My Project

Generated by Doxygen 1.8.14

Contents

Chapter 1

Hierarchical Index

1.1 Class Hierarchy

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

Chapter 2

Class Index

2.1 Class List

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

Chapter 3

Class Documentation

3.1 Atom Struct Reference

Public Member Functions

- bool **operator==** (const Atom &other) const
- bool **operator!=** (const Atom &other) const
- bool **operator**< (const Atom &other) const
- bool **operator**> (const Atom &other) const

Public Attributes

- std::size_t **id** {0}
- std::string **name** {}
- REALVEC **position** {0, 0, 0}
- REALVEC **velocity** {0, 0, 0}

Friends

- std::ostream & **operator**<< (std::ostream &, const Atom &)

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

- container/atom.hpp

3.2 ContainerBase< T > Struct Template Reference

Public Member Functions

- auto & **operator()** (std::size_t i)
- constexpr auto & **operator()** (std::size_t i) const
- auto & **operator[ ]** (std::size_t i)
- constexpr auto & **operator[ ]** (std::size_t i) const
- auto **begin** ()
- auto **end** ()
- auto **begin** () const
- auto **end** () const
- auto **cbegin** () const
- auto **cend** () const
- auto **rbegin** ()
- auto **rend** ()
- auto **rbegin** () const
- auto **rend** () const
- auto **crbegin** () const
- auto **crend** () const
- auto **size** () const
- auto & **front** ()
- const auto & **front** () const
- auto & **back** ()
- const auto & **back** () const

Public Attributes

- T **data** {}

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

- container/containerBase.hpp

3.3 Controller Class Reference

Public Member Functions

- void **setup** (int argc, char ∗argv[ ])
- void **start** ()
- void **stop** ()

Static Public Member Functions

- static void **signal** (int SIG)

Static Public Attributes

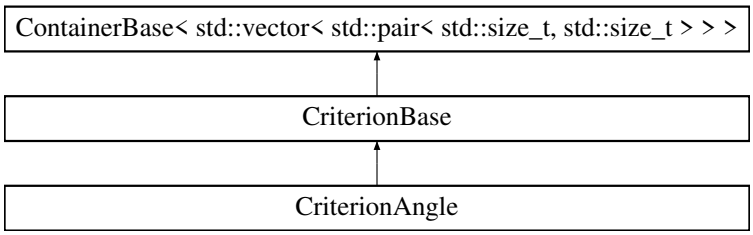
- static std::atomic< int > **SIGNAL** = {0}
- static std::atomic< bool > **CIVILISED_SHUTDOWN** = {false}

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

- control/controller.hpp
- control/controller.cpp

3.4 CriterionAngle Class Reference

Inheritance diagram for CriterionAngle:



Public Member Functions

- virtual std::string **getType** () const override
- bool **valid** (const std::vector< Molecule > &reactants, const REALVEC &boxDimensions)

Protected Member Functions

- virtual CriterionAngle * **clone_impl** () const override

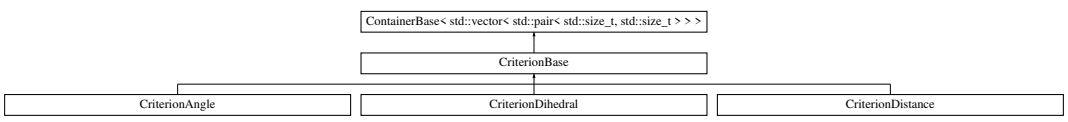
Additional Inherited Members

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

- reaction/criterionDerived.hpp

3.5 CriterionBase Class Reference

Inheritance diagram for CriterionBase:



Public Member Functions

- virtual std::string **getType** () const =0
- void **setThresholds** (const REAL &min, const REAL &max)
- void **setThresholds** (const std::pair< REAL, REAL > &values)
- void **setMin** (const REAL &value)
- void **setMax** (const REAL &value)
- const auto & **getMin** () const
- const auto & **getMax** () const
- const auto & **getLatest** () const
- void **addAtomIndices** (const std::size_t &molix, const std::size_t &atomix)
- void **addAtomIndices** (const std::pair< std::size_t, std::size_t > &indices)
- virtual bool **valid** (const std::vector< Molecule > &, const REALVEC &)=0
- auto **clone** () const

Protected Member Functions

- virtual CriterionBase * **clone_impl** () const =0

Protected Attributes

- REAL **minValue** {0}
- REAL **maxValue** {0}
- REAL **latestValue** {0}

Friends

- std::ostream & **operator<<** (std::ostream &, const CriterionBase &)

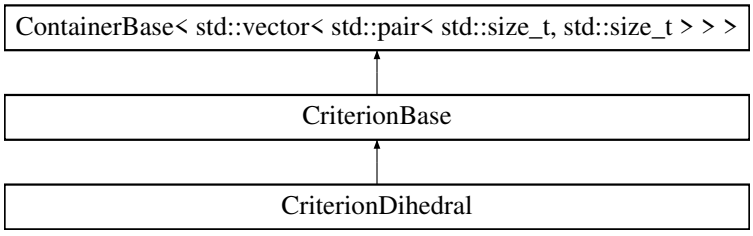
Additional Inherited Members

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

- reaction/criterionBase.hpp

3.6 CriterionDihedral Class Reference

Inheritance diagram for CriterionDihedral:



Public Member Functions

- virtual std::string **getType** () const override
- bool **valid** (const std::vector< Molecule > &reactants, const REALVEC &boxDimensions)

Protected Member Functions

- virtual CriterionDihedral * **clone_impl** () const override

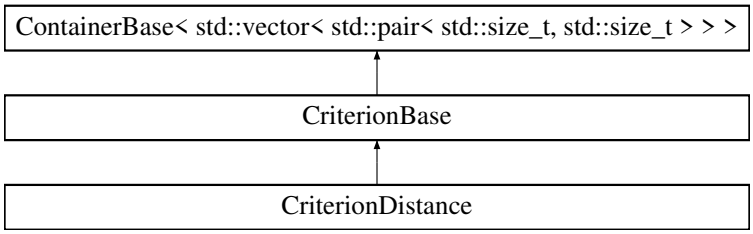
Additional Inherited Members

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

- reaction/criterionDerived.hpp

3.7 CriterionDistance Class Reference

Inheritance diagram for CriterionDistance:



Public Member Functions

- virtual std::string **getType** () const override
- bool **valid** (const std::vector< Molecule > &reactants, const REALVEC &boxDimensions)

Protected Member Functions

- virtual CriterionDistance * **clone_impl** () const override

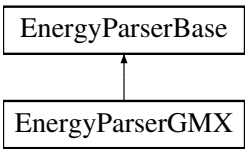
Additional Inherited Members

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

- reaction/criterionDerived.hpp

3.8 EnergyParserBase Class Reference

Inheritance diagram for EnergyParserBase:



Public Member Functions

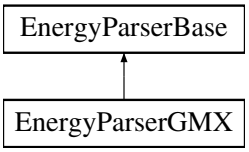
- virtual REAL **readPotentialEnergyDifference** (const std::size_t &, const std::size_t &)=0
- virtual void **setup** (const Parameters &)=0

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

- parser/energyParserBase.hpp

3.9 EnergyParserGMX Class Reference

Inheritance diagram for EnergyParserGMX:



Public Member Functions

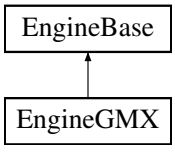
- REAL **readPotentialEnergyDifference** (const std::size_t &, const std::size_t &)
- void **setup** (const Parameters &)

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

- parser/energyParserGMX.hpp
- parser/energyParserGMX.cpp

3.10 EngineBase Class Reference

Inheritance diagram for EngineBase:



Public Member Functions

- virtual void **setup** (const Parameters &)=0
- virtual void **verifyExecutable** ()=0
- virtual void **runMD** (const std::size_t &)=0
- virtual void **runMDInitial** ()=0
- virtual void **runMDAppending** (const std::size_t &, const std::size_t &)=0
- virtual bool **runRelaxation** (const std::size_t &)=0
- virtual void **runEnergyComputation** (const std::size_t &, const std::size_t &)=0
- virtual void **cleanup** (const std::size_t &)=0

Protected Member Functions

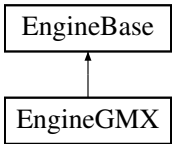
- template<typename... Args>
  void **execute** (const char *, Args &&... args)
- template<typename... Args>
  void **execute** (std::string &, const char *, Args &&... args)

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

- engine/engineBase.hpp

3.11 EngineGMX Class Reference

Inheritance diagram for EngineGMX:



Public Member Functions

- void **setup** (const Parameters &)
- void **verifyExecutable** ()
- void **runMD** (const std::size_t &)
- void **runMDInitial** ()
- void **runMDAppending** (const std::size_t &, const std::size_t &)
- bool **runRelaxation** (const std::size_t &)
- void **runEnergyComputation** (const std::size_t &, const std::size_t &)
- void **cleanup** (const std::size_t &)

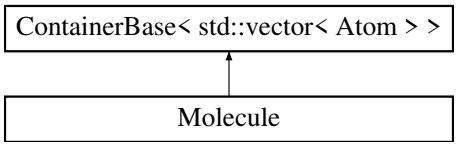
Additional Inherited Members

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

- engine/engineGMX.hpp
- engine/engineGMX.cpp

3.12 Molecule Class Reference

Inheritance diagram for Molecule:



Public Member Functions

- void **setID** (std::size_t id)
- void **setName** (std::string name)
- const auto & **getID** () const
- const auto & **getName** () const
- auto **addAtom** (Atom a)
- auto **addAtom** (std::size_t id, std::string name)
- const Atom & **getAtom** (std::size_t id) const
- void **removeAtom** (Atom &element)
- void **removeAtom** (std::size_t id)
- bool **containsAtom** (Atom &element) const
- bool **containsAtom** (std::size_t id) const
- bool **containsAtom** (std::string name) const
- bool **empty** () const
- bool **operator==** (const Molecule &other) const
- bool **operator!=** (const Molecule &other) const
- bool **operator**< (const Molecule &other) const
- bool **operator**> (const Molecule &other) const

Friends

- std::ostream & **operator**<< (std::ostream &, const Atom &)

Additional Inherited Members

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

- container/molecule.hpp
- container/molecule.cpp

3.13 Parameters Class Reference

Public Member Functions

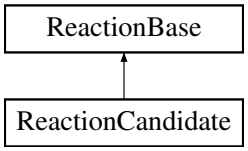
- **Parameters** (int, char ∗[ ])
- const auto & **getOption** (const std::string &s) const
- const auto & **getEngineType** () const
- const auto & **getSimulationMode** () const
- const auto & **getSimulationAlgorithm** () const
- std::string **str** () const
- template<>
  std::string **formatted** (const std::string &name, const std::vector< std::string > &values) const

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

- parameters/parameters.hpp
- parameters/parameters.cpp

3.14 ReactionBase Class Reference

Inheritance diagram for ReactionBase:



Public Member Functions

- **ReactionBase** (const ReactionBase &)
- **ReactionBase** (ReactionBase &&)=default
- ReactionBase & **operator=** (const ReactionBase &)=delete
- ReactionBase & **operator=** (ReactionBase &&)=default
- void **setName** (const std::string &n)
- const auto & **getName** () const
- void **setReactionEnergy** (const REAL &e)
- const auto & **getReactionEnergy** () const
- void **setActivationEnergy** (const REAL &e)
- const auto & **getActivationEnergy** () const
- void **setRate** (const std::vector< std::pair< REAL, REAL >> r)
- const auto & **getRate** () const
- const auto **getReactant** (const std::size_t &) const
- const auto & **getReactants** () const
- auto & **getReactants** ()
- const auto **getProduct** (const std::size_t &) const
- const auto & **getProducts** () const
- auto & **getProducts** ()
- Molecule & **getAddReactant** (const std::size_t &)
- Molecule & **getAddProduct** (const std::size_t &)
- void **addTransition** (const std::size_t &, const std::size_t &, const std::size_t &, const std::size_t &)
- void **addCriterion** (const std::vector< std::pair< std::size_t, std::size_t >> &, const std::pair< REAL, REAL > &)
- void **addTranslation** (const std::vector< std::pair< std::size_t, std::size_t >> &, const REAL &)
- void **consistencyCheck** () const

Protected Member Functions

- virtual std::string **str** () const

Protected Attributes

- std::string **name** {}
- std::vector< Molecule > **reactants** {}
- std::vector< Molecule > **products** {}
- std::vector< TransitionTable > **transitionTables** {}
- std::vector< TranslationTable > **translationTables** {}
- REAL **reactionEnergy** {0}
- REAL **activationEnergy** {0}
- std::vector< std::pair< REAL, REAL > > **reactionRate** {}
- std::vector< std::unique_ptr< CriterionBase > > **criterions** {}

Friends

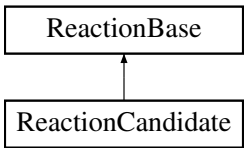
- std::ostream & **operator**<< (std::ostream &stream, const ReactionBase &reaction)

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

- reaction/reactionBase.hpp
- reaction/reactionBase.cpp

3.15 ReactionCandidate Class Reference

Inheritance diagram for ReactionCandidate:



Public Member Functions

- **ReactionCandidate** (const ReactionBase &)
- **ReactionCandidate** (const ReactionCandidate &)=default
- ReactionCandidate & **operator=** (const ReactionCandidate &)=delete
- **ReactionCandidate** (ReactionCandidate &&)=default
- ReactionCandidate & **operator=** (ReactionCandidate &&)=default
- REAL **getCurrentReactionRateValue** () const
- REAL **getCurrentDistanceValue** () const
- void **updateReactant** (const std::size_t, const Molecule &)
- void **applyTransitions** ()
- void **applyTranslations** ()
- bool **valid** (const REALVEC &)
- std::string **shortInfo** () const

Additional Inherited Members

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

- reaction/reactionCandidate.hpp
- reaction/reactionCandidate.cpp

3.16 ReactionParser Class Reference

Public Member Functions

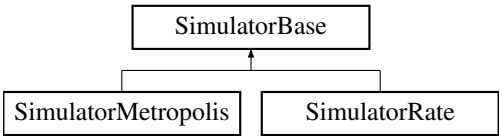
- ReactionBase **read** (const std::string &)
- std::string **writeExample** ()

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

- parser/reactionParser.hpp
- parser/reactionParser.cpp

3.17 SimulatorBase Class Reference

Inheritance diagram for SimulatorBase:



Public Member Functions

- void **run** ()
- void **writeRestartFile** (const Parameters &) const
- virtual void **setup** (const Parameters &)
- virtual void **finish** ()=0
- auto **getNCycles** () const

Protected Member Functions

- void **mdSequence** ()
- virtual void **reactiveStep** ()=0
- virtual bool **acceptance** (const ReactionCandidate &)=0

Protected Attributes

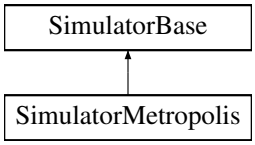
- Universe **universe** {}
- std::unique_ptr< EngineBase > **mdEngine** {nullptr}
- std::unique_ptr< EnergyParserBase > **energyParser** {nullptr}
- std::size_t **currentCycle** {1}
- std::size_t **lastReactiveCycle** {0}
- std::size_t **nCycles** {0}
- std::size_t **nCyclesCompleted** {0}
- bool **writeStatistics** {false}
- std::ofstream **STATISTICS_FILE** {}
- std::unique_ptr< UnitSystem > **unitSystem** {nullptr}

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

- control/simulatorBase.hpp
- control/simulatorBase.cpp

3.18 SimulatorMetropolis Class Reference

Inheritance diagram for SimulatorMetropolis:



Public Member Functions

- void **finish** ()
- void **setup** (const Parameters &)

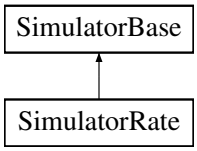
Additional Inherited Members

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

- control/simulatorMetropolis.hpp
- control/simulatorMetropolis.cpp

3.19 SimulatorRate Class Reference

Inheritance diagram for SimulatorRate:



Public Member Functions

- void **finish** ()
- void **setup** (const Parameters &)

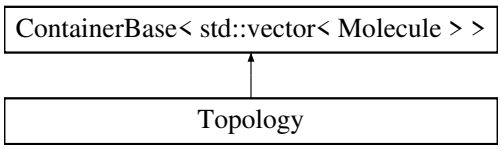
Additional Inherited Members

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

- control/simulatorRate.hpp
- control/simulatorRate.cpp

3.20 Topology Class Reference

Inheritance diagram for Topology:



Public Member Functions

- void **setDimensions** (const REALVEC &d)
- const auto & **getDimensions** () const
- void **addReactionRecord** (const std::size_t &molid)
- const auto & **getReactionRecordsAtoms** ()
- const auto & **getReactionRecordsMolecules** ()
- const std::size_t & **getReactionRecordMolecule** (const std::size_t &oldmolid)
- auto **addMolecule** (Molecule m)
- auto **addMolecule** (std::size_t id, std::string name)
- void **removeMolecule** (Molecule &)
- void **removeMolecule** (std::size_t)
- bool **containsMolecule** (const Molecule &) const
- bool **containsMolecule** (const std::size_t &) const
- const Molecule & **getMolecule** (std::size_t) const
- std::vector< std::reference_wrapper< Molecule > > **getMolecules** (std::string)
- Molecule & **getAddMolecule** (std::size_t, std::string)
- std::vector< std::string > **getMoleculetypes** () const
- const auto **getNAtoms** () const
- void **sort** ()
- void **repairMoleculePBC** (Molecule &)
- bool **empty** () const
- void **clear** ()
- void **clearReactionRecords** ()

Friends

- std::ostream & **operator**<< (std::ostream &os, const Topology &obj)

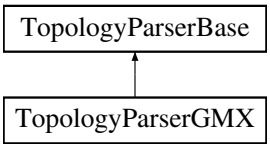
Additional Inherited Members

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

- container/topology.hpp
- container/topology.cpp

3.21 TopologyParserBase Class Reference

Inheritance diagram for TopologyParserBase:



Public Member Functions

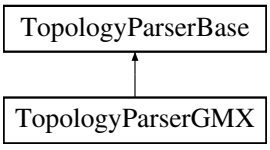
- virtual void **read** (Topology &, const std::size_t &)=0
- virtual void **readRelaxed** (Topology &, const std::size_t &)=0
- virtual void **write** (Topology &, const std::size_t &)=0

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

- parser/topologyParserBase.hpp

3.22 TopologyParserGMX Class Reference

Inheritance diagram for TopologyParserGMX:



Public Member Functions

- void **read** (Topology &, const std::size_t &)
- void **readRelaxed** (Topology &, const std::size_t &)
- void **write** (Topology &, const std::size_t &)

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

- parser/topologyParserGMX.hpp
- parser/topologyParserGMX.cpp

3.23 TransitionTable Struct Reference

Public Member Functions

- **TransitionTable** (const std::size_t &ix1, const std::size_t &ix2, const std::size_t &ix3, const std::size_t &ix4)

Public Attributes

- std::size_t **oldMolix** {0}
- std::size_t **oldix** {0}
- std::size_t **newMolix** {0}
- std::size_t **newix** {0}

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

- reaction/reactionBase.hpp

3.24 TranslationTable Struct Reference

Public Member Functions

- **TranslationTable** (const std::pair< std::size_t, std::size_t > &ix1, const std::pair< std::size_t, std::size_t > &ix2, const REAL &val)

Public Attributes

- std::pair< std::size_t, std::size_t > **indices1** {}
- std::pair< std::size_t, std::size_t > **indices2** {}
- REAL **value** {0}

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

- reaction/reactionBase.hpp

3.25 Universe Class Reference

Public Member Functions

- void **setup** (const Parameters &)
- void **update** (const std::size_t &)
- void **write** (const std::size_t &)
- void **readRelaxed** (const std::size_t &)
- std::vector< ReactionCandidate > **searchReactionCandidates** ()
- bool **isAvailable** (const ReactionCandidate &)
- void **react** (ReactionCandidate &)
- void **checkMovement** (const ReactionCandidate &)
- const auto & **getReactionTemplates** () const

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

- container/universe.hpp
- container/universe.cpp

3.26 enhance::Vector3d< T > Class Template Reference

Public Member Functions

- **Vector3d** (const T)
- **Vector3d** (const T, const T, const T)
- **Vector3d** (const Vector3d< T > &other)=default
- **Vector3d** (Vector3d< T > &&other)=default
- template<typename O >
  Vector3d (const Vector3d< O > &)
- T & **operator()** (std::size_t i)
- constexpr T **operator()** (std::size_t i) const
- T & **operator[ ]** (std::size_t i)
- constexpr T **operator[ ]** (std::size_t i) const
- Vector3d< T > & **operator=** (const Vector3d< T > &)
- Vector3d< T > & **operator=** (Vector3d< T > &&)
- template<typename O >
  const Vector3d< T > **operator*** (const O &) const
- template<typename O >
  Vector3d< T > **operator*** (O &&) const
- template<typename O >
  const Vector3d< T > **operator/** (const O &) const
- template<typename O >
  Vector3d< T > **operator/** (O &&) const
- template<typename O >
  const Vector3d< T > **operator+** (const Vector3d< O > &) const
- template<typename O >
  Vector3d< T > **operator+** (Vector3d< O > &&) const
- template<typename O >
  const Vector3d< T > **operator-** (const Vector3d< O > &) const
- template<typename O >
  Vector3d< T > **operator-** (Vector3d< O > &&) const

- const Vector3d< T > **operator-** () const
- template<typename O >
  Vector3d< T > **operator*=** (const O &)
- template<typename O >
  Vector3d< T > **operator/=** (const O &)
- template<typename O >
  Vector3d< T > **operator+=** (const Vector3d< O > &)
- template<typename O >
  Vector3d< T > **operator-=** (const Vector3d< O > &)
- bool **operator==** (const Vector3d< T > &)
- bool **operator!=** (const Vector3d< T > &)
- auto **begin** ()
- auto **end** ()
- auto **begin** () const
- auto **end** () const
- auto **cbegin** () const
- auto **cend** () const
- auto **rbegin** ()
- auto **rend** ()
- auto **rbegin** () const
- auto **rend** () const
- auto **crbegin** () const
- auto **crend** () const
- float **norm** () const
- template<typename O >
  T **dot** (const Vector3d< O > &) const
- template<typename O >
  Vector3d< T > **cross** (const Vector3d< O > &) const
- void **setZero** ()
- bool **isZero** () const

Protected Attributes

- std::array< T, 3 > **data**

Friends

- template<typename O >
  Vector3d< T > **operator*** (O scalar, Vector3d< T > vector)
- std::ostream & **operator<<** (std::ostream &os, const Vector3d< T > &vec)

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

- enhance/vector3d.hpp