QMC2 Documentation

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Contents

Chapter 1

Class Index

1.1 Class Hierarchy

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

Chapter 2

Class Index

2.1 Class List

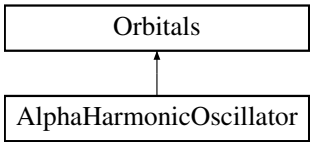
Here are the classes, structs, unions and interfaces with brief descriptions:

Chapter 3

Class Documentation

3.1 AlphaHarmonicOscillator Class Reference

Inheritance diagram for AlphaHarmonicOscillator:



Public Member Functions

- **AlphaHarmonicOscillator** (GeneralParams &, VariationalParams &)
- **AlphaHarmonicOscillator** (GeneralParams &)
- virtual void **set_qnum_indie_terms** (const Walker ∗walker, int i)

Protected Member Functions

- virtual double **get_variational_derivative** (const Walker ∗walker, int n)
- void **get_qnums** ()
- double **H** (int n, double x) const
- virtual double **get_parameter** (int n)
- virtual void **set_parameter** (double parameter, int n)

Protected Attributes

- double ∗ **alpha**
- double ∗ **k**
- double ∗ **k2**

- double * **w_over_a**
- double * **exp_factor**
- arma::Mat< int > **qnums**
- double **w**

Friends

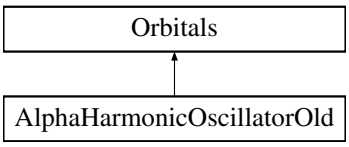
- class **ExpandedBasis**

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

- src/Orbitals/AlphaHarmonicOscillator/AlphaHarmonicOscillator.h
- src/Orbitals/AlphaHarmonicOscillator/AlphaHarmonicOscillator.cpp

3.2 AlphaHarmonicOscillatorOld Class Reference

Inheritance diagram for AlphaHarmonicOscillatorOld:



Public Member Functions

- **AlphaHarmonicOscillatorOld** (GeneralParams &, VariationalParams &)

Friends

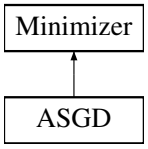
- class **ExpandedBasis**

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

- src/Orbitals/AlphaHarmonicOscillatorOld/AlphaHarmonicOscillatorOld.h
- src/Orbitals/AlphaHarmonicOscillatorOld/AlphaHarmonicOscillatorOld.cpp

3.3 ASGD Class Reference

Inheritance diagram for ASGD:



Public Member Functions

- **ASGD** (VMC ∗, MinimizerParams &, const ParParams &)
- virtual VMC ∗ **minimize** ()

Protected Member Functions

- void **get_total_grad** ()
- virtual void **update_parameters** ()
- void **output_cycle** ()
- void **thermalize_walkers** ()
- double **f** (double x)
- void **get_variational_gradients** (Walker ∗walker, double e_local)

Protected Attributes

- int **n_c**
- int **n_c_SGD**
- int **SGDsamples**
- int **n_walkers**
- int **thermalization**
- int **sample**
- double **t_prev**
- double **t**
- double **step**
- double **max_step**
- double **E**
- double **a**
- double **A**
- double **f_min**
- double **f_max**
- double **w**
- Walker ∗∗ **walkers**
- Walker ∗∗ **trial_walkers**
- arma::rowvec **parameter**
- arma::rowvec **gradient**
- arma::rowvec **gradient_local**
- arma::rowvec **gradient_old**
- arma::rowvec **gradient_tot**

Friends

- class **stdoutASGD**

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

- src/Minimizer/ASGD/ASGD.h
- src/Minimizer/ASGD/ASGD.cpp

3.4 BasisFunctions Class Reference

Public Member Functions

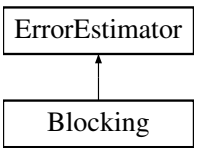
- virtual double **eval** (const Walker ∗walker, int i)=0

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

- src/BasisFunctions/BasisFunctions.h
- src/BasisFunctions/BasisFunctions.cpp

3.5 Blocking Class Reference

Inheritance diagram for Blocking:



Public Member Functions

- **Blocking** (int n_c, ParParams &pp, std::string filename="blocking_out", std::string path="./", int n_b=100, int maxb=10000, int minb=10, bool rerun=false)
- **Blocking** (int n_c, std::string filename="blocking_out", std::string path="./", int n_b=100, int maxb=10000, int minb=10)
- double **estimate_error** ()
- void **get_initial_error** ()
- void **get_unique_blocks** (arma::Row< int > &block_sizes, int &n)

Protected Member Functions

- void **block_data** (int block_size, double &var, double &mean)

Protected Attributes

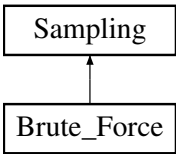
- arma::rowvec **local_block**
- int **min_block_size**
- int **max_block_size**
- int **n_block_samples**

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

- src/ErrorEstimator/Blocking/Blocking.h
- src/ErrorEstimator/Blocking/Blocking.cpp

3.6 Brute_Force Class Reference

Inheritance diagram for Brute_Force:



Public Member Functions

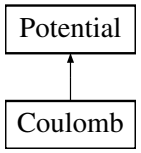
- **Brute_Force** (GeneralParams &)
- void **update_walker** (Walker ∗walker_pre, const Walker ∗walker_post, int particle) const
- virtual void **get_necessities** (Walker ∗walker)
- virtual void **update_necessities** (const Walker ∗walker_pre, Walker ∗walker_post, int particle) const
- virtual void **calculate_energy_necessities** (Walker ∗walker) const
- virtual void **copy_walker** (const Walker ∗parent, Walker ∗child) const
- virtual void **reset_walker** (const Walker ∗walker_pre, Walker ∗walker_post, int particle) const

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

- src/Sampling/Brute_Force/Brute_Force.h
- src/Sampling/Brute_Force/Brute_Force.cpp

3.7 Coulomb Class Reference

Inheritance diagram for Coulomb:



Public Member Functions

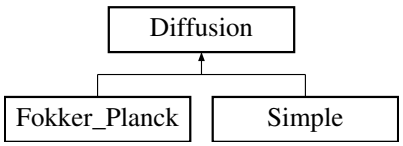
- **Coulomb** (GeneralParams &)
- virtual double **get_pot_E** (const Walker ∗walker) const

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

- src/Potential/Coulomb/Coulomb.h
- src/Potential/Coulomb/Coulomb.cpp

3.8 Diffusion Class Reference

Inheritance diagram for Diffusion:



Public Member Functions

- **Diffusion** (int n_p, int dim, double timestep, long random_seed, double D)
- double **ran2** (long ∗idum)
- double **gaussian_deviate** (long ∗idum)
- virtual double **get_new_pos** (const Walker ∗walker, int i, int j)
- virtual double **get_g_ratio** (const Walker ∗walker_post, const Walker ∗walker_pre) const =0
- double **get_GBfunc** (double E_x, double E_y, double E_T) const
- double **call_RNG** ()
- void **set_qmc_ptr** (QMC ∗qmc)
- void **set_dt** (double dt)
- double **get_dt** () const

Protected Attributes

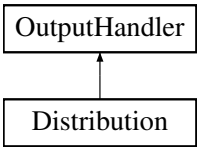
- int **n_p**
- int **dim**
- QMC * **qmc**
- double **timestep**
- double **D**
- long **random_seed**
- double **std**

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

- src/Diffusion/Diffusion.h
- src/Diffusion/Diffusion.cpp

3.9 Distribution Class Reference

Inheritance diagram for Distribution:



Public Member Functions

- **Distribution** (ParParams &, std::string filename="dist_out", std::string path="./")
- virtual void **dump** ()

Protected Attributes

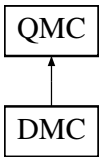
- int **i**

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

- src/OutputHandler/Distribution/Distribution.h
- src/OutputHandler/Distribution/Distribution.cpp

3.10 DMC Class Reference

Inheritance diagram for DMC:



Public Member Functions

- **DMC** (GeneralParams &, DMCparams &, SystemObjects &, ParParams &)
- virtual void **run_method** ()
- virtual void **output** ()

Static Public Attributes

- static const int **K** = 2

Protected Member Functions

- void **initialize** ()
- virtual bool **move_autherized** (double A)
- void **iterate_walker** (int k, int n_b=1, bool production=false)
- void **Evolve_walker** (int k, double GB)
- void **bury_the_dead** ()
- void **update_energies** ()
- void **reset_parameters** ()
- virtual void **node_comm** ()

Protected Attributes

- int **n_w**
- int **n_w_last**
- int **deaths**
- int **block_size**
- int **samples**
- double **dmc_E**
- double **E_T**
- double **E**
- bool **dist_from_file**
- std::string **dist_in_path**
- Walker ∗∗ **original_walkers**
- Walker ∗ **trial_walker**

Friends

- class **stdoutDMC**

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

- src/QMC/DMC/DMC.h
- src/QMC/DMC/DMC.cpp

3.11 DMCparams Struct Reference

Public Attributes

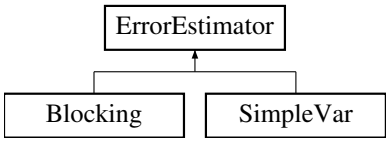
- int **n_c**
- int **therm**
- int **n_w**
- int **n_b**
- double **dt**
- double **E_T**
- bool **dist_in**
- std::string **dist_in_path**

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

- src/QMCheaders.h

3.12 ErrorEstimator Class Reference

Inheritance diagram for ErrorEstimator:



Public Member Functions

- **ErrorEstimator** (int n_c, std::string filename, std::string path, bool parallel, int node, int n_nodes, bool rerun=false)
- double **combine_variance** (double var, double mean=0)
- void **finalize** ()
- void **node_comm_gather_data** ()

- void **node_comm_scatter_data** ()
- void **init_file** ()
- virtual double **estimate_error** ()=0
- void **normalize** ()
- virtual void **update_data** (double val)
- void **clear** ()

Public Attributes

- bool **data_to_file**
- bool **output_to_file**

Protected Attributes

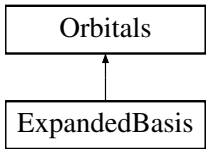
- int **n_c**
- int **i**
- bool **parallel**
- bool **is_master**
- int **node**
- int **n_nodes**
- bool **rerun**
- std::string **filename**
- std::string **path**
- std::ofstream **file**
- arma::rowvec **data**

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

- src/ErrorEstimator/ErrorEstimator.h
- src/ErrorEstimator/ErrorEstimator.cpp

3.13 ExpandedBasis Class Reference

Inheritance diagram for ExpandedBasis:



Public Member Functions

- **ExpandedBasis** (GeneralParams &gp, Orbitals *basis, int m, std::string coeffPath)
- virtual double **phi** (const Walker *walker, int particle, int q_num)
- virtual double **del_phi** (const Walker *walker, int particle, int q_num, int d)
- virtual double **lapl_phi** (const Walker *walker, int particle, int q_num)

Protected Attributes

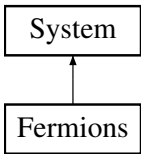
- int **basis_size**
- arma::mat **coeffs**
- Orbitals * **basis**

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

- src/Orbitals/ExpandedBasis/ExpandedBasis.h
- src/Orbitals/ExpandedBasis/ExpandedBasis.cpp

3.14 Fermions Class Reference

Inheritance diagram for Fermions:



Public Member Functions

- **Fermions** (GeneralParams &, Orbitals *)
- virtual void **get_spatial_grad** (Walker *walker, int particle) const
- virtual void **get_spatial_grad_full** (Walker *walker) const
- virtual double **get_spatial_ratio** (const Walker *walker_post, const Walker *walker_pre, int particle) const
- virtual double **get_spatial_lapl_sum** (const Walker *walker) const
- virtual void **copy_walker** (const Walker *parent, Walker *child) const
- void **update_walker** (Walker *walker_pre, const Walker *walker_post, int particle) const
- virtual void **reset_walker** (const Walker *walker_pre, Walker *walker_post, int particle) const
- virtual double **get_spatial_wf** (const Walker *walker)
- virtual void **initialize** (Walker *walker)
- virtual void **calc_for_newpos** (const Walker *walker_old, Walker *walker_new, int i)

Protected Member Functions

- void **make_merged_inv** (Walker ∗walker)
- void **update_inverse** (const Walker ∗walker_old, Walker ∗walker_new, int particle)

Protected Attributes

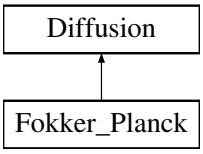
- arma::rowvec **l**

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

- src/System/Fermions/Fermions.h
- src/System/Fermions/Fermions.cpp

3.15 Fokker_Planck Class Reference

Inheritance diagram for Fokker_Planck:



Public Member Functions

- **Fokker_Planck** (int n_p, int dim, double timestep, long random_seed, double D=0.5)
- virtual double **get_g_ratio** (const Walker ∗walker_post, const Walker ∗walker_pre) const
- virtual double **get_new_pos** (const Walker ∗walker, int i, int j)

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

- src/Diffusion/Fokker_Planck/Fokker_Planck.h
- src/Diffusion/Fokker_Planck/Fokker_Planck.cpp

3.16 GeneralParams Struct Reference

Public Attributes

- int **n_p**

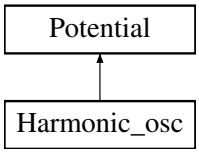
- int **dim**
- long **random_seed**
- double **D**
- double **h**
- double **w**
- bool **doMIN**
- bool **doVMC**
- bool **doDMC**
- bool **estimate_error**
- bool **use_jastrow**
- bool **use_coulomb**
- std::string **system**
- std::string **sampling**

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

- src/QMCheaders.h

3.17 Harmonic_osc Class Reference

Inheritance diagram for Harmonic_osc:



Public Member Functions

- **Harmonic_osc** (GeneralParams &)
- virtual double **get_pot_E** (const Walker *walker) const

Protected Attributes

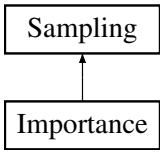
- double **w**

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

- src/Potential/Harmonic_osc/Harmonic_osc.h
- src/Potential/Harmonic_osc/Harmonic_osc.cpp

3.18 Importance Class Reference

Inheritance diagram for Importance:



Public Member Functions

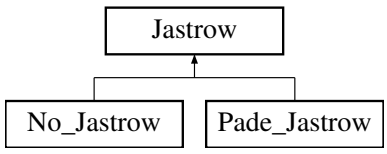
- **Importance** (GeneralParams &)
- void **update_walker** (Walker ∗walker_pre, const Walker ∗walker_post, int particle) const
- virtual void **get_necessities** (Walker ∗walker)
- virtual void **update_necessities** (const Walker ∗walker_pre, Walker ∗walker_post, int particle) const
- virtual void **calculate_energy_necessities** (Walker ∗walker) const
- virtual void **copy_walker** (const Walker ∗parent, Walker ∗child) const
- virtual void **reset_walker** (const Walker ∗walker_pre, Walker ∗walker_post, int particle) const

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

- src/Sampling/Importance/Importance.h
- src/Sampling/Importance/Importance.cpp

3.19 Jastrow Class Reference

Inheritance diagram for Jastrow:



Public Member Functions

- **Jastrow** (int n_p, int dim)
- virtual void **initialize** ()=0
- virtual double **get_val** (const Walker ∗walker) const =0

- virtual double **get_j_ratio** (const Walker ∗walker_new, const Walker ∗walker_old, int i) const =0
- virtual void **get_grad** (Walker ∗walker) const =0
- virtual void **get_grad** (const Walker ∗walker_pre, Walker ∗walker_post, int i) const =0
- virtual void **get_dJ_matrix** (Walker ∗walker, int i) const =0
- void **get_dJ_matrix** (Walker ∗walker) const
- virtual double **get_lapl_sum** (const Walker ∗walker) const =0

Protected Member Functions

- virtual double **get_parameter** (int n)=0
- virtual void **set_parameter** (double param, int n)=0
- virtual double **get_variational_derivative** (const Walker ∗walker, int n)

Protected Attributes

- int **n_p**
- int **n2**
- int **dim**
- bool **active**

Friends

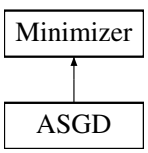
- class **Minimizer**
- class **ASGD**
- class **stdoutASGD**

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

- src/Jastrow/Jastrow.h
- src/Jastrow/Jastrow.cpp

3.20 Minimizer Class Reference

Inheritance diagram for Minimizer:



Public Member Functions

- **Minimizer** (VMC ∗vmc, const ParParams &, const arma::rowvec &alpha, const arma::rowvec &beta)
- void **add_output** (OutputHandler ∗output_handler)
- Orbitals ∗ **get_orbitals** ()
- Jastrow ∗ **get_jastrow** ()
- virtual VMC ∗ **minimize** ()=0
- void **output** (std::string message, double number=-1)
- void **add_error_estimator** (ErrorEstimator ∗error_estimator)

Protected Member Functions

- void **dump_output** ()
- void **finalize_output** ()
- void **error_output** ()
- virtual void **update_parameters** ()=0

Protected Attributes

- int **n_nodes**
- bool **is_master**
- VMC ∗ **vmc**
- STDOUT ∗ **std_out**
- std::stringstream **s**
- int **Nspatial_params**
- int **Njastrow_params**
- int **Nparams**
- std::vector< OutputHandler ∗ > **output_handler**
- std::vector< ErrorEstimator ∗ > **error_estimators**

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

- src/Minimizer/Minimizer.h
- src/Minimizer/Minimizer.cpp

3.21 MinimizerParams Struct Reference

Public Attributes

- double **max_step**
- double **f_max**
- double **f_min**
- double **omega**

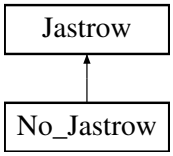
- double **A**
- double **a**
- int **SGDsamples**
- int **n_walkers**
- int **thermalization**
- int **n_cm**
- int **n_c_SGD**
- arma::rowvec **alpha**
- arma::rowvec **beta**

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

- src/QMCheaders.h

3.22 No_Jastrow Class Reference

Inheritance diagram for No_Jastrow:



Public Member Functions

- virtual void **get_grad** (Walker ∗walker) const
- virtual void **get_grad** (const Walker ∗walker_pre, Walker ∗walker_post, int i) const

- virtual void **initialize** ()
- virtual void **get_dJ_matrix** (Walker ∗walker, int i) const
- virtual double **get_j_ratio** (const Walker ∗walker_post, const Walker ∗walker_pre, int i) const
- virtual double **get_val** (const Walker ∗walker) const
- virtual double **get_lapl_sum** (const Walker ∗walker) const

Protected Member Functions

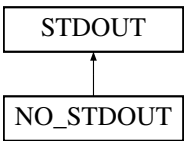
- virtual double **get_parameter** (int n)
- virtual void **set_parameter** (double param, int n)
- virtual double **get_variational_derivative** (const Walker ∗walker, int n)

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

- src/Jastrow/No_Jastrow/No_Jastrow.h
- src/Jastrow/No_Jastrow/No_Jastrow.cpp

3.23 NO_STDOUT Class Reference

Inheritance diagram for NO_STDOUT:



Public Member Functions

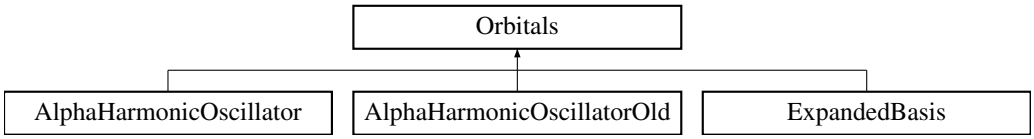
- virtual void **cout** (std::stringstream &a)

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

- src/QMCheaders.h

3.24 Orbitals Class Reference

Inheritance diagram for Orbitals:



Public Member Functions

- **Orbitals** (int n_p, int dim)
- virtual void **set_qnum_indie_terms** (const Walker ∗walker, int i)
- virtual double **phi** (const Walker ∗walker, int particle, int q_num)
- virtual double **del_phi** (const Walker ∗walker, int particle, int q_num, int d)
- virtual double **lapl_phi** (const Walker ∗walker, int particle, int q_num)
- void **set_qmc_ptr** (QMC ∗qmc)

Protected Member Functions

- virtual double **get_parameter** (int n)=0
- virtual void **set_parameter** (double parameter, int n)=0
- virtual double **get_variational_derivative** (const Walker ∗walker, int n)
- double **num_diff** (const Walker ∗walker, int particle, int q_num, int d)
- double **num_ddiff** (const Walker ∗walker, int particle, int q_num)

Protected Attributes

- int **n_p**
- int **n2**
- int **dim**
- int **max_implemented**
- QMC * **qmc**
- double **h**
- double **h2**
- double **two_h**
- BasisFunctions ** **basis_functions**
- BasisFunctions *** **dell_basis_functions**
- BasisFunctions ** **lapl_basis_functions**

Friends

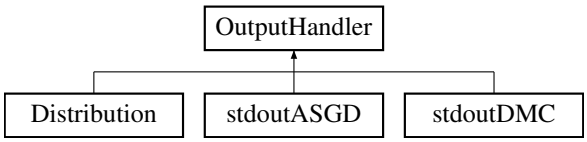
- class **Minimizer**
- class **ASGD**
- class **stdoutASGD**

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

- src/Orbitals/Orbitals.h
- src/Orbitals/Orbitals.cpp

3.25 OutputHandler Class Reference

Inheritance diagram for OutputHandler:



Public Member Functions

- **OutputHandler** (std::string filename, std::string path, bool parallel, int node, int n_nodes)
- virtual void **dump** ()=0
- virtual void **finalize** ()
- void **set_qmc_ptr** (QMC *qmc)
- void **set_min_ptr** (Minimizer *min)

Protected Member Functions

- void **init_file** ()

Protected Attributes

- bool **is_vmc**
- bool **is_dmc**
- bool **is_ASGD**
- bool **parallel**
- int **node**
- int **n_nodes**
- bool **use_file**
- std::stringstream **s**
- std::string **filename**
- std::string **path**
- std::ofstream **file**
- QMC * **qmc**
- DMC * **dmc**
- VMC * **vmc**
- Minimizer * **min**
- ASGD * **asgd**

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

- src/OutputHandler/OutputHandler.h
- src/OutputHandler/OutputHandler.cpp

3.26 OutputParams Struct Reference

Public Attributes

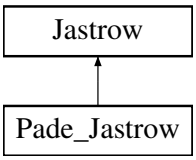
- bool **dist_out**
- bool **blocking_out**
- bool **dmc_out**
- bool **ASGD_out**
- std::string **outputSuffix**
- std::string **outputPath**

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

- src/QMCheaders.h

3.27 Pade_Jastrow Class Reference

Inheritance diagram for Pade_Jastrow:



Public Member Functions

- **Pade_Jastrow** (GeneralParams &, VariationalParams &)
- virtual void **initialize** ()
- virtual void **get_grad** (Walker ∗walker) const
- virtual void **get_grad** (const Walker ∗walker_pre, Walker ∗walker_post, int i) const
- virtual void **get_dJ_matrix** (Walker ∗walker, int i) const
- virtual double **get_j_ratio** (const Walker ∗walker_new, const Walker ∗walker_old, int i) const
- virtual double **get_val** (const Walker ∗walker) const
- virtual double **get_lapl_sum** (const Walker ∗walker) const

Protected Member Functions

- virtual double **get_variational_derivative** (const Walker ∗walker, int n)
- virtual void **set_parameter** (double param, int n)
- virtual double **get_parameter** (int n)

Protected Attributes

- double **beta**
- arma::mat **a**

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

- src/Jastrow/Pade_Jastrow/Pade_Jastrow.h
- src/Jastrow/Pade_Jastrow/Pade_Jastrow.cpp

3.28 ParParams Struct Reference

Public Attributes

- bool **parallel**

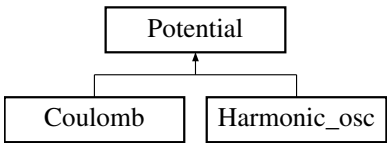
- bool **is_master**
- int **n_nodes**
- int **node**

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

- src/QMCheaders.h

3.29 Potential Class Reference

Inheritance diagram for Potential:



Public Member Functions

- **Potential** (int n_p, int dim)
- virtual double **get_pot_E** (const Walker *walker) const =0

Protected Attributes

- int **n_p**
- int **dim**

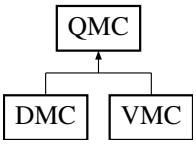
The documentation for this class was generated from the following files:

- src/Potential/Potential.h
- src/Potential/Potential.cpp

3.30 QMC Class Reference

The QMC superduper class!

Inheritance diagram for QMC:



Public Member Functions

- **QMC** (int n_p, int dim, int n_c, SystemObjects &, ParParams &)
- void **add_output** (OutputHandler *output_handler)
- virtual void **run_method** ()=0
- virtual void **output** ()=0
- double **get_KE** (const Walker *walker) const
- void **get_QF** (Walker *walker) const
- void **get_gradients** (const Walker *walker_pre, Walker *walker_post, int particle) const
- void **get_gradients** (Walker *walker) const
- void **get_laplsum** (Walker *walker) const
- double **get_wf_value** (Walker *walker) const
- double **calculate_local_energy** (const Walker *walker) const
- System * **get_system_ptr** () const
- Sampling * **get_sampling_ptr** () const
- Jastrow * **get_jastrow_ptr** () const
- Orbitals * **get_orbitals_ptr** () const
- double **get_accepted_ratio** (int total_cycles) const
- void **set_error_estimator** (ErrorEstimator *error_estimator)

Protected Member Functions

- virtual void **node_comm** ()=0
- virtual void **initialize** ()=0
- virtual bool **move_autherized** (double A)=0
- void **dump_output** ()
- void **finalize_output** ()
- void **diffuse_walker** (Walker *original, Walker *trial)
- double **get_acceptance_ratio** (const Walker *walker_pre, const Walker *walker_post, int particle) const
- void **set_spin_state** (int particle) const
- bool **metropolis_test** (double A)
- void **update_walker** (Walker *walker_pre, const Walker *walker_post, int particle) const
- void **reset_walker** (const Walker *walker_pre, Walker *walker_post, int particle) const
- void **copy_walker** (const Walker *parent, Walker *child) const
- void **calculate_energy_necessities** (Walker *walker) const
- void **estimate_error** () const

Protected Attributes

- STDOUT * **std_out**
- std::stringstream s

  This stream is awesome!
- bool **is_master**
- bool **parallel**
- int **node**
- int **n_nodes**
- int **n_c**
- int **n_p**
- int **n2**
- int **dim**
- int **cycle**
- int **accepted**
- int **thermalization**
- double **local_E**
- Jastrow * **jastrow**
- Sampling * **sampling**
- System * **system**
- ErrorEstimator * **error_estimator**
- std::vector< OutputHandler * > **output_handler**

3.30.1 Detailed Description

The QMC superduper class!

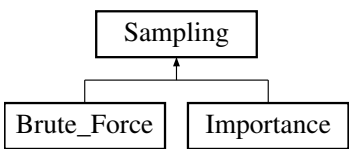
This class is so cool!

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

- src/QMC/QMC.h
- src/QMC/QMC.cpp

3.31 Sampling Class Reference

Inheritance diagram for Sampling:



Public Member Functions

- **Sampling** (int n_p, int dim)
- void **update_pos** (const Walker ∗walker_pre, Walker ∗walker_post, int particle) const
- virtual void **update_necessities** (const Walker ∗walker_pre, Walker ∗walker_post, int particle) const =0
- virtual void **update_walker** (Walker ∗walker_pre, const Walker ∗walker_post, int particle) const =0
- void **set_trial_pos** (Walker ∗walker, bool set_pos=true)
- void **set_trial_states** (Walker ∗walker)
- virtual void **get_necessities** (Walker ∗walker)=0
- virtual void **calculate_energy_necessities** (Walker ∗walker) const =0
- virtual void **copy_walker** (const Walker ∗parent, Walker ∗child) const =0
- virtual void **reset_walker** (const Walker ∗walker_pre, Walker ∗walker_post, int particle) const =0
- virtual double **get_g_ratio** (const Walker ∗walker_post, const Walker ∗walker_pre) const
- double **get_branching_Gfunc** (double E_x, double E_y, double E_T) const
- double **get_spatialjast_ratio** (const Walker ∗walker_post, const Walker ∗walker_pre, int particle) const
- void **set_qmc_ptr** (QMC ∗qmc)
- void **set_dt** (double dt)
- double **get_dt** () const
- double **call_RNG** ()
- void **set_spin_state** (int start, int end)

Protected Attributes

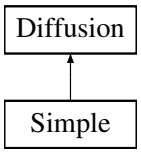
- int **n_p**
- int **n2**
- int **dim**
- int **start**
- int **end**
- Diffusion ∗ **diffusion**
- QMC ∗ **qmc**

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

- src/Sampling/Sampling.h
- src/Sampling/Sampling.cpp

3.32 Simple Class Reference

Inheritance diagram for Simple:



Public Member Functions

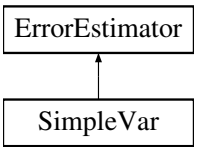
- **Simple** (int n_p, int dim, double timestep, long random_seed, double D=0.5)
- virtual double **get_new_pos** (const Walker ∗walker, int i, int j)
- virtual double **get_g_ratio** (const Walker ∗walker_post, const Walker ∗walker_-pre) const

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

- src/Diffusion/Simple/Simple.h
- src/Diffusion/Simple/Simple.cpp

3.33 SimpleVar Class Reference

Inheritance diagram for SimpleVar:



Public Member Functions

- **SimpleVar** (int n_c, ParParams &)
- **SimpleVar** (int n_c)
- double **estimate_error** ()

Protected Attributes

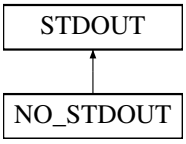
- double **E**
- double **E2**

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

- src/ErrorEstimator/SimpleVar/SimpleVar.h
- src/ErrorEstimator/SimpleVar/SimpleVar.cpp

3.34 STDOUT Class Reference

Inheritance diagram for STDOUT:



Public Member Functions

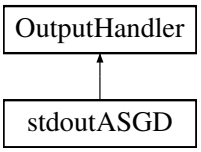
- virtual void **cout** (std::stringstream &a)

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

- src/QMCheaders.h

3.35 stdoutASGD Class Reference

Inheritance diagram for stdoutASGD:



Public Member Functions

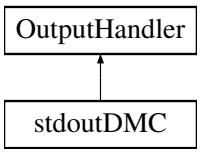
- **stdoutASGD** (std::string filename="ASGD_out", std::string path="./")
- virtual void **dump** ()

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

- src/OutputHandler/stdoutASGD/stdoutASGD.h
- src/OutputHandler/stdoutASGD/stdoutASGD.cpp

3.36 stdoutDMC Class Reference

Inheritance diagram for stdoutDMC:



Public Member Functions

- **stdoutDMC** (std::string filename="DMC_out", std::string path="./", bool parallel=false, int node=0, int n_nodes=1)
- virtual void **dump** ()

Protected Attributes

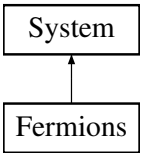
- int **n**
- double **sumE**
- double **sumN**

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

- src/OutputHandler/stdoutDMC/stdoutDMC.h
- src/OutputHandler/stdoutDMC/stdoutDMC.cpp

3.37 System Class Reference

Inheritance diagram for System:



Public Member Functions

- **System** (int n_p, int dim, Orbitals ∗orbital)
- void **add_potential** (Potential ∗pot)
- double **get_potential_energy** (const Walker ∗walker)

- virtual void **update_walker** (Walker *walker_pre, const Walker *walker_post, int particle) const =0
- virtual void **calc_for_newpos** (const Walker *walker_old, Walker *walker_new, int particle)=0
- virtual double **get_spatial_ratio** (const Walker *walker_pre, const Walker *walker_post, int particle) const =0
- virtual double **get_spatial_wf** (const Walker *walker)=0
- virtual void **get_spatial_grad** (Walker *walker, int particle) const =0
- virtual void **get_spatial_grad_full** (Walker *walker) const =0
- virtual double **get_spatial_lapl_sum** (const Walker *walker) const =0
- virtual void **initialize** (Walker *walker)=0
- virtual void **copy_walker** (const Walker *parent, Walker *child) const =0
- virtual void **reset_walker** (const Walker *walker_pre, Walker *walker_post, int particle) const =0
- Orbitals * **get_orbital_ptr** ()
- void **set_spin_state** (int start, int end)

Protected Attributes

- int **n_p**
- int **n2**
- int **dim**
- int **start**
- int **end**
- std::vector< Potential * > **potentials**
- Orbitals * **orbital**

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

- src/System/System.h
- src/System/System.cpp

3.38 SystemObjects Struct Reference

Public Attributes

- Orbitals * **SP_basis**
- Potential * **onebody_pot**
- System * **SYSTEM**
- Sampling * **sample_method**
- Jastrow * **jastrow**

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

- src/QMCheaders.h

3.39 VariationalParams Struct Reference

Public Attributes

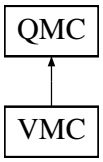
- double **alpha**
- double **beta**

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

- src/QMCheaders.h

3.40 VMC Class Reference

Inheritance diagram for VMC:



Public Member Functions

- **VMC** (GeneralParams &, VMCparams &, SystemObjects &, ParParams &)
- void **set_e** (double E)
- double **get_energy** () const
- virtual void **run_method** ()
- virtual void **output** ()

Protected Member Functions

- virtual void **initialize** ()
- virtual bool **move_autherized** (double A)
- void **scale_values** ()
- virtual void **node_comm** ()

Protected Attributes

- double **vmc_E**
- Walker * **original_walker**
- Walker * **trial_walker**

Friends

- class **Minimizer**
- class **ASGD**
- class **Distribution**
- class **BlockingData**

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

- src/QMC/VMC/VMC.h
- src/QMC/VMC/VMC.cpp

3.41 VMCparams Struct Reference

Public Attributes

- int **n_c**
- double **dt**

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

- src/QMCheaders.h

3.42 Walker Class Reference

Public Member Functions

- **Walker** (int n_p, int dim, bool do_init=true)
- void **calc_r_i2** (int i)
- void **calc_r_i2** ()
- double **abs_relative** (int i, int j) const
- void **make_rel_matrix** ()
- double **get_r_i2** (int i) const
- void **kill** ()
- bool **is_dead** ()
- bool **is_alive** ()
- void **ressurect** ()
- void **set_E** (double E)
- double **get_E** () const
- void **print** (std::string header="----")

Public Attributes

- double **spatial_ratio**
- double **value**
- double **lapl_sum**
- double **E**
- arma::mat **r**
- arma::mat **r_rel**
- arma::mat **qforce**
- arma::mat **spatial_grad**
- arma::mat **jast_grad**
- arma::mat **inv**
- arma::mat **phi**
- arma::field< arma::mat > **dell_phi**
- arma::cube **dJ**
- arma::rowvec **r2**

Protected Attributes

- int **n_p**
- int **n2**
- int **dim**
- bool **is_murdered**

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

- src/Walker/Walker.h
- src/Walker/Walker.cpp