

Molecular Dynamics General

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Chapter 1

MDGeneral

This is a repository for making a fast and general molecular dynamics program

Chapter 2

Hierarchical Index

2.1 Class Hierarchy

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

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Chapter 3

Class Index

3.1 Class List

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

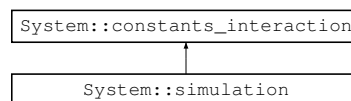
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Chapter 4

Class Documentation

4.1 System::constants_interaction Class Reference

Inheritance diagram for System::constants_interaction:



Public Member Functions

- **constants_interaction** (int n_types)

Public Attributes

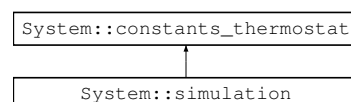
- std::vector< std::vector< std::vector< double > > > **interaction_const**

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

- C:/Users/SamarthH/Documents/GitHub/MDGeneral/Backend/include/system.h

4.2 System::constants_thermostat Class Reference

Inheritance diagram for System::constants_thermostat:



Public Member Functions

- **constants_thermostat** (int n_types)

Public Attributes

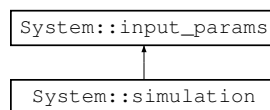
- std::vector< std::vector< double > > **thermostat_const**

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

- C:/Users/SamarthH/Documents/GitHub/MDGeneral/Backend/include/system.h

4.3 System::input_params Class Reference

Inheritance diagram for System::input_params:



Public Member Functions

- **input_params** (std::string input)

Public Attributes

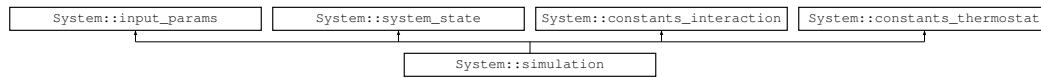
- int **n_types**
- int **n_dimensions**
- std::vector< int > **n_particles**
- double **timestep**
- double **runtime**
- int **parallelize**
- std::vector< double > **mass**
- std::vector< double > **temperature_required**
- int **periodic_boundary**

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

- C:/Users/SamarthH/Documents/GitHub/MDGeneral/Backend/include/system.h

4.4 System::simulation Class Reference

Inheritance diagram for System::simulation:



Public Member Functions

- **simulation** (std::string input, double size[])

Public Attributes

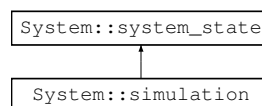
- std::vector< void(*)(<code>simulation</code> &, int)> **thermostat**
- std::vector< std::vector< void(*)(<code>simulation</code> &, int, int)> > **interaction**
- std::vector< double > **box_size_limits**

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

- C:/Users/SamarthH/Documents/GitHub/MDGeneral/Backend/include/system.h

4.5 System::system_state Class Reference

Inheritance diagram for System::system_state:



Public Member Functions

- **system_state** (int n_types, int n_dimensions, std::vector< int > &n_particles)

Public Attributes

- std::vector< std::vector< std::vector< double > > > **position**
- std::vector< std::vector< std::vector< double > > > **orientation**
- std::vector< std::vector< std::vector< double > > > **velocity**
- std::vector< std::vector< std::vector< double > > > **acceleration**
- std::vector< double > **temperature**
- double **energy_total**
- double **energy_potential**
- std::vector< double > **energy_kinetic**
- double **time**
- int **state**

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

- C:/Users/SamarthH/Documents/GitHub/MDGeneral/Backend/include/system.h

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