defines

- #define WINDOW_SIZE 800
- #define MAX_WINDOW_WIDTH 800
- #define MAX_WINDOW_HEIGHT 600
- #define LEFT_BUTTON 1
- #define MIDDLE_BUTTON 2
- #define RIGHT_BUTTON 3

Enumerations

- enum Gui::Elements {

  Gui::points = 0, Gui::nodes, Gui::edges, Gui::faces,

  Gui::cells, Gui::frame, Gui::mesh, Gui::boundary_nodes,

  Gui::boundary_edges, Gui::boundary_faces, Gui::boundary_cells, Gui::maxelements }

- enum Gui::Color {
  Gui::red = 0, Gui::green, Gui::blue, Gui::skyblue,
  Gui::brown, Gui::magenta, Gui::yellow, Gui::color6,
  Gui::color7, Gui::color8, Gui::color9, Gui::color10,
  Gui::color11, Gui::color12, Gui::color13, Gui::color14,
  Gui::color15, Gui::maxcolor }
- enum Gui::ColorSchemes {
  Gui::colorByType = 0, Gui::colorByBoundary, Gui::colorByTime, Gui::colorByMass,
  Gui::maxColorSchemes }
- enum Gui::PointParameters {
  Gui::variable = maxcolor, Gui::vmin, Gui::vmax, Gui::size,
  Gui::sizevar, Gui::massvar, Gui::maxpointprm }
- enum Gui::LineParameters { Gui::thickness = maxcolor, Gui::length, Gui::maxlineprm }
- enum Gui::AxesParameters {
  Gui::axeswidth = 0, Gui::xaxislength, Gui::yaxislength, Gui::zaxislength,
  Gui::arrowheight, Gui::arrowidth, Gui::maxaxesprm }
- enum Gui::SurfDispType { Gui::gridlines = 0, Gui::solidsurface, Gui::maxsurfdisptypes }
- enum Gui::Movement { Gui::stay = 0, Gui::rotate, Gui::moveuv, Gui::movew }
- enum Gui::ShowPars {
  Gui::showRun = 0, Gui::showAxes, Gui::showSpheres, Gui::showBonds,
  Gui::showGrid, Gui::showNodes, Gui::showVariables, Gui::showBoundaryVertexes,
  Gui::showBoundaryVectors, Gui::showToolVertexes, Gui::showBoundaryFaceCenters, Gui::showBoundaryFaces,
  Gui::showBoundaryGrid, Gui::showToolGrid, Gui::showFrame, Gui::showCellCenters,
  Gui::showFaceCenters, Gui::showIsoSurfaces, Gui::dumpWindow, Gui::maxshowpars }

Functions

- void Gui::Exit ()
- void Gui::Quit ()
- void Gui::readconf ()
- void Gui::helpDisplay ()
- int Gui::readparam (char *s, char *param[ ], int maxparam, char *filename, REAL val[ ])
- void Gui::initdisp ()
- void Gui::Materials (int argc, char *argv[ ])
- void Gui::display ()
- void Gui::displayAxes ()
- void Gui::writeData ()
- void Gui::helpCommand ()
- void Gui::printGridXLimits ()
- void Gui::printGridVecLimits ()
- void Gui::getXLimits (REAL *xmin, REAL *xmax)
- void Gui::getScaling (REAL &lmin, REAL &lmax)
- void Gui::printPartVelLimits ()
- void Gui::printParticleVariables ()
- void Gui::showGridElements (int ne, double *X, REAL color[ ])

- void Gui::showVectorComponent (int ivar, int icomp, double *X, double vmn, double vmx)
- void Gui::showVector (int ivar, double *X)
- void Gui::commandMode ()
- void Gui::printVariables (int n)
- void Gui::init (int argc, char *argv[ ], Domain *newdomain)
- void Gui::finish ()
- void Gui::InitMaterials (void)
- void Gui::getScaling (double &l0, double &l1)
- void Gui::getXLimits (double *x0, double *x1)
- void Gui::selectVariable ()
- void Gui::setBackgroundRun ()
- void Gui::setForegroundRun ()
- void Gui::animate ()
- void Gui::reshape (int w, int h)
- void Gui::mouse (int button, int state, int x, int y)
- void Gui::motion (int x, int y)
- void Gui::keyboard (unsigned char key, int x, int y)
- void Gui::menu (int value)
- void Gui::run ()
- void Gui::drawSegment (REAL *x, REAL *y)
- void Gui::displaymessage (char *msg)
- void Gui::setElementColor (int element_type, REAL rgbcolor[ ])
- void Gui::getElementColor (int element_type, REAL rgbcolor[ ])
- void Palette::init (REAL vmin, REAL vmax)
- void Palette::pickcolor (REAL var, REAL color[ ])

14.13.1 Define Documentation

14.13.1.1 #define LEFT_BUTTON 1

Definition at line 10 of file gui.h.

Referenced by Gui::mouse().

14.13.1.2 #define MAX_WINDOW_HEIGHT 600

Definition at line 8 of file gui.h.

Referenced by Gui::initdisp().

14.13.1.3 #define MAX_WINDOW_WIDTH 800

Definition at line 7 of file gui.h.

Referenced by Gui::initdisp().

14.13.1.4 #define MIDDLE_BUTTON 2

Definition at line 11 of file gui.h.

Referenced by Gui::mouse().

14.13.1.5 #define RIGHT_BUTTON 3

Definition at line 12 of file gui.h.

Referenced by Gui::mouse().

14.13.1.6 #define WINDOW_SIZE 800

Definition at line 6 of file gui.h.

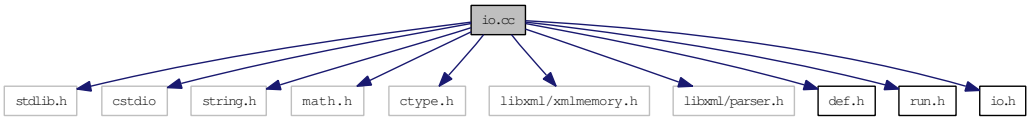
Referenced by Gui::initdisp().

14.14 implementation.dox File Reference

14.15 io.cc File Reference

```
#include <stdlib.h>
#include <cstdio>
#include <string.h>
#include <math.h>
#include <ctype.h>
#include <libxml/xmlmemory.h>
#include <libxml/parser.h>
#include "def.h"
#include "run.h"
#include "io.h"
```

Include dependency graph for io.cc:



Namespaces

- namespace IO

  Some IO routines.

Functions

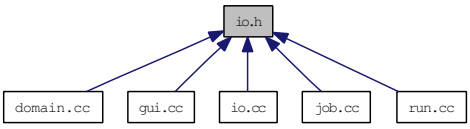
- void IO::initxwd (int i)
- void IO::xwd (char *windowname)
- int IO::getCharAttr (xmlNodePtr cur, char *attr, char *result)
- int IO::getIntAttr (xmlNodePtr cur, char *attr)
- int IO::getIntAttr (xmlDocPtr doc, char *tag, char *keyname, char *key, char *attr)
- int IO::parseWord (xmlDocPtr doc, xmlNodePtr cur, char *keyword, char *result)
- int IO::parseInt (xmlDocPtr doc, xmlNodePtr cur, char *keyword)
- int IO::parseFloat (xmlDocPtr doc, xmlNodePtr cur, char *keyword, REAL &result)
- double IO::parseFloat (xmlDocPtr doc, xmlNodePtr cur, char *keyword)
- void IO::getTimeXML (char inpfilename[ ])
- void IO::getTime (char inpfilename[ ])
- int IO::getIter (char inpfilename[ ])

Variables

- int IO::ioutput = 0
- int IO::nxwdump = 0

14.16 io.h File Reference

This graph shows which files directly or indirectly include this file:



Namespaces

- namespace IO

  Some IO routines.

Functions

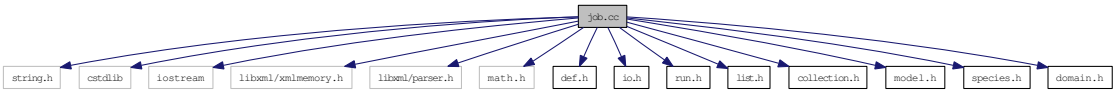
- int IO::getCharAttr (xmlNodePtr cur, char ∗attr, char ∗result)
- int IO::getIntAttr (xmlNodePtr cur, char ∗attr)
- int IO::getIntAttr (xmlDocPtr doc, char ∗tag, char ∗keyname, char ∗key, char ∗attr)
- int IO::parseWord (xmlDocPtr doc, xmlNodePtr cur, char ∗keyword, char ∗result)
- int IO::parseInt (xmlDocPtr doc, xmlNodePtr cur, char ∗keyword)
- double IO::parseFloat (xmlDocPtr doc, xmlNodePtr cur, char ∗keyword)
- int IO::parseFloat (xmlDocPtr doc, xmlNodePtr cur, char ∗keyword, REAL &result)
- int IO::getIter (char inpfilename[ ])
- void IO::getTime (char inpfilename[ ])
- void IO::xwd (char ∗windowname)

14.17 job.cc File Reference

The ReMoDy backend.

```
#include <string.h>
#include <cstdlib>
#include <iostream>
#include <libxml/xmlmemory.h>
#include <libxml/parser.h>
#include <math.h>
#include "def.h"
#include "io.h"
#include "run.h"
#include "list.h"
#include "collection.h"
#include "model.h"
#include "species.h"
#include "domain.h"
```

Include dependency graph for job.cc:



Functions

- void usage ()
- void parsename (char *name, char *filename)

  Strips the suffix from the filename.

- int main (int argc, char *argv[ ])

  The Main routine for a batch mode. Executes a background job.

14.17.1 Detailed Description

The ReMoDy backend.

Executes background job.

Definition in file job.cc.

14.17.2 Function Documentation

14.17.2.1 int main (int *argc*, char * *argv*[ ])

The Main routine for a batch mode. Executes a background job.

Parameters:

argc,argv,: standard command line arguments

Returns:

exit code 0 - success, 1 - failure.

parses command line arguments

creates a domain instance

erases screen

runs the code

retrieves taskname

retrieves taskname

saves data

Definition at line 41 of file job.cc.

References Run::configfile, Gui::domain, ESC, IO::getIter(), Run::init(), Run::inputfile, Run::option, parsename(), Run::programname, Domain::run(), Domain::save(), and WORDLENGTH.

14.17.2.2 void parsename (char * *name*, char * *filename*)

Strips the suffix from the filename.

Parameters:

filename,: file name including suffix

Returns:

name: file name with suffix removed

Definition at line 30 of file job.cc.

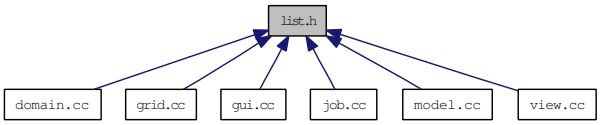
Referenced by main().

14.17.2.3 void usage ()

Definition at line 23 of file job.cc.

14.18 list.h File Reference

This graph shows which files directly or indirectly include this file:



Classes

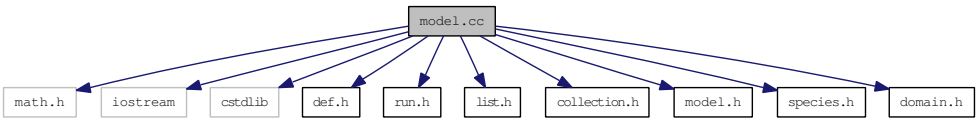
- struct Pointer< Element >
- class List< Element >

14.19 main.dox File Reference

14.20 model.cc File Reference

```
#include <math.h>
#include <iostream>
#include <cstdlib>
#include "def.h"
#include "run.h"
#include "list.h"
#include "collection.h"
#include "model.h"
#include "species.h"
#include "domain.h"
```

Include dependency graph for model.cc:



Namespaces

- namespace Potential

  Interaction-potential functions, such as LJ.

Functions

- REAL Potential::invdist (REAL x)

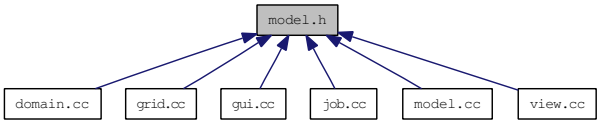
Variables

- REAL Potential::sigma = 1.0
- REAL Potential::eta = 1.0
- REAL Potential::cutoff = 2.0

14.21 model.dox File Reference

14.22 model.h File Reference

This graph shows which files directly or indirectly include this file:



Classes

- union State
- class Molecule

Namespaces

- namespace Potential

  Interaction-potential functions, such as LJ.

- namespace Geom

  Provides some trigeometry functions.

Defines

- #define HARDBALLS

  hardball collision as opposed to interaction via a potential

Enumerations

- enum AtomType {
  undefined = 0, hydrogen = 1, helium = 2, carbon = 12,
  oxygen = 16, maxAtomTypes }

Functions

- void Potential::strength (REAL strength)
- REAL Potential::strength ()
- void Potential::lengthscale (REAL lengthscale)
- REAL Potential::lengthscale ()
- void Potential::Cutoff (REAL newcutoff)
- REAL Potential::Cutoff ()
- REAL Potential::value (REAL r)
- REAL Potential::force (REAL r)
- REAL Potential::derivative (REAL r)
- void Geom::distvec (REAL a[ ], REAL b[ ], REAL c[ ])

- REAL Geom::distance (REAL a[ ], REAL b[ ])
- REAL Geom::distance (int dim, REAL a[ ], REAL b[ ])
- REAL Geom::sclp (REAL a[ ], REAL b[ ])
- REAL Geom::length (REAL a[ ])
- REAL Geom::area (REAL a[ ], REAL b[ ])
- REAL Geom::normalize (REAL a[ ])
- int Geom::hash (int i, int j, int n)

Variables

- const REAL Potential::small = 1.0e-20
- const REAL Potential::large = 1.0e20

14.22.1 Define Documentation

14.22.1.1 #define HARDBALLS

hardball collision as opposed to interaction via a potential

Definition at line 2 of file model.h.

14.22.2 Enumeration Type Documentation

14.22.2.1 enum AtomType

Define the ADSORPTION flag below to enable the time delay for the adsorbed species to be released from the surface

Enumerator:

undefined

hydrogen

helium

carbon

oxygen

maxAtomTypes

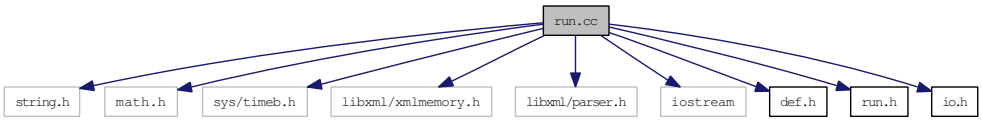
Definition at line 8 of file model.h.

14.23 output.dox File Reference

14.24 run.cc File Reference

```
#include <string.h>
#include <math.h>
#include <sys/timeb.h>
#include <libxml/xmlmemory.h>
#include <libxml/parser.h>
#include <iostream>
#include "def.h"
#include "run.h"
#include "io.h"
```

Include dependency graph for run.cc:



Namespaces

- namespace Run

  Processing command-line and execution control parameters.

Defines

- #define RAND_MAX 2147483647

Functions

- void Run::testrnd ()

  Test random numer generator.

- REAL Run::rnd ()

  Seeds random number.

- REAL Run::gauss ()

  normal random number generator

- void Run::init (int argc, char *argv[ ])

  Initialize all variables, and execution options.

- void Run::readcmdline (int argc, char *argv[ ])

  Parses command-line options.

- int Run::elapsed ()

  time (sec) elapsed since the start of the run

Variables

- struct Option Run::option = {0,0,0,0}

  command-line options

- void(* Run::usage)()
- char Run::programname [MAXLINLEN]
- char Run::configfile [MAXLINLEN]
- char Run::outputfile [MAXLINLEN]
- char Run::inputfile [MAXLINLEN]
- char Run::outputname [MAXLINLEN]
- int Run::nthreads
- struct timeb Run::worldtime
- struct Time Run::time

14.24.1 Define Documentation

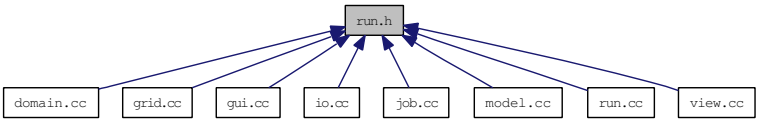
14.24.1.1 #define RAND_MAX 2147483647

Definition at line 14 of file run.cc.

Referenced by Run::rnd(), and Run::testrnd().

14.25 run.h File Reference

This graph shows which files directly or indirectly include this file:



Classes

- struct Option

  Execution options.

- struct Run::Time

  Execution time-control structure.

Namespaces

- namespace Run

  Processing command-line and execution control parameters.

Functions

- void Run::init (int argc, char ∗argv[ ])

  Initialize all variables, and execution options.

- void Run::readcmdline (int argc, char ∗argv[ ])

  Parses command-line options.

- int Run::elapsed ()

  time (sec) elapsed since the start of the run

- void Run::seed ()

  seed random number generator

- REAL Run::rnd ()

  Seeds random number.

- REAL Run::gauss ()

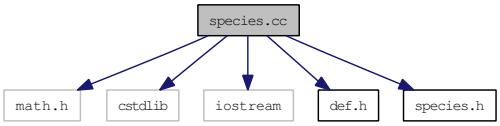
  normal random number generator

- void(∗) Run::usage ()

14.26 species.cc File Reference

```
#include <math.h>
#include <cstdlib>
#include <iostream>
#include "def.h"
#include "species.h"
```

Include dependency graph for species.cc:



Namespaces

- namespace Species

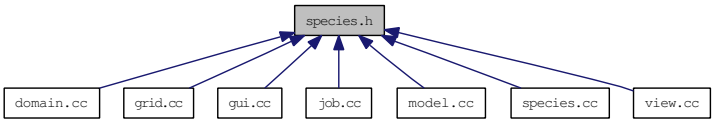
  Description of Specie and Reaction classes.

Variables

- int Species::nspecies
- Specie * Species::species
- Reaction * Species::reactions

14.27 species.h File Reference

This graph shows which files directly or indirectly include this file:



Classes

- class Species::Specie
- struct Species::Gas

  Gas is a specie with some additional parameters.

- struct Species::Reaction

  Reaction determines the two products only.

- struct Species::Reaction::Outcome

  Possible outcomes of a reaction.

Namespaces

- namespace Species

  Description of Specie and Reaction classes.

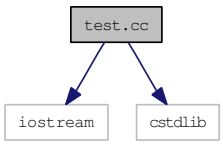
Enumerations

- enum Species::Interaction { Species::missed = 0, Species::collided, Species::reacted, Species::annihalated }

14.28 test.cc File Reference

```
#include <iostream>
#include <cstdlib>
```

Include dependency graph for test.cc:



Functions

- main ()

14.28.1 Function Documentation

14.28.1.1 main ()

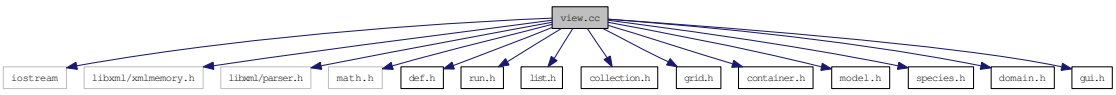
Definition at line 4 of file test.cc.

14.29 view.cc File Reference

The frontend of ReMoDy with the OpenGL Visualizer.

```
#include <iostream>
#include <libxml/xmlmemory.h>
#include <libxml/parser.h>
#include <math.h>
#include "def.h"
#include "run.h"
#include "list.h"
#include "collection.h"
#include "grid.h"
#include "container.h"
#include "model.h"
#include "species.h"
#include "domain.h"
#include "gui.h"
```

Include dependency graph for view.cc:



Functions

- void usage ()
- int main (int argc, char *argv[ ])

  The main routine.

14.29.1 Detailed Description

The frontend of ReMoDy with the OpenGL Visualizer.

Executes a job and displays the computational domain in an OpenGL window.

Definition in file view.cc.

14.29.2 Function Documentation

14.29.2.1 int main (int *argc*, char * *argv*[ ])

The main routine.

parses command line arguments

creates a domain instance

initializes the domain

executes the job

Definition at line 29 of file view.cc.

References Gui::domain, Gui::init(), Run::init(), Run::inputfile, and Gui::run().

14.29.2.2 void usage ()

Definition at line 25 of file view.cc.

References Run::programname.

Index