M7

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 AbInitioHamiltonian Class Reference

Inheritance diagram for AbInitioHamiltonian:

3.2 Aliaser Class Reference

Public Member Functions

- **Aliaser** (const size_t nprob, PrivateStore< PRNG > &prng)
- void **update** (const defs::prob_t ∗probs, const size_t nprob)
- void **update** (const std::vector< defs::prob_t > &probs)
- **Aliaser** (const defs::prob_t ∗probs, const size_t nprob, PrivateStore< PRNG > &prng)
- **Aliaser** (const std::vector< defs::prob_t > &probs, const size_t nprob, PrivateStore< PRNG > &prng)
- **Aliaser** (const std::vector< defs::prob_t > &probs, PrivateStore< PRNG > &prng)
- size_t **draw** () const
- defs::prob_t **norm** () const
- defs::prob_t **prob** (const size_t &i) const

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/sample/Aliaser.h

3.3 AlignedAllocator< T, alignment > Class Template Reference

Classes

- struct rebind

Public Types

- typedef T **value_type**
- typedef T ∗ **pointer**
- typedef const T ∗ **const_pointer**
- typedef T & **reference**
- typedef const T & **const_reference**
- typedef std::size_t **size_type**

Public Member Functions

- pointer **address** (reference value) const
- const_pointer **address** (const_reference value) const
- **AlignedAllocator** (const AlignedAllocator &alloc) throw ()
- template<class U >
  AlignedAllocator (const AlignedAllocator< U, alignment > &) throw ()
- size_type **max_size** () const throw ()
- pointer **allocate** (size_type num, const void ∗=0)
- void **construct** (pointer p, const T &value)
- void **destroy** (pointer p)
- void **deallocate** (pointer p, size_type num)

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/thread/AlignedAllocator.h

3.4 AlignedAllocator2< T, alignment > Class Template Reference

Classes

- struct rebind

Public Types

- typedef T **value_type**
- typedef T ∗ **pointer**
- typedef const T ∗ **const_pointer**
- typedef T & **reference**
- typedef const T & **const_reference**
- typedef std::size_t **size_type**
- typedef std::ptrdiff_t **difference_type**

Public Member Functions

- pointer **address** (reference value) const
- const_pointer **address** (const_reference value) const
- **AlignedAllocator2** (const AlignedAllocator2 &) throw ()
- template<class U >
  AlignedAllocator2 (const AlignedAllocator2< U, alignment > &) throw ()
- size_type **max_size** () const throw ()
- pointer **allocate** (size_type num, const void ∗=0)
- void **construct** (pointer p, const T &value)
- void **destroy** (pointer p)
- void **deallocate** (pointer p, size_type num)

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/thread/AlignedAllocator2.h

3.5 DeterminantElement::AntiDatawordEnumerator Class Reference

Inheritance diagram for DeterminantElement::AntiDatawordEnumerator:

Collaboration diagram for DeterminantElement::AntiDatawordEnumerator:

Public Member Functions

- **AntiDatawordEnumerator** (const DeterminantElement &data)

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/DeterminantField.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/DeterminantField.cpp

3.6 AntisymConnection Class Reference

Inheritance diagram for AntisymConnection:

Collaboration diagram for AntisymConnection:

Public Member Functions

- **AntisymConnection** (const Field ∗field)
- **AntisymConnection** (const DeterminantElement &ket, const DeterminantElement &bra)
- **AntisymConnection** (const DeterminantElement &ket)
- void **connect** (const DeterminantElement &ket, const DeterminantElement &bra) override
- void **apply** (const DeterminantElement &ket)
- void **apply** (const DeterminantElement &ket, DeterminantElement &bra) override
- const defs::det_work & **com** () const
- const size_t & **com** (const size_t &i) const
- const size_t & **ncom** () const
- const bool & **phase** () const

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/fermion/Connection.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/fermion/Connection.cpp

3.7 ArrayIndexer< nind > Class Template Reference

Public Member Functions

- **ArrayIndexer** (const std::array< size_t, nind > &shape)
- const std::array< size_t, nind > & **shape** () const
- const std::array< size_t, nind > & **strides** () const
- size_t **nelement** () const
- bool **operator==** (const ArrayIndexer &rhs) const
- bool **operator!=** (const ArrayIndexer &rhs) const
- size_t **get** (const std::array< size_t, nind > &inds) const

Protected Attributes

- std::array< size_t, nind > **m_shape** {}
- std::array< size_t, nind > **m_strides** {}

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/multidim/ArrayIndexer.h

3.8 Atomic< T > Struct Template Reference

Public Member Functions

- **Atomic** (T &v)
- T & **operator+=** (const T &rhs)
- T & **operator-=** (const T &rhs)
- T & **operator∗=** (const T &rhs)
- T & **operator/=** (const T &rhs)

Public Attributes

- T & **m_v**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/thread/Atomic.h

3.9 Atomic< bool > Struct Template Reference

Public Member Functions

- **Atomic** (bool &v)
- bool & **operator&=** (const bool &rhs)
- bool & **operator|=** (const bool &rhs)

Public Attributes

- bool & **m_v**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/thread/Atomic.h

3.10 Atomic< std::complex< T > > Struct Template Reference

Public Member Functions

- **Atomic** (std::complex< T > &v)
- std::complex< T > & **operator+=** (const std::complex< T > &rhs)
- std::complex< T > & **operator-=** (const std::complex< T > &rhs)
- std::complex< T > & **operator∗=** (const std::complex< T > &rhs)
- std::complex< T > & **operator/=** (const std::complex< T > &rhs)

Public Attributes

- T & **m_real**
- T & **m_imag**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/thread/Atomic.h

3.11 Bitset Class Reference

Inheritance diagram for Bitset:

Collaboration diagram for Bitset:

Public Member Functions

- **Bitset** (size_t nbit)

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/Bitset.h

3.12 BitsetClrEnumerator Class Reference

Inheritance diagram for BitsetClrEnumerator:

Collaboration diagram for BitsetClrEnumerator:

Public Member Functions

- **BitsetClrEnumerator** (const BitsetElement &data1, Enumerator< size_t > ∗subsequent=nullptr, size_↩
  t offset=0)

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/enumerator/BitsetEnumerator.h

3.13 BitsetElement Class Reference

Inheritance diagram for BitsetElement:

Collaboration diagram for BitsetElement:

Public Types

- typedef BitsetField **Field_T**

Public Member Functions

- **BitsetElement** ([BitsetField](#) ∗field, char ∗begin)
- void **set** (const defs::pair &pair)
- virtual void **set** (const size_t &ibit)
- void **set** (const defs::inds &inds)
- void **clr** (const defs::pair &pair)
- virtual void **clr** (const size_t &ibit)
- bool **get** (const defs::pair &pair) const
- bool **get** (const size_t &ibit) const
- std::string **to_string** () override
- size_t **nsetbit** () const
- bool **is_zero** () const override

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/BitsetField.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/BitsetField.cpp

3.14 BitsetEnumerator< op > Class Template Reference

Inheritance diagram for BitsetEnumerator< op >:

Collaboration diagram for BitsetEnumerator< op >:

Public Member Functions

- **BitsetEnumerator** (const [BitsetElement](#) &data1, const [BitsetElement](#) &data2, [Enumerator](#) ∗subsequent=nullptr, size_t offset=0)
- bool **next_element** (size_t &result) override
- defs::data_t **get_work** (const size_t &idata) const

Protected Attributes

- const [BitsetElement](#) & **m_data1**
- const [BitsetElement](#) & **m_data2**
- size_t **m_offset**
- size_t **m_idata** = ∼0ul
- defs::data_t **m_work** = 0ul

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/enumerator/BitsetEnumerator.h

3.15 BitsetField Class Reference

Inheritance diagram for BitsetField:

Collaboration diagram for BitsetField:

Public Member Functions

- **BitsetField** (Table ∗table, size_t nelement, size_t nbit, const std::string &description="")
- size_t **nbit** () const override
- BitsetElement **operator()** (const size_t &irow, const size_t &isegment=0, const size_t &ielement=0)
- std::string **to_string** (size_t irow, size_t isegment, size_t ielement) override

Static Public Member Functions

- static defs::pair **rectify_offset** (const defs::pair &pair)

Protected Member Functions

- virtual void **update_nbit** (size_t nbit)
- void **increment_nbit** (size_t nbit)

Protected Attributes

- size_t **m_nbit**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/BitsetField.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/BitsetField.cpp

3.16 BitsetSetEnumerator Class Reference

Inheritance diagram for BitsetSetEnumerator:

Collaboration diagram for BitsetSetEnumerator:

Public Member Functions

- **BitsetSetEnumerator** (const BitsetElement &data1, Enumerator< size_t > ∗subsequent=nullptr, size_↩
  t offset=0)

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/enumerator/BitsetEnumerator.h

3.17 CombinationEnumerator Class Reference

Inheritance diagram for CombinationEnumerator:

Collaboration diagram for CombinationEnumerator:

Public Member Functions

- **CombinationEnumerator** (size_t n, size_t r, Enumerator ∗subsequent=nullptr)
- virtual bool **next_element** (defs::inds &result)
- defs::inds **default_result** () override

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/enumerator/CombinationEnumerator.↩
h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/enumerator/CombinationEnumerator.↩
cpp

3.18 consts::component_t< T > Struct Template Reference

Public Types

- typedef T **type**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/util/consts.h

3.19 consts::component_t< const std::complex< T > & > Struct Template Reference

Public Types

- typedef T **type**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/util/consts.h

3.20 consts::component_t< std::complex< T > > Struct Template Reference

Public Types

- typedef T **type**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/util/consts.h

3.21 Connection Class Reference

Inheritance diagram for Connection:

Public Member Functions

- **Connection** (const Field ∗field)
- **Connection** (const DeterminantElement &ket, const DeterminantElement &bra)
- **Connection** (const DeterminantElement &ket)
- const defs::det_work & **ann** () const
- const size_t & **ann** (const size_t &i) const
- const size_t & **nann** () const
- const defs::det_work & **cre** () const
- const size_t & **cre** (const size_t &i) const
- const size_t & **ncre** () const
- virtual void **connect** (const DeterminantElement &ket, const DeterminantElement &bra)
- virtual void **apply** (const DeterminantElement &ket, DeterminantElement &bra)
- void **zero** ()
- void **add_cre** (const size_t &i)
- void **add_ann** (const size_t &i)
- void **add** (const size_t &ann, const size_t &cre)
- void **add** (const size_t &ann1, const size_t &ann2, const size_t &cre1, const size_t &cre2)
- void **sort** ()
- const size_t & **nexcit** () const

Protected Attributes

- const size_t **m_nbit**
- defs::det_work **m_ann** {}
- defs::det_work **m_cre** {}
- size_t **m_nann**
- size_t **m_ncre**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/fermion/Connection.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/fermion/Connection.cpp

3.22 Hamiltonian::ConnectionList Class Reference

Inheritance diagram for Hamiltonian::ConnectionList:

Collaboration diagram for Hamiltonian::ConnectionList:

Public Member Functions

- **ConnectionList** (size_t nsite, size_t nbucket)

Public Attributes

- DeterminantField **determinant**
- NumericField< defs::ham_t > **helement**

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/hamiltonian/Hamiltonian.h

3.23 ContainerCombinationEnumerator< T > Class Template Reference

Inheritance diagram for ContainerCombinationEnumerator< T >:

Collaboration diagram for ContainerCombinationEnumerator< T >:

Public Member Functions

- **ContainerCombinationEnumerator** (const T &container, size_t n, size_t r, Enumerator ∗subsequent=nullptr)
- **ContainerCombinationEnumerator** (const T &container, size_t r, Enumerator ∗subsequent=nullptr)
- bool **next_element** (defs::inds &result) override

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/enumerator/ContainerCombination↩
  Enumerator.h

3.24 DeterminantElement::DatawordEnumerator Class Reference

Inheritance diagram for DeterminantElement::DatawordEnumerator:

Collaboration diagram for DeterminantElement::DatawordEnumerator:

Public Member Functions

- **DatawordEnumerator** (const DeterminantElement &data)

Protected Member Functions

- virtual size_t **get_dataword** (const size_t &idataword)
- virtual size_t **get_dataword** (const size_t &idataword, const size_t &nbit)
- bool **next_element** (defs::data_t &result) override

Protected Attributes

- size_t **m_idataword** = 0ul
- const DeterminantElement & **m_data**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/DeterminantField.h

3.25 DecodedDeterminant Struct Reference

Inheritance diagram for DecodedDeterminant:

Public Member Functions

- **DecodedDeterminant** (const Field ∗field)
- **DecodedDeterminant** (const DeterminantElement &det_elem)
- virtual void **update** (const DeterminantElement &det_elem)=0

Public Attributes

- const size_t **m_nbit**
- const size_t **m_element_dsize**
- defs::det_work **m_inds** {}
- size_t **m_nind** = 0ul

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/fermion/DecodedDeterminant.h

3.26 DenseHamiltonian Class Reference

Inheritance diagram for DenseHamiltonian:

Collaboration diagram for DenseHamiltonian:

Public Member Functions

- **DenseHamiltonian** (const Hamiltonian &source)

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/linalg/DenseHamiltonian.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/linalg/DenseHamiltonian.cpp

3.27 Determinant Class Reference

Inheritance diagram for Determinant:

Collaboration diagram for Determinant:

Public Member Functions

- **Determinant** (size_t nsite)
- Determinant & **operator=** (const DeterminantElement &rhs)
- Determinant & **operator=** (const Determinant &rhs)
- **Determinant** (const Determinant &obj)

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/fermion/Determinant.h

3.28 DeterminantClrEnumerator Class Reference

Inheritance diagram for DeterminantClrEnumerator:

Collaboration diagram for DeterminantClrEnumerator:

Public Member Functions

- **DeterminantClrEnumerator** (const DeterminantElement &data1, Enumerator< size_t > ∗subsequent=nullptr, size_t offset=0)

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/enumerator/BitsetEnumerator.h

3.29 DeterminantElement Class Reference

Inheritance diagram for DeterminantElement:

Collaboration diagram for DeterminantElement:

Classes

- class AntiDatawordEnumerator
- class DatawordEnumerator

Public Types

- typedef DeterminantField **Field_T**

Public Member Functions

- **DeterminantElement** (DeterminantField ∗field, char ∗begin)
- virtual std::string **to_string** () const
- void **set** (const size_t &ispin, const size_t &iorb)
- void **set** (const defs::inds &ispinorbs)
- void **clr** (const size_t &ispin, const size_t &iorb)
- bool **get** (const size_t &ispin, const size_t &iorb) const
- size_t **nsite** () const
- void **excite** (const size_t &i, const size_t &j)
- void **excite** (const size_t &i, const size_t &j, const size_t &k, const size_t &l)
- int **spin** () const
- int **nalpha** () const

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/DeterminantField.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/DeterminantField.cpp

3.30 DeterminantEnumerator< op > Class Template Reference

Inheritance diagram for DeterminantEnumerator< op >:

Collaboration diagram for DeterminantEnumerator< op >:

Public Member Functions

- **DeterminantEnumerator** (const DeterminantElement &data1, const DeterminantElement &data2, Enumerator< size_t > *subsequent=nullptr, size_t offset=0)
- bool **next_element** (size_t &result) override

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/enumerator/BitsetEnumerator.h

3.31 DeterminantField Class Reference

Inheritance diagram for DeterminantField:

Collaboration diagram for DeterminantField:

Public Member Functions

- **DeterminantField** (Table *table, size_t nelement, size_t nsite, const std::string &description="")
- DeterminantElement **operator()** (const size_t &irow, const size_t &isegment=0, const size_t &ielement=0)
- std::string **to_string** (size_t irow, size_t isegment, size_t ielement) override

Public Attributes

- const size_t **m_nsite**

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/DeterminantField.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/DeterminantField.cpp

3.32 DeterminantSampler Class Reference

Public Types

- enum **Outcome** { **no_excitations**, **single_excitation**, **double_excitation**, **both_excitations** }

Public Member Functions

- **DeterminantSampler** (const HeatBathSampler &precomputed)
- void **update** (const DeterminantElement &det)
- void **set_P1** (std::vector< defs::prob_t > &P1)
- void **set_P2** (std::vector< defs::prob_t > &P2, const size_t &p)
- void **draw_pq** (size_t &p, size_t &q)
- void **draw_pq** (size_t &p, size_t &q, defs::prob_t &prob)
- void **draw_r** (const size_t &p, const size_t &q, size_t &r)
- void **draw_r** (const size_t &p, const size_t &q, size_t &r, defs::prob_t &prob)
- void **draw_pqr** (size_t &p, size_t &q, size_t &r)
- void **draw_pqr** (size_t &p, size_t &q, size_t &r, defs::prob_t &prob)
- void **draw_s** (const size_t &p, const size_t &q, const size_t &r, size_t &s)
- void **draw_s** (const size_t &p, const size_t &q, const size_t &r, size_t &s, defs::prob_t &prob)
- void **draw** (size_t p, size_t q, size_t r, size_t s, defs::prob_t &prob_single, defs::prob_t &prob_double, defs::ham_t &helement_single, defs::ham_t &helement_double)
- void **draw** ()
- bool **single_generated** () const
- bool **double_generated** () const
- AntisymConnection & **get_single** ()
- AntisymConnection & **get_double** ()
- const Determinant & **get_single_dst_det** ()
- const Determinant & **get_double_dst_det** ()
- const defs::prob_t & **get_single_prob** () const
- const defs::prob_t & **get_double_prob** () const

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/heatbath/DeterminantSampler.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/heatbath/DeterminantSampler.cpp

3.33 DeterminantSetEnumerator Class Reference

Inheritance diagram for DeterminantSetEnumerator:

Collaboration diagram for DeterminantSetEnumerator:

Public Member Functions

- **DeterminantSetEnumerator** (const DeterminantElement &data1, Enumerator< size_t > ∗subsequent=nullptr, size_t offset=0)

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/enumerator/BitsetEnumerator.h

3.34 DeterministicSubspace Class Reference

Public Member Functions

- **DeterministicSubspace** ([WalkerList](#) ∗walker_list)
- void **add_determinant** (size_t irow_walker_list)
- const size_t & **nrow_local** () const
- const size_t & **nrow_full** () const
- void **build_hamiltonian** (const [Hamiltonian](#) ∗ham)

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/dynamics/DeterministicSubspace.h

3.35 Distributed< T > Class Template Reference

Public Member Functions

- [Distributed](#)< T > & **operator=** (const T &rhs)
- T & **local** ()
- T & **reduced** ()
- T & **sum** ()
- T & **max** ()
- T & **min** ()
- T & **bcast** (size_t irank)
- [Atomic](#)< T > **as_atomic** ()

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/parallel/Distributed.h

3.36 EigenSolver< T > Class Template Reference

Public Member Functions

- **EigenSolver** (const [Matrix](#)< T > &matrix)

Public Attributes

- [Matrix](#)< T > **m_evecs**
- std::vector< typename [consts::component_t](#)< T >::type > **m_evals**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/linalg/EigenSolver.h

3.37 Element Class Reference

Inheritance diagram for Element:

Collaboration diagram for Element:

Public Types

- typedef Field **Field_T**

Public Member Functions

- **Element** (Field ∗field, char ∗begin)
- virtual size_t **hash** () const
- virtual size_t **size** () const
- virtual size_t **dsize** () const
- virtual std::string **to_string** ()
- void **print** ()
- bool **compatible_with** (const Element &rhs) const
- defs::data_t & **dataword** (const size_t &idataword) const
- defs::data_t **get_dataword** (const size_t &idataword) const
- defs::data_t **get_dataword** (const size_t &idataword, const size_t &nbit) const
- defs::data_t **get_antidataword** (const size_t &idataword) const
- defs::data_t **get_antidataword** (const size_t &idataword, const size_t &nbit) const
- int **cmp** (const Element &rhs) const
- Element & **operator=** (const Element &rhs)
- bool **operator==** (const Element &rhs) const
- bool **operator!=** (const Element &rhs) const
- char ∗ **begin** () const
- size_t **nbit** () const
- void **zero** ()
- virtual bool **is_zero** () const
- const Field ∗ **field** () const
- virtual bool **is_complex** () const

Protected Attributes

- Field ∗ **m_field**
- char ∗ **m_begin**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/Element.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/Element.cpp

3.38 Enumerator< result_T > Class Template Reference

Collaboration diagram for Enumerator< result_T >:

Public Member Functions

- virtual bool **next** (result_T &result)
- virtual bool **next** (result_T &result, size_t &i)
- void **set_subsequent** ([Enumerator](#) ∗subsequent)
- bool **has_subsequent** ()
- virtual result_T **default_result** ()
- std::vector< result_T > **enumerate** ()
- size_t **count** ()
- bool **has_fewer_than_n_elements** (size_t nmax)

Protected Member Functions

- **Enumerator** ([Enumerator](#) ∗subsequent)

Protected Attributes

- [Enumerator](#) ∗ **m_subsequent** = nullptr
- [Enumerator](#) ∗ **m_current** = this

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/enumerator/Enumerator.h

3.39 ExactPropagator Class Reference

Inheritance diagram for ExactPropagator:

Collaboration diagram for ExactPropagator:

Public Member Functions

- **ExactPropagator** ([FciqmcCalculation](#) ∗fciqmc)
- void **off_diagonal** (const [DeterminantElement](#) &determinant, const [NumericElement](#)< defs::ham_t > &weight, [SpawnList](#) &spawn_list, bool flag_deterministic, bool flag_initiator) override
- void **diagonal** (const [NumericElement](#)< defs::ham_comp_t > &hdiag, [NumericElement](#)< defs::ham_t > &weight, defs::ham_comp_t &delta_square_norm, defs::ham_comp_t &delta_nw) override

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/dynamics/ExactPropagator.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/dynamics/ExactPropagator.cpp

3.40 ExcitationGenerator Class Reference

Inheritance diagram for ExcitationGenerator:

Collaboration diagram for ExcitationGenerator:

Public Member Functions

- **ExcitationGenerator** (const Hamiltonian ∗h, PrivateStore< PRNG > &prng)
- virtual bool **draw_single** (const DeterminantElement &src_det, DeterminantElement &dst_det, const OccupiedOrbitals &occ, const VacantOrbitals &vac, defs::prob_t &prob, defs::ham_t &helem, Antisym↵ Connection &anticonn)=0
- virtual bool **draw_double** (const DeterminantElement &src_det, DeterminantElement &dst_det, const OccupiedOrbitals &occ, defs::prob_t &prob, defs::ham_t &helem, AntisymConnection &anticonn)=0
- const Hamiltonian ∗ **ham** ()

Protected Attributes

- const Hamiltonian ∗ **m_h**
- PrivateStore< PRNG > & **m_prng**
- const size_t **m_norb**
- const size_t **m_nelec**
- const size_t **m_norb_pair**
- const size_t **m_nelec_pair**
- const bool **m_spin_conserving**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/sample/ExcitationGenerator.h

3.41 FcidumpFileIterator< T > Class Template Reference

Inheritance diagram for FcidumpFileIterator< T >:

Collaboration diagram for FcidumpFileIterator< T >:

Public Member Functions

- **FcidumpFileIterator** (const std::string &filename)
- size_t **nspinorb** () const
- size_t **nsite** () const

Public Attributes

- const size_t **m_norb**
- const size_t **m_isymm**
- const size_t **m_nelec**
- const defs::inds **m_orbsym**
- const bool **m_spin_resolved**

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/io/FcidumpFileIterator.h

3.42 FciqmcCalculation Class Reference

Collaboration diagram for FciqmcCalculation:

Public Member Functions

- **FciqmcCalculation** (const Options &input)
- void **execute** ()
- void **write_iter_stats** (size_t icycle)

Public Attributes

- const Options **m_input**
- RankAllocator< DeterminantElement > **m_rank_allocator**
- std::unique_ptr< FciqmcStatsFile > **m_stats_file** = nullptr
- std::unique_ptr< Hamiltonian > **m_ham**
- Determinant **m_reference**
- std::unique_ptr< Propagator > **m_prop**
- Wavefunction **m_wf**
- std::unique_ptr< FciqmcScratch > **m_scratch**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/dynamics/FciqmcCalculation.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/dynamics/FciqmcCalculation.cpp

3.43 FciqmcScratch Struct Reference

Public Member Functions

- **FciqmcScratch** (const DeterminantElement &ref)

Public Attributes

- std::unique_ptr< PrivateStore< OccupiedOrbitals > > **occ**
- std::unique_ptr< PrivateStore< VacantOrbitals > > **vac**
- std::unique_ptr< PrivateStore< Connection > > **conn**
- std::unique_ptr< PrivateStore< AntisymConnection > > **anticonn**

Static Public Attributes

- static const size_t **nelement_occ**
- static const size_t **nelement_vac**
- static const size_t **nelement_conn**
- static const size_t **nelement_anticonn**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/dynamics/FciqmcScratch.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/dynamics/FciqmcScratch.cpp

3.44 FciqmcStatsFile Struct Reference

Inheritance diagram for FciqmcStatsFile:

Collaboration diagram for FciqmcStatsFile:

Public Member Functions

- **FciqmcStatsFile** (const Options &input)

Public Attributes

- StatsField< size_t > **m_cycle_number**
- StatsField< defs::ham_comp_t > **m_diagonal_shift**
- StatsField< double > **m_timestep**
- StatsField< defs::ham_t > **m_ref_proj_energy_num**
- StatsField< defs::ham_t > **m_ref_weight**
- StatsField< defs::ham_t > **m_ref_proj_energy**
- StatsField< defs::ham_comp_t > **m_nwalker**
- StatsField< size_t > **m_ninitiator**
- StatsField< defs::wf_t > **m_aborted_weight**
- StatsField< size_t > **m_noccupied_det**
- StatsField< defs::prob_t > **m_psingle**

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/io/FciqmcStatsFile.h

3.45 Field Class Reference

Inheritance diagram for Field:

Collaboration diagram for Field:

Public Member Functions

- **Field** ([Table](#) *table, size_t element_size, size_t nelement, const std::type_info &type_info, const std::string &description="")
- [Element](#) **operator()** (const size_t &irow, const size_t &isegment=0, const size_t &ielement=0)
- bool **compatible_with** (const [Field](#) &rhs) const
- virtual size_t **nbit** () const
- virtual size_t **element_dsize** () const
- virtual bool **is_complex** () const
- virtual const std::string **description** () const
- void **expand_table** (size_t delta_nrow)
- bool **is_allocated** () const
- virtual std::string **to_string** (size_t irow, size_t isegment, size_t ielement)
- void **zero** (size_t irow, size_t isegment=0)

Protected Member Functions

- char * **begin** (const size_t &irow, const size_t &isegment=0)
- char * **element_begin** (const size_t &irow, const size_t &isegment=0, const size_t &ielement=0)

Protected Attributes

- [Table](#) * **m_table**
- size_t **m_element_size**
- size_t **m_element_dsize**
- const size_t **m_nelement**
- const std::type_index **m_type_index**
- size_t **m_offset**
- std::string **m_description**

Friends

- class **Table**
- class **Element**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/Field.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/Field.cpp

3.46 FileIterator Class Reference

Inheritance diagram for FileIterator:

Public Member Functions

- **FileIterator** (const std::string &filename, const size_t &ifirstline)
- **FileIterator** (const std::string &filename)
- **FileIterator** (const std::string &filename, const std::regex &regex)
- bool **next** (std::string &)
- std::string **next** ()

Static Public Member Functions

- static const size_t **line_number_from_regex** (const std::string &, const std::regex &)

Protected Attributes

- std::unique_ptr< std::ifstream > **m_file**
- const size_t **m_ifirstline**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/io/FileIterator.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/io/FileIterator.cpp

3.47 Flag Class Reference

Public Member Functions

- **Flag** (FlagField ∗field, size_t nelement, const std::string &description="")
- FlagElement **operator()** (const size_t &irow, const size_t &isegment=0)
- const defs::pair & **offset** () const

Friends

- class **FlagField**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/Flag.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/Flag.cpp

3.48 FlagElement Class Reference

Public Member Functions

- **FlagElement** (Flag ∗flag, BitsetElement bitset_element)
- void **operator=** (bool v)
- **operator bool** ()

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/Flag.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/Flag.cpp

3.49 FlagField Class Reference

Inheritance diagram for FlagField:

Collaboration diagram for FlagField:

Public Member Functions

- **FlagField** ([Table](#) ∗table, size_t nelement, const std::string &description)
- defs::pair **add_flag** ([Flag](#) ∗flag)
- const std::string **description** () const override

Friends

- class **Flag**

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/FlagField.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/FlagField.cpp

3.50 Hamiltonian Class Reference

Inheritance diagram for Hamiltonian:

Classes

- class [ConnectionList](#)

Public Member Functions

- **Hamiltonian** (const size_t &nsite)
- [consts::component_t](#)< defs::ham_t >::type **get_energy** (const [DeterminantElement](#) &det) const
- virtual defs::ham_t **get_element_0** (const defs::det_work &occs, const size_t &nocc) const =0
- defs::ham_t **get_element_0** (const [OccupiedOrbitals](#) &occs) const
- defs::ham_t **get_element_0** (const [DeterminantElement](#) &det) const
- defs::ham_t **get_element_0** (const [AntisymConnection](#) &connection) const
- virtual defs::ham_t **get_element_1** (const [AntisymConnection](#) &connection) const =0
- virtual defs::ham_t **get_element_2** (const size_t &i, const size_t &j, const size_t &k, const size_t &l) const =0
- defs::ham_t **get_element_2** (const [Connection](#) &connection) const
- defs::ham_t **get_element_2** (const [AntisymConnection](#) &connection) const
- defs::ham_t **get_element** (const [AntisymConnection](#) &connection) const
- defs::ham_t **get_element** (const [DeterminantElement](#) &bra, const [DeterminantElement](#) &ket) const
- size_t **nsite** () const
- size_t **nci** () const
- virtual bool **spin_conserving** () const =0
- virtual size_t **nelec** () const =0
- virtual bool **spin_resolved** () const =0
- [Determinant](#) **guess_reference** (const int &spin_level) const
- [Determinant](#) **refine_guess_reference** (const [DeterminantElement](#) &ref) const
- [Determinant](#) **choose_reference** (const int &spin_level) const
- void **all_connections_of_det** ([ConnectionList](#) ∗list, const [Determinant](#) &ref, const defs::ham_comp_t eps) const

Protected Attributes

- const size_t **m_nsite**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/hamiltonian/Hamiltonian.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/hamiltonian/Hamiltonian.cpp

3.51 HashMap< T > Class Template Reference

Inheritance diagram for HashMap< T >:

Public Member Functions

- **HashMap** (const size_t &nbucket)
- **HashMap** (const HashMap &old, const size_t &nbucket)
- virtual T **get_key** (const size_t &key_index) const =0
- virtual void **set_key** (const size_t &key_index, const T &key)=0
- size_t **bucket** (const T &key) const
- virtual size_t **lookup** (const size_t &ibucket, const T &key) const
- virtual size_t **lookup** (const T &key) const
- virtual void **insert** (const size_t &ibucket, const T &key, const size_t &key_index)
- virtual void **insert** (const T &key, const size_t &key_index)
- virtual size_t **remove** (const size_t &ibucket, const size_t &key_index)
- virtual size_t **remove** (const T &key)
- size_t **size** () const
- bool **operator==** (const HashMap &other) const
- void **print** () const

Protected Attributes

- std::vector< std::forward_list< size_t > > **m_buckets**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/hash/HashMap.h

3.52 HeatBathSampler Class Reference

Collaboration diagram for HeatBathSampler:

Public Member Functions

- **HeatBathSampler** (const Hamiltonian ∗m_h, PrivateStore< PRNG > &prng)

Public Attributes

- const [Hamiltonian](#) ∗ **m_h**
- [PrivateStore](#)< [PRNG](#) > & **m_prng**
- const size_t **m_nbit**
- const bool **m_spin_conserving**
- [NdArray](#)< defs::prob_t, 2 > **m_D**
- [NdArray](#)< defs::prob_t, 1 > **m_S**
- [NdArray](#)< defs::prob_t, 3 > **m_P3**
- [NdArray](#)< defs::prob_t, 3 > **m_H_tot**
- [NdArray](#)< defs::prob_t, 4 > **m_P4**
- std::unique_ptr< [PrivateStore](#)< [DeterminantSampler](#) > > **det_sampler**

Static Public Attributes

- static const size_t **nelement_det_sampler** = 1

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/heatbath/HeatBathSampler.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/heatbath/HeatBathSampler.cpp

3.53 HeatBathSamplers Class Reference

Inheritance diagram for HeatBathSamplers:

Collaboration diagram for HeatBathSamplers:

Public Member Functions

- **HeatBathSamplers** (const [Hamiltonian](#) ∗h, [PrivateStore](#)< [PRNG](#) > &prng)
- bool **draw_single** (const [DeterminantElement](#) &src_det, [DeterminantElement](#) &dst_det, const [Occupied↩](#) [Orbitals](#) &occ, const [VacantOrbitals](#) &vac, defs::prob_t &prob, defs::ham_t &helem, [AntisymConnection](#) &anticonn) override
- bool **draw_double** (const [DeterminantElement](#) &src_det, [DeterminantElement](#) &dst_det, const [Occupied↩](#) [Orbitals](#) &occ, defs::prob_t &prob, defs::ham_t &helem, [AntisymConnection](#) &anticonn) override

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/pchb/HeatBathSamplers.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/pchb/HeatBathSamplers.cpp

3.54 Indexer< nind > Class Template Reference

Public Member Functions

- template<typename... Args>
  Indexer (const size_t &first, Args...shape)
- **Indexer** (const std::array< size_t, nind > &shape)
- const std::array< size_t, nind > & **shape** () const
- const std::array< size_t, nind > & **strides** () const
- size_t **nelement** () const
- template<typename... Args>
  size_t **get_sub** (Args...inds) const
- template<typename... Args>
  size_t **get** (Args...inds) const

Protected Attributes

- std::array< size_t, nind > **m_shape** {}
- std::array< size_t, nind > **m_strides** {}

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/multidim/Indexer.h

3.55 InputError Class Reference

Inheritance diagram for InputError:

Collaboration diagram for InputError:

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/io/InputOptions.h

3.56 InputOptions Class Reference

Inheritance diagram for InputOptions:

Collaboration diagram for InputOptions:

Public Member Functions

- **InputOptions** (CLI::App &app)
- template<typename T >
  void **add_option** (const std::string cli_options, T &variable_to_bind, const std::string description, bool re-
  quired=false)
- void **add_flag** (const std::string cli_options, bool &variable_to_bind, const std::string description)

Static Public Attributes

- static const std::string **description**

Additional Inherited Members

3.56.1 Member Data Documentation

3.56.1.1 const std::string InputOptions::description [static]

Initial value:

```
=
        "\nM7: Many-body Stochastic Expectation Value Estimation Networks\n"
        "Command line interface\n"
```

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/io/InputOptions.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/io/InputOptions.cpp

3.57 Integrals Class Reference

Inheritance diagram for Integrals:

Public Attributes

- const size_t **m_norb**
- const bool **m_spin_resolved**
- const size_t **m_nspinorb**
- const size_t **m_nspatorb**

Protected Member Functions

- **Integrals** (size_t norb, bool spin_resolved)
- size_t **spinorb** (const size_t &ispat, const size_t &ispin) const

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/integrals/Integrals.h

3.58 Integrals_1e< T, isym > Class Template Reference

Inheritance diagram for Integrals_1e< T, isym >:

Collaboration diagram for Integrals_1e< T, isym >:

Public Member Functions

- **Integrals_1e** (const size_t &norb, bool spin_resolved)
- **Integrals_1e** (std::string fname)
- size_t **flat_index** (const size_t &i, const size_t &j) const
- void **set** (const size_t &i, const size_t &j, const T &value)
- void **set** (const size_t &ispat, const size_t &ispin, const size_t &jspat, const size_t &jspin, const T &value)
- void **set** (const defs::inds &inds, const T &value)
- void **set_from_fcidump** (const defs::inds &inds, const T &value, bool spin_major=false)
- T **get** (const size_t &i, const size_t &j) const
- T **get** (const size_t &ispat, const size_t &ispin, const size_t &jspat, const size_t &jspin) const
- T **operator()** (const size_t &i, const size_t &j) const
- bool **spin_conserving** () const

Static Public Member Functions

- static bool **valid_inds** (const defs::inds &inds)

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/integrals/Integrals_1e.h

3.59 Integrals_2e< T, isym > Class Template Reference

Inheritance diagram for Integrals_2e< T, isym >:

Collaboration diagram for Integrals_2e< T, isym >:

Public Member Functions

- **Integrals_2e** (const size_t &norb, bool spin_resolved)
- **Integrals_2e** (std::string fname, bool spin_major=false)
- size_t **flat_index** (const size_t &icase, const size_t &i, const size_t &j, const size_t &k, const size_t &l) const
- void **set** (const size_t &i, const size_t &j, const size_t &k, const size_t &l, const T &value)
- void **set** (const size_t &ispat, const size_t &ispin, const size_t &jspat, const size_t &jspin, const size_t &kspat, const size_t &kspin, const size_t &lspat, const size_t &lspin, const T &value)
- void **set** (const defs::inds &inds, const T &value)
- void **set_from_fcidump** (const defs::inds &inds, const T &value, bool spin_major=false)
- T **get** (const size_t &i, const size_t &j, const size_t &k, const size_t &l) const
- T **element** (const size_t &i, const size_t &j, const size_t &k, const size_t &l) const
- T **element** (const size_t &ispat, const size_t &ispin, const size_t &jspat, const size_t &jspin, const size_t &kspat, const size_t &kspin, const size_t &lspat, const size_t &lspin) const
- T **phys_element** (const size_t &i, const size_t &j, const size_t &k, const size_t &l) const
- T **phys_element** (const size_t &ispat, const size_t &ispin, const size_t &jspat, const size_t &jspin, const size_t &kspat, const size_t &kspin, const size_t &lspat, const size_t &lspin)
- T **phys_antisym_element** (const size_t &i, const size_t &j, const size_t &k, const size_t &l) const
- T **phys_antisym_element** (const size_t &ispat, const size_t &ispin, const size_t &jspat, const size_t &jspin, const size_t &kspat, const size_t &kspin, const size_t &lspat, const size_t &lspin) const

Static Public Member Functions

- static bool **valid_inds** (defs::inds inds)

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/integrals/Integrals_2e.h

3.60 consts::is_complex_t< T > Struct Template Reference

Inheritance diagram for consts::is_complex_t< T >:

Collaboration diagram for consts::is_complex_t< T >:

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/util/consts.h

3.61 consts::is_complex_t< const std::complex< T > & > Struct Template Reference

Inheritance diagram for consts::is_complex_t< const std::complex< T > & >:

Collaboration diagram for consts::is_complex_t< const std::complex< T > & >:

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/util/consts.h

3.62 consts::is_complex_t< const std::complex< T > > Struct Template Reference

Inheritance diagram for consts::is_complex_t< const std::complex< T > >:

Collaboration diagram for consts::is_complex_t< const std::complex< T > >:

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/util/consts.h

3.63 consts::is_complex_t< std::complex< T > & > Struct Template Reference

Inheritance diagram for consts::is_complex_t< std::complex< T > & >:

Collaboration diagram for consts::is_complex_t< std::complex< T > & >:

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/util/consts.h

3.64 consts::is_complex_t< std::complex< T > > Struct Template Reference

Inheritance diagram for consts::is_complex_t< std::complex< T > >:

Collaboration diagram for consts::is_complex_t< std::complex< T > >:

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/util/consts.h

3.65 List Class Reference

Inheritance diagram for List:

Collaboration diagram for List:

Public Member Functions

- **List** (size_t nsegment=1)
- void **recv** (List *list)
- void **expand** (size_t delta_nrow) override
- const defs::inds & **high_water_mark** () const
- const size_t & **high_water_mark** (const size_t isegment) const
- virtual size_t **push** (const size_t &isegment=0)
- size_t **push** (const size_t &isegment, const size_t &nrow)
- size_t **expand_push** (const size_t &isegment, const size_t &nrow, double factor=1.5)
- size_t **expand_push** (const size_t &isegment=0, double factor=1.5)
- void **zero** () override
- std::string **to_string** ()
- void **communicate** ()
- void **all_gather** (List &local)

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/list/List.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/list/List.cpp

3.66 ListSafeHashMap< T > Struct Template Reference

Inheritance diagram for ListSafeHashMap< T >:

Collaboration diagram for ListSafeHashMap< T >:

Public Member Functions

- **ListSafeHashMap** (MappedList< T > &list, const size_t &nbucket)
- T **get_key** (const size_t &key_index) const override
- void **set_key** (const size_t &key_index, const T &key) override

Public Attributes

- MappedList< T > & **m_list**

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/list/MappedList.h

3.67 MagnitudeLogger Class Reference

Public Member Functions

- **MagnitudeLogger** (const Options &input)
- void **log** (size_t nexcit, defs::ham_t helem, defs::prob_t prob)
- void **synchronize** ()

Public Attributes

- double **m_tau**
- defs::prob_t **m_psingle** = 0.001

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/dynamics/MagnitudeLogger.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/dynamics/MagnitudeLogger.cpp

3.68 MappedList< T > Class Template Reference

Inheritance diagram for MappedList< T >:

Collaboration diagram for MappedList< T >:

Public Member Functions

- **MappedList** (Field_T &key_field, size_t nbucket)
- Field_T & **key_field** () const
- Mutex **get_mutex** (const size_t &ibucket)
- Mutex **key_mutex** (const T &key)
- size_t **lookup** (const T &key)
- size_t **lookup** (Mutex &mutex, const T &key)
- virtual size_t **push** (Mutex &mutex, const T &key)
- virtual size_t **push** (const T &key)
- size_t **lookup_push** (Mutex &mutex, const T &key)
- size_t **lookup_push** (const T &key)
- bool **row_empty** (const size_t &irow) const
- void **print_map** () const

Protected Attributes

- Field_T & **m_key_field**
- ListSafeHashMap< T > **m_map**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/list/MappedList.h

3.69 Matrix< T > Class Template Reference

Public Member Functions

- **Matrix** (size_t nrow, size_t ncol)
- **Matrix** (size_t n)
- T & **operator()** (const size_t &irow, const size_t &icol)
- void **zero** ()
- bool **is_square** () const
- void **set_row** (const size_t &irow, const std::vector< T > &v)
- EigenSolver< T > **diagonalize** () const
- void **multiply** (const std::vector< T > &in, std::vector< T > &out)
- void **print** ()
- template<>
  void **multiply** (const std::vector< double > &in, std::vector< double > &out)
- template<>
  void **multiply** (const std::vector< std::complex< double >> &in, std::vector< std::complex< double >> &out)

Public Attributes

- const size_t **m_nrow**
- const size_t **m_ncol**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/linalg/Matrix.h

3.70 mpi Struct Reference

Public Types

- enum **MpiOp** {
  MpiMax, **MpiMin**, **MpiSum**, **MpiLand**,
  MpiLor }

Static Public Member Functions

- static size_t **nrank** ()
- static size_t **irank** ()
- static std::string **processor_name** ()
- static void **barrier** ()
- template<typename T >
  static bool **max** (const T ∗send, T ∗recv, size_t ndata=1, size_t iroot=0)
- template<typename T >
  static bool **all_max** (const T ∗send, T ∗recv, size_t ndata=1)
- template<typename T >
  static T **max** (const T ∗send, size_t iroot=0)
- template<typename T >
  static T **all_max** (const T ∗send)
- template<typename T >
  static T **all_max** (const T &send)
- template<typename T >
  static bool **min** (const T ∗send, T ∗recv, size_t ndata=1, size_t iroot=0)
- template<typename T >
  static bool **all_min** (const T ∗send, T ∗recv, size_t ndata=1)
- template<typename T >
  static T **min** (const T ∗send, size_t iroot=0)
- template<typename T >
  static T **all_min** (const T ∗send)
- template<typename T >
  static T **all_min** (const T &send)
- template<typename T >
  static bool **sum** (const T ∗send, T ∗recv, size_t ndata=1, size_t iroot=0)
- template<typename T >
  static bool **all_sum** (const T ∗send, T ∗recv, size_t ndata=1)
- template<typename T >
  static T **sum** (const T ∗send, size_t iroot=0)
- template<typename T >
  static T **all_sum** (const T ∗send)
- template<typename T >
  static T **all_sum** (const T &send)
- template<typename T >
  static bool **land** (const T ∗send, T ∗recv, size_t ndata=1, size_t iroot=0)
- template<typename T >
  static bool **all_land** (const T ∗send, T ∗recv, size_t ndata=1)
- template<typename T >
  static T **land** (const T ∗send, size_t iroot=0)
- template<typename T >
  static T **all_land** (const T ∗send)
- template<typename T >
  static T **all_land** (const T &send)

- template<typename T >
  static bool **bcast** (T ∗data, const size_t ndata=1, size_t iroot=0)
- template<typename T >
  static bool **bcast** (T &data, size_t iroot=0)
- template<typename T >
  static bool **bcast** (std::vector< T > &data, size_t ndata=0, size_t iroot=0)
- template<typename T >
  static bool **all_to_all** (const T ∗send, const size_t nsend, T ∗recv, const size_t nrecv)
- template<typename T >
  static bool **all_to_all** (const std::vector< T > &send, std::vector< T > &recv)
- template<typename T >
  static bool **all_to_allv** (const T ∗send, const defs::inds &sendcounts, const defs::inds &senddispls, T ∗recv, const defs::inds &recvcounts, const defs::inds &recvdispls)
- template<typename T >
  static bool **all_gatherv** (const T ∗send, const size_t &sendcount, T ∗recv, const defs::inds &recvcounts, const defs::inds &recvdispls)
- template<typename T >
  static bool **all_gather** (const T ∗send, const int sendcount, T ∗recv, const int recvcount)
- static bool **i_am** (const size_t i)
- static bool **i_am_root** ()
- static void **rank_print** (const std::string s, size_t irank)
- static void **root_print** (const std::string s)
- static bool **initialized** ()
- static bool **finalized** ()
- static void **initialize** (int ∗argc=NULL, char ∗∗∗argv=NULL)
- static void **finalize** ()

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/parallel/MPIWrapper.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/parallel/MPIWrapper.cpp

3.71 Mutex Class Reference

Public Member Functions

- **Mutex** (omp_lock_t &lock, const size_t &index)
- size_t **index** () const

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/hash/MutexVector.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/hash/MutexVector.cpp

3.72 MutexVector Class Reference

Public Member Functions

- **MutexVector** (size_t n)
- size_t **size** () const
- void **resize** (const size_t &n)
- void **grow** (const size_t &n_add)
- Mutex **get** (const size_t &i)

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/hash/MutexVector.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/hash/MutexVector.cpp

3.73 NdArray< T, nind > Class Template Reference

Public Member Functions

- template<typename... Args>
  NdArray (const size_t &first, Args...shape)
- template<typename... Args>
  NdArray (T ∗data, const std::array< size_t, nind > &shape)
- template<typename... Args>
  T ∗ **view** (Args...inds) const
- template<typename... Args>
  NdArray< T, nind-sizeof...(Args)> **subarray** (Args...subs)
- void **operator=** (NdArray &src)
- void **operator=** (std::vector< T > &src)
- void **operator∗=** (const T &factor)
- void **operator/=** (const T &factor)
- const std::array< size_t, nind > & **shape** () const
- const std::array< size_t, nind > & **strides** () const
- size_t **nelement** () const

Protected Attributes

- const Indexer< nind > **m_indexer**
- std::vector< T > **m_data_internal**
- T ∗ **m_data** = nullptr

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/multidim/NdArray.h

3.74 NumericElement< T > Class Template Reference

Inheritance diagram for NumericElement< T >:

Collaboration diagram for NumericElement< T >:

Public Types

- typedef NumericField< T > **Field_T**

Public Member Functions

- **NumericElement** (NumericField< T > ∗field, char ∗begin)
- **NumericElement** (const T &value)
- T & **operator**∗ () const
- **operator T** () const
- virtual NumericElement< T > & **operator=** (const T &v)
- virtual NumericElement< T > & **operator=** (const NumericElement< T > &v)
- bool **operator==** (const T &v) const
- bool **operator==** (const NumericElement< T > &other) const
- bool **operator!=** (const T &v) const
- bool **operator!=** (const NumericElement< T > &other) const
- NumericElement< T > & **operator**∗**=** (const T &v)
- NumericElement< T > & **operator/=** (const T &v)
- NumericElement< T > & **operator+=** (const T &v)
- NumericElement< T > & **operator-=** (const T &v)
- bool **is_zero** () const override
- size_t **size** () const override
- virtual std::string **to_string** ()

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/NumericElement.h

3.75 NumericField< T > Class Template Reference

Inheritance diagram for NumericField< T >:

Collaboration diagram for NumericField< T >:

Public Member Functions

- **NumericField** (Table ∗table, size_t nelement=1, const std::string &description="")
- NumericElement< T > **operator()** (const size_t &irow, const size_t &isegment=0, const size_t &ielement=0)
- bool **is_complex** () const override
- std::string **to_string** (size_t irow, size_t isegment, size_t ielement) override

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/NumericElement.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/NumericField.h

3.76 OccupiedOrbitals Struct Reference

Inheritance diagram for OccupiedOrbitals:

Collaboration diagram for OccupiedOrbitals:

Public Member Functions

- **OccupiedOrbitals** (const Field ∗field)
- **OccupiedOrbitals** (const DeterminantElement &det_elem)
- void **update** (const DeterminantElement &det_elem) override

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/fermion/DecodedDeterminant.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/fermion/DecodedDeterminant.cpp

3.77 Options Struct Reference

Inheritance diagram for Options:

Public Member Functions

- bool **validate** () const

Public Attributes

- std::string **fcidump_path** = "FCIDUMP"
- std::string **stats_path** = "M7.stats"
- bool **exact_propagation** = false
- double **nwalker_initial** = 1.0
- double **nwalker_target** = 0.0
- double **nadd_initiator** = 3.0
- double **max_bloom** = 1.0
- size_t **prng_seed** = 0
- size_t **prng_ngen** = 1000
- size_t **ndet_semistoch** = 0
- size_t **spin_restrict** = 0
- double **walker_factor_initial** = 1.0
- double **buffer_factor_initial** = 10.0
- double **min_spawn_mag** = 0.0
- size_t **nload_balance_block** = 10
- double **tau_initial** = 0.05
- bool **dynamic_tau** = false
- size_t **nenough_spawns_for_dynamic_tau** = 100
- double **shift_initial** = 0.0
- double **shift_damp** = 1.0
- size_t **shift_update_period** = 1
- size_t **ncycle** = $\sim$0ul

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/io/Options.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/io/Options.cpp

3.78 PerforableMappedList< T > Class Template Reference

Inheritance diagram for PerforableMappedList< T >:

Collaboration diagram for PerforableMappedList< T >:

Public Member Functions

- **PerforableMappedList** (Field_T &key_field, size_t nbucket)
- void **synchronize** ()
- size_t **push** ([Mutex](#) &mutex, const T &key) override
- size_t **push** (const T &key) override
- size_t **remove** ([Mutex](#) &mutex, const size_t &key_index)
- size_t **remove** (const T &key, const size_t &key_index)
- size_t **remove** (const T &key)
- size_t **nfilled** () const
- size_t **nzero_rows** (size_t isegment=0) const
- void **expand** (size_t delta_rows) override

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/list/PerforableMappedList.h

3.79 PrivateStore< T > Class Template Reference

Public Member Functions

- template<typename... Args>
  PrivateStore (Args &&...construct_args)
- T & **get** ()
- const size_t & **nthread** () const
- template<typename U = T>
  enable_if_t< true, U > **reduce_land** ()
- template<typename U = T>
  enable_if_t< true, U > **reduce_lor** ()
- template<typename U = T>
  enable_if_t< true, U > **reduce_sum** ()
- template<typename U = T>
  enable_if_t< true, U > **reduce_prod** ()
- template<typename U = T>
  enable_if_t< std::is_integral< U >::value, U > **reduce_max** ()
- template<typename U = T>
  enable_if_t<!std::is_integral< U >::value, U > **reduce_max** ()
- template<typename U = T>
  enable_if_t< std::is_integral< U >::value, U > **reduce_min** ()
- template<typename U = T>
  enable_if_t<!std::is_integral< U >::value, U > **reduce_min** ()

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/thread/PrivateStore.h

3.80 PRNG Class Reference

Public Member Functions

- **PRNG** (const size_t &seed, const size_t &block_size)
- void **refresh** ()
- uint32_t **draw_uint** ()
- uint32_t **draw_uint** (uint32_t)
- double **draw_float** ()
- template<typename T >
  T **stochastic_round** (const T &v, const double &magnitude)
- template<typename T >
  std::complex< T > **stochastic_round** (const std::complex< T > &v, const double &magnitude)
- template<typename T >
  T **stochastic_threshold** (const T &v, const double &magnitude)

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/sample/PRNG.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/sample/PRNG.cpp

3.81 Propagator Class Reference

Inheritance diagram for Propagator:

Collaboration diagram for Propagator:

Public Member Functions

- **Propagator** (FciqmcCalculation ∗fciqmc)
- void **spawn** (SpawnList &spawn_list, const DeterminantElement &dst_det, const defs::wf_t &delta, bool flag_initiator)
- virtual void **diagonal** (const NumericElement< defs::ham_comp_t > &hdiag, NumericElement< defs::ham↵ _t > &weight, defs::ham_comp_t &delta_square_norm, defs::ham_comp_t &delta_nw)=0
- virtual void **off_diagonal** (const DeterminantElement &determinant, const NumericElement< defs::ham_t > &weight, SpawnList &spawn_list, bool flag_deterministic, bool flag_initiator)=0
- virtual defs::ham_t **round** (const defs::ham_t &weight)
- void **update** (const size_t icycle, defs::wf_comp_t nwalker, defs::wf_comp_t nwalker_growth)
- void **write_iter_stats** (FciqmcStatsFile ∗stats_file)

Public Attributes

- FciqmcCalculation ∗ **m_fciqmc**
- const Options & **m_input**
- const std::unique_ptr< Hamiltonian > & **m_ham**
- const RankAllocator< DeterminantElement > & **m_rank_allocator**
- MagnitudeLogger **m_magnitude_logger**
- double **m_tau**
- defs::ham_comp_t **m_shift**
- bool **vary_shift** = false
- Distributed< defs::wf_comp_t > **m_largest_spawn_magnitude**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/dynamics/Propagator.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/dynamics/Propagator.cpp

3.82 RankAllocator< T > Class Template Reference

Public Member Functions

- **RankAllocator** (size_t nblock)
- size_t **get_rank** (const T &key) const

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/parallel/RankAllocator.h

3.83 AlignedAllocator2< T, alignment >::rebind< U > Struct Template Reference

Public Types

- typedef AlignedAllocator2< U, alignment > **other**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/thread/AlignedAllocator2.h

3.84 AlignedAllocator< T, alignment >::rebind< U > Struct Template Reference

Public Types

- typedef AlignedAllocator< U, alignment > **other**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/thread/AlignedAllocator.h

3.85 SafeHashMap< T > Class Template Reference

Inheritance diagram for SafeHashMap< T >:

Collaboration diagram for SafeHashMap< T >:

Public Member Functions

- **SafeHashMap** (const size_t &nbucket)
- **SafeHashMap** (const HashMap< T > &old, const size_t &nbucket)
- Mutex **get_mutex** (const size_t &ibucket) const
- Mutex **key_mutex** (const T &key) const
- size_t **lookup** (Mutex &mutex, const T &key) const
- size_t **lookup** (const T &key) const override
- void **insert** (Mutex &mutex, const T &key, const size_t &key_index)
- void **insert** (const T &key, const size_t &key_index) override
- size_t **remove** (Mutex &mutex, const size_t &key_index)

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/hash/SafeHashMap.h

3.86 Scratch Class Reference

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/global/Scratch.h

3.87 SparseEntry< T > Struct Template Reference

Collaboration diagram for SparseEntry< T >:

Public Attributes

- size_t **icol**
- T **element**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/sparse/SparseMatrix.h

3.88 SparseMatrix< T > Class Template Reference

Public Member Functions

- size_t **nrow** ()
- void **resize** (const size_t nrow)
- void **expand** (const size_t delta_nrow)
- T & **operator()** (const size_t &irow, const size_t &icol)
- bool **empty** ()
- void **multiply** (const std::vector< T > &in, std::vector< T > &out)

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/sparse/SparseMatrix.h

3.89 SpawnList Struct Reference

Inheritance diagram for SpawnList:

Collaboration diagram for SpawnList:

Public Member Functions

- **SpawnList** (size_t nsite, size_t nsegment)
- size_t **add** (const size_t isegment, const DeterminantElement &determinant, const defs::wf_t &weight, bool flag_parent_initiator)

Public Attributes

- DeterminantField **m_determinant**
- NumericField< defs::wf_t > **m_weight**
- Flags **m_flags**

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/dynamics/SpawnList.h

3.90 StatsElement< T > Class Template Reference

Inheritance diagram for StatsElement< T >:

Collaboration diagram for StatsElement< T >:

Public Member Functions

- **StatsElement** (StatsField< T > ∗field, char ∗begin)
- StatsElement< T > & **operator=** (const T &v) override
- const size_t & **fp_precision** () const
- StatsElement< T > & **operator=** (const NumericElement< T > &v) override
- std::string **to_string** () override

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/io/StatsFile.h

3.91 StatsField< T > Class Template Reference

Inheritance diagram for StatsField< T >:

Collaboration diagram for StatsField< T >:

Public Member Functions

- **StatsField** (StatsFile ∗file, size_t nelement=1, const std::string &description="", size_t fp_precision=6, bool retention=false)
- std::pair< T, T > **mean_std** (size_t istart, size_t iend) const
- std::pair< T, T > **mean_std** (size_t istart)
- std::pair< T, T > **mean_std** ()
- void **write** (const T &v, size_t ielement=0)
- bool **is_complex** () const override
- std::string **to_string** (size_t irow, size_t isegment, size_t ielement) override

Public Attributes

- const size_t **m_fp_precision**
- const bool **m_retention**
- std::vector< T > **m_series**

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/io/StatsFile.h

3.92 StatsFile Class Reference

Inheritance diagram for StatsFile:

Collaboration diagram for StatsFile:

Public Member Functions

- **StatsFile** (const std::string &fname)
- void **flush** ()
- std::string **to_string** () override

Protected Member Functions

- void **write_header** ()

Protected Attributes

- const std::string **m_fname**
- std::unique_ptr< std::ofstream > **m_file**
- size_t **m_nflush** = 0

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/io/StatsFile.h

3.93 StochasticPropagator Class Reference

Inheritance diagram for StochasticPropagator:

Collaboration diagram for StochasticPropagator:

Public Member Functions

- **StochasticPropagator** (FciqmcCalculation ∗fciqmc)
- void **off_diagonal** (const DeterminantElement &src_det, const NumericElement< defs::ham_t > &weight, SpawnList &spawn_list, bool flag_deterministic, bool flag_initiator) override
- void **diagonal** (const NumericElement< defs::ham_comp_t > &hdiag, NumericElement< defs::ham_t > &weight, defs::ham_comp_t &delta_square_norm, defs::ham_comp_t &delta_nw) override

Public Attributes

- PrivateStore< PRNG > **m_prng**
- std::unique_ptr< ExcitationGenerator > **m_exgen** = nullptr
- PrivateStore< Determinant > **m_dst_det**
- PrivateStore< OccupiedOrbitals > **m_occ**
- PrivateStore< VacantOrbitals > **m_vac**
- PrivateStore< AntisymConnection > **m_anticonn**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/dynamics/StochasticPropagator.h

3.94 Table Class Reference

Inheritance diagram for Table:

Public Member Functions

- **Table** (size_t nsegment=1)
- char ∗ **field_begin** (const Field ∗field, const size_t &irow, const size_t isegment=0)
- char ∗ **row_begin** (const size_t &irow, const size_t isegment=0)
- virtual void **expand** (size_t delta_nrow)
- virtual void **resize** (size_t nrow)
- size_t **irow** (const size_t &irow, const size_t &isegment=0) const
- virtual void **zero** ()
- void **zero_row** (const size_t &irow, const size_t &isegment)
- size_t **add_field** (Field ∗field)
- void **update_last_field** ()
- void **print** ()
- const size_t & **nrow_per_segment** () const
- bool **compatible_with** (const Table &other) const
- bool **is_allocated** () const
- std::string **row_to_string** (size_t irow, size_t isegment)
- virtual std::string **to_string** ()
- virtual std::string **to_string** (const defs::inds &nrows)
- void **print_row** (size_t irow, size_t isegment)
- size_t **dsize** () const

Protected Attributes

- std::vector< defs::data_t, AlignedAllocator< defs::data_t, defs::cache_line_size > > **m_data**
- std::vector< Field ∗ > **m_fields**
- size_t **m_row_size** = 0
- size_t **m_padded_row_size** = 0
- size_t **m_padded_row_dsize** = 0
- const size_t **m_nsegment**
- size_t **m_nrow_per_segment** = 0
- size_t **m_segment_size** = 0
- size_t **m_segment_dsize** = 0
- defs::inds **m_segment_doffsets**
- std::vector< std::function< std::string(const Element ∗)> > **m_printers**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/Table.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/table/Table.cpp

3.95 TensorFileIterator< T > Class Template Reference

Inheritance diagram for TensorFileIterator< T >:

Collaboration diagram for TensorFileIterator< T >:

Public Member Functions

- **TensorFileIterator** (const std::string filename, const size_t nind, const bool indsfirst)
- bool **next** (defs::inds &inds, T &value)

Static Public Member Functions

- static std::string **uint_space_list_regex_string** (const size_t &n)
- static std::string **data_regex_string** (const size_t &nind, const bool &indsfirst)
- static size_t **nind** (const std::string &filename)
- static size_t **nreal_given** (const std::string &filename, const std::regex &data_regex)
- static size_t **indsfirst** (const std::string &filename)
- static bool **extract_line** (const std::string &line, const size_t &nind, const size_t &nreal_given, const bool &indsfirst, defs::inds &inds, T &value)
- static defs::inds **shape** (const std::string &filename, const size_t &nind, const size_t &nreal_given, const bool &indsfirst, const std::regex &data_regex)

Public Attributes

- const size_t **m_nind**
- const bool **m_indsfirst**
- const size_t **m_nreal_given**
- const defs::inds **m_shape**

Static Public Attributes

- static constexpr size_t **m_nreal** = std::__is_static_castable<T, float>::value ? 1 : 2

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/io/TensorFileIterator.h

3.96 VacantOrbitals Struct Reference

Inheritance diagram for VacantOrbitals:

Collaboration diagram for VacantOrbitals:

Public Member Functions

- **VacantOrbitals** (const Field ∗field)
- **VacantOrbitals** (const DeterminantElement &det_elem)
- void **update** (const DeterminantElement &det_elem) override

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/fermion/DecodedDeterminant.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/fermion/DecodedDeterminant.cpp

3.97 WalkerList Struct Reference

Inheritance diagram for WalkerList:

Collaboration diagram for WalkerList:

Public Member Functions

- **WalkerList** (size_t nsite, size_t nbucket)
- size_t **add** (Mutex &mutex, const DeterminantElement &key, const defs::wf_t &weight, const defs::ham_←
  comp_t &hdiag, bool initiator=false, bool reference_connection=false, bool deterministic=false)
- size_t **add** (const DeterminantElement &key, const defs::wf_t &weight, const defs::ham_comp_t &hdiag, bool
  initiator=false, bool reference_connection=false, bool deterministic=false)
- size_t **verify_ninitiator** (const double &nadd)
- std::list< size_t > **top_weighted** (size_t n)

Public Attributes

- DeterminantField **m_determinant**
- NumericField< defs::wf_t > **m_weight**
- NumericField< defs::ham_comp_t > **m_hdiag**
- Flags **m_flags**

Additional Inherited Members

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/dynamics/WalkerList.h

3.98 Wavefunction Class Reference

Collaboration diagram for Wavefunction:

Public Member Functions

- **Wavefunction** (FciqmcCalculation ∗fciqmc)
- defs::wf_t **get_reference_weight** ()
- void **propagate** ()
- void **communicate** ()
- void **consolidate_incoming_weight** ()
- void **annihilate** ()
- void **write_iter_stats** (FciqmcStatsFile ∗stats_file)

Public Attributes

- Distributed< defs::wf_comp_t > **m_square_norm**
- Distributed< defs::wf_comp_t > **m_delta_square_norm**
- Distributed< defs::wf_comp_t > **m_nw**
- Distributed< defs::wf_comp_t > **m_delta_nw**
- defs::wf_comp_t **m_nw_growth_rate**
- Distributed< size_t > **m_noccupied_determinant**

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

- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/dynamics/Wavefunction.h
- /home/teamcity/TeamCity/buildAgent/work/5343cdffda4690e5/src/core/dynamics/Wavefunction.cpp

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