QMC2 Documentation

Generated by Doxygen 1.7.6.1

Mon Apr 1 2013 14:18:52

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:

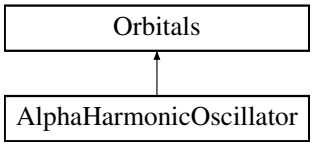
Chapter 3

Class Documentation

3.1 AlphaHarmonicOscillator Class Reference

Harmonic Oscillator single particle wave function class. Uses the HarmonicOscillator - BasisFunction subclasses auto-generated by SymPy through the orbitalsGenerator tool.

Inheritance diagram for AlphaHarmonicOscillator:



Public Member Functions

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

Protected Member Functions

- double get_variational_derivative (const Walker ∗walker, int n)
- void get_qnums ()
- double H (int n, double x) const

  Method for calculating Hermite polynomials.
- double get_parameter (int n)
- void set_parameter (double parameter, int n)

Protected Attributes

- double w

  The oscillator frequency.
- double * alpha

  Pointer to the variational parameter alpha. Shared address with all the BasisFunction subclasses.
- double * k

  *Pointer to sqrt(alpha*w). Shared address with all the BasisFunction subclasses.*
- double * k2

  *Pointer to alpha*w. Shared address with all the BasisFunction subclasses.*
- double * **w_over_a**
- double * exp_factor

  Pointer to a factor precalculated by set_qnum_indie_terms(). Shared address with all the BasisFunction subclasses.
- arma::Mat< int > qnums

  Quantum number matrix needed by the variational derivatives.

Friends

- class **ExpandedBasis**

3.1.1 Detailed Description

Harmonic Oscillator single particle wave function class. Uses the HarmonicOscillator - BasisFunction subclasses auto-generated by SymPy through the orbitalsGenerator tool.

3.1.2 Member Function Documentation

3.1.2.1 double AlphaHarmonicOscillator::get_parameter (int *n*) [inline, protected, virtual]

Returns

The variational parameter alpha.

Implements Orbitals.

3.1.2.2 void AlphaHarmonicOscillator::get_qnums ( ) [protected]

Calculates the quantum numbers of the oscillator and stores them in the matrix qnums.

3.1.2.3 double AlphaHarmonicOscillator::get_variational_derivative (const Walker * *walker,* int *n*) [protected, virtual]

Overridden superclass method implementing closed form expressions using Hermite polynomials.

Reimplemented from Orbitals.

3.1.2.4 double AlphaHarmonicOscillator::H (int *n,* double *x*) const [protected]

Method for calculating Hermite polynomials.

Parameters

n	The degree of the Hermite polynomial.
x	The argument for evaluating the polynomial.

3.1.2.5 void AlphaHarmonicOscillator::set_parameter (double *parameter,* int *n*) [inline, protected, virtual]

Sets a new value for the alpha and updates all the pointer values.

Implements Orbitals.

3.1.2.6 void AlphaHarmonicOscillator::set_qnum_indie_terms (const Walker * *walker,* int *i*) [inline, virtual]

Calculates the exponential term shared by all oscillator function once pr. particle to save CPU-time.

See also

Orbitals::set_qnum_indie_terms()

Reimplemented from Orbitals.

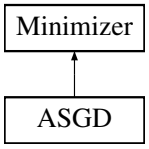
The documentation for this class was generated from the following files:

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

3.2 ASGD Class Reference

Implementation for the Adaptive Stochastic Gradient Descent method (ASGD) Used to find optimal variational parameters using adaptive step lengths.

Inheritance diagram for ASGD:



Public Member Functions

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

  Method for executing the minimization main solver.

Protected Member Functions

- void get_total_grad ()

  Method for calculating the total gradient.
- void update_parameters ()

  Calculates the step and updates parameters.
- void output_cycle ()

  Standard output of the progress.
- void thermalize_walkers ()

  Thermalizes a set of walkers before the main loop.
- double f (double x)

  Function for calculating the adaptive step.
- void get_variational_gradients (Walker ∗walker, double e_local)

  Method for updating the vectors needed to calculate the total variational derivative.

Protected Attributes

- int n_c

  The correlation length between storing two walkers after thermalization.
- int n_c_SGD

  The number of samples used to estimate expectation values.
- int SGDsamples

  The number of ASGD cycles.
- int n_walkers

  The number of walkers.
- int thermalization

  The number of thermalization cycles used on walkers.
- int sample

  The current ASGD cycle.
- double t_prev

The previous t.

- double t

  The current t.

- double step

  The current calculates step.

- double max_step

  The maximum threshold on a step.

- double E

  The energy summation variable used to calculate the mean.

- double a

  ASGD step parameter.

- double A

  ASGD step parameter.

- double f_min

  ASGD step parameter.

- double f_max

  ASGD step parameter.

- double w

  ASGD step parameter.

- Walker ** walkers

  The walkers used to sample expectation values.

- Walker ** **trial_walkers**
- arma::rowvec **parameter**
- arma::rowvec gradient

  Sumamtion vector for the trial wave function's variational derivatives.

- arma::rowvec gradient_local

  Sumamtion vector for the trial wave function's variational derivatives times the energy.

- arma::rowvec gradient_old

  The previous total gradient.

- arma::rowvec gradient_tot

  The current total gradient.

Friends

- class **stdoutASGD**

3.2.1 Detailed Description

Implementation for the Adaptive Stochastic Gradient Descent method (ASGD) Used to find optimal variational parameters using adaptive step lengths.

3.2.2 Member Function Documentation

3.2.2.1 void ASGD::get_total_grad ( ) [protected]

Method for calculating the total gradient.

Updates the error estimator with statistics.

3.2.2.2 void ASGD::get_variational_gradients (Walker * *walker,* double *e_local*) [protected]

Method for updating the vectors needed to calculate the total variational derivative.

Calculates the single particle variational derivatives V and accumulates V and V∗e_-local.

Parameters

e_local	The local energy of the current walker at the current time step.

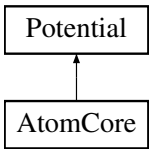
The documentation for this class was generated from the following files:

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

3.3 AtomCore Class Reference

Implementation of the Atom Core potential. -Z/r.

Inheritance diagram for AtomCore:



Public Member Functions

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

  Method for calculating a walker's potential energy.

Protected Attributes

- int Z

  The core charge.

3.3.1 Detailed Description

Implementation of the Atom Core potential. -Z/r.

3.3.2 Member Function Documentation

3.3.2.1 double AtomCore::get_pot_E (const Walker * *walker*) const [virtual]

Method for calculating a walker's potential energy.

Method overridden by subclasses.

Parameters

walker	The walker for which the potential energy should be calculated.

Returns

The potential energy.

Implements Potential.

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

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

3.4 BasisFunctions Class Reference

The Superclass shell for orbital basis functions.

Public Member Functions

- virtual double eval (const Walker *walker, int i)=0
  The method representing the orbitals functional expression.

3.4.1 Detailed Description

The Superclass shell for orbital basis functions.

Each single particle orbital has it's own implementation as a subclass of this class. A set of orbitals can then be loaded into the Orbitals basis_function vectors. An orbital-Generator script is supplied to autogenerate CPP files using this class.

See also

Orbitals::basis_functions
Orbitals::dell_basis_functions
Orbitals::lapl_basis_functions

3.4.2 Member Function Documentation

3.4.2.1 virtual double BasisFunctions::eval (const Walker * *walker*, int *i*) [pure virtual]

The method representing the orbitals functional expression.

Parameters

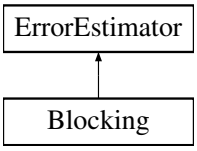
walker	The Walker whose position the orbital is to be evaluted at.
i	The particle to be evaluated (Single particle function).

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 ()

  Estimates the error based on the subclass implementation.
- void get_initial_error ()
- void get_unique_blocks (arma::Row< int > &block_sizes, int &n)

  Calculates the block sizes.

Protected Member Functions

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

  Calculates the variance and mean of the dataset with the specified block size.

Protected Attributes

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

  The minimum amount of samples in one block.
- int max_block_size

  The maximum amount of samples in one block.
- int n_block_samples

  The total amount of different block sizes.

3.5.1 Member Function Documentation

3.5.1.1 void Blocking::block_data (int *block_size*, double & *var*, double & *mean*) [protected]

Calculates the variance and mean of the dataset with the specified block size.

Parameters

block_size	The number of samples in each block.
var	Reference to the variance of the block's means.
mean	Reference to the mean of the block's means. Needed to combine the variances from different processes.

3.5.1.2 void Blocking::get_initial_error ( )

Calculates the variance as in SimpleVar

3.5.1.3 void Blocking::get_unique_blocks (arma::Row< int > & *block_sizes*, int & *n*)

Calculates the block sizes.

Due to integer division, alot of sizes becomes equal. Only unique block sizes are returned.

Parameters

block_sizes	Vector containing the block sizes
n	The number of unqiue block sizes

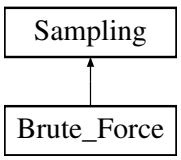
The documentation for this class was generated from the following files:

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

3.6 Brute_Force Class Reference

Implementation of the Brute Force QMC. Uses the Simle diffusion class. All methods are empty except for the energy necessities part which requires the gradients to be calculated (not using the Quantum Force).

Inheritance diagram for Brute_Force:



Public Member Functions

- **Brute_Force** (GeneralParams &)
- void update_walker (Walker ∗walker_pre, const Walker ∗walker_post, int particle) const
- void get_necessities (Walker ∗walker)

  Method for calculating the sampling specific necessary values.
- void update_necessities (const Walker ∗walker_pre, Walker ∗walker_post, int particle) const

  Method for updating the sampling specific necessary values.
- void calculate_energy_necessities (Walker ∗walker) const

  Method for calculating the sampling specific necessary values in order to compute the local energy.
- void copy_walker (const Walker ∗parent, Walker ∗child) const

  Method for copying the sampling specific parts of a walker.
- void reset_walker (const Walker ∗walker_pre, Walker ∗walker_post, int particle) const

3.6.1 Detailed Description

Implementation of the Brute Force QMC. Uses the Simle diffusion class. All methods are empty except for the energy necessities part which requires the gradients to be calculated (not using the Quantum Force).

3.6.2 Member Function Documentation

3.6.2.1 void Brute_Force::copy_walker (const Walker ∗ *parent*, Walker ∗ *child*) const [inline, virtual]

Method for copying the sampling specific parts of a walker.

See also

QMC::copy_walker()

Implements Sampling.

3.6.2.2 void Brute_Force::get_necessities (Walker * *walker*) [inline, virtual]

Method for calculating the sampling specific necessary values.

Called after a trial position is set.

Implements Sampling.

3.6.2.3 void Brute_Force::reset_walker (const Walker * *walker_pre*, Walker * *walker_post*, int *particle*) const [inline, virtual]

See also

QMC::reset_walker()

Implements Sampling.

3.6.2.4 void Brute_Force::update_walker (Walker * *walker_pre*, const Walker * *walker_post*, int *particle*) const [inline, virtual]

See also

QMC::update_walker()

Implements Sampling.

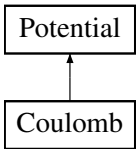
The documentation for this class was generated from the following files:

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

3.7 Coulomb Class Reference

Implementation of the Coulomb potential. 1/r_{ij}.

Inheritance diagram for Coulomb:



Public Member Functions

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

  Method for calculating a walker's potential energy.

3.7.1 Detailed Description

Implementation of the Coulomb potential. 1/r_{ij}.

3.7.2 Member Function Documentation

3.7.2.1 double Coulomb::get_pot_E (const Walker * *walker*) const [virtual]

Method for calculating a walker's potential energy.

Method overridden by subclasses.

Parameters

walker	The walker for which the potential energy should be calculated.

Returns

The potential energy.

Implements Potential.

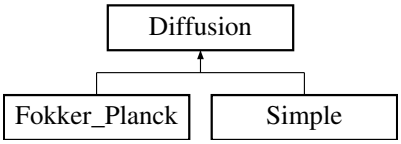
The documentation for this class was generated from the following files:

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

3.8 Diffusion Class Reference

Class containing rules for walker movement based on diffusion models. Serves as class member in the Sampling class. Brute force implies the Simple diffusion model, while - Importance Sampling implies the Fokker Planck diffusion.

Inheritance diagram for Diffusion:



Public Member Functions

- **Diffusion** (int n_p, int dim, double timestep, seed_type random_seed, double D)
- virtual double get_new_pos (const Walker *walker, int i, int j)

  Virtual function returning the new position.
- virtual double get_g_ratio (const Walker *walker_post, const Walker *walker_pre) const =0

  Calculates the Diffusion Green's function ratio needed by metropolis.
- double get_GBfunc (double E_x, double E_y, double E_T) const

  Calculates the Branching Green's function ratio needed by DMC.
- double call_RNG ()

  Calls a uniform random number generator.
- void **set_qmc_ptr** (QMC *qmc)
- void set_dt (double dt)

  Function for altering the time step.
- double **get_dt** () const
- double **get_std** () const

Protected Attributes

- int **n_p**
- int **dim**
- QMC * qmc

  The qmc main solver object. Not needed?
- double timestep

  The discrete time step.
- double D

  The diffusion constant.
- long random_seed

  The random seed. Needs to be stored for some RNGs to work.
- double std

  *The standard deviation from QMC stored for efficiency. sqrt(2D*timestep).*

3.8.1 Detailed Description

Class containing rules for walker movement based on diffusion models. Serves as class member in the Sampling class. Brute force implies the Simple diffusion model, while -Importance Sampling implies the Fokker Planck diffusion.

See also

Brute_Force, Importance.

3.8.2 Member Function Documentation

3.8.2.1 double Diffusion::call_RNG ( )

Calls a uniform random number generator.

Returns a random uniform number on [0,1).

3.8.2.2 virtual double Diffusion::get_g_ratio (const Walker * *walker_post,* const Walker * *walker_pre*) const [pure virtual]

Calculates the Diffusion Green's function ratio needed by metropolis.

Parameters

walker_post	Walker at current time step.
walker_pre	Walker at previous time step.

Returns

The Diffusion Green's function ratio.

Implemented in Simple, and Fokker_Planck.

3.8.2.3 double Diffusion::get_GBfunc (double *E_x,* double *E_y,* double *E_T*) const [inline]

Calculates the Branching Green's function ratio needed by DMC.

Parameters

E_x	Energy at current time step
E_y	Energy at previous time step

Returns

The Branching Green's function ratio

3.8.2.4 double Diffusion::get_new_pos (const Walker * *walker,* int *i,* int *j*) [virtual]

Virtual function returning the new position.

Returns the simple diffusion step if not overridden.

Parameters

i	Particle number.
j	dimension (x,y,z).

Returns

The new position (relative to the old).

Reimplemented in Fokker_Planck, and Simple.

3.8.2.5 void Diffusion::set_dt (double *dt*) [inline]

Function for altering the time step.

Takes care of consequences. Time step should only be altered using this function.

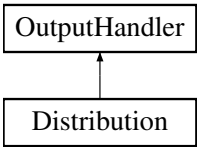
The documentation for this class was generated from the following files:

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

3.9 Distribution Class Reference

Class for calculating distribution functions such as the one-body density. Does not collect data itself, but works merely as a control organ for the QMC class, calling it's methods for storing position data.

Inheritance diagram for Distribution:



Public Member Functions

- Distribution (ParParams &, std::string path, std::string name)

  Constructor.
- void dump ()
- void finalize ()

  Method for calculating the distribution.
- void rerun (int n_p, int N, double bin_edge)

  Method for re-calculating the distribution given a stores set of position data.

3.9.1 Detailed Description

Class for calculating distribution functions such as the one-body density. Does not collect data itself, but works merely as a control organ for the QMC class, calling it's methods for storing position data.

3.9.2 Constructor & Destructor Documentation

3.9.2.1 Distribution::Distribution (ParParams & *pp,* std::string *path,* std::string *name*)

Constructor.

Parameters

path	The path where output is stored (or read).
name	Name of the file.

3.9.3 Member Function Documentation

3.9.3.1 void Distribution::dump ( ) [virtual]

Signals QMC solver to store position data.

Implements OutputHandler.

3.9.3.2 void Distribution::finalize ( ) [virtual]

Method for calculating the distribution.

Overrides the superclass implementation.

Reimplemented from OutputHandler.

3.9.3.3 void Distribution::rerun (int *n_p,* int *N,* double *bin_edge*)

Method for re-calculating the distribution given a stores set of position data.

Scatters the data across nodes.

Parameters

n_p	Number of particles in the set.
N	Number of mesh points used in the histogram.
bin_edge	The Cartesian position of the end points of the histogram.

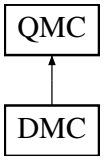
The documentation for this class was generated from the following files:

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

3.10 DMC Class Reference

Implementation of the Diffusion Monte-Carlo Method. Very little needs to be added when the QMC superclass holds all the general functionality.

Inheritance diagram for DMC:



Public Member Functions

- DMC (GeneralParams &, DMCparams &, SystemObjects &, ParParams &, VMC *vmc, bool dist_out)

  Constructor.
- void run_method ()

  Method used for executing the solver.
- void output ()

  Method for standard output.

Static Public Attributes

- static const int K = 50

  Factor of empty space for walkers over initial walkers.
- static const int **check_thresh** = 25
- static const int **sendcount_thresh** = 20

Protected Member Functions

- void set_trial_positions ()

  Method for setting the trial position of all DMC walkers.
- void iterate_walker (int k, int n_b=1)

  Method for iterating a walker one time step.
- void Evolve_walker (int k, double GB)

  Method for the birth/death process of a walker.
- void bury_the_dead ()

  Method for cleaning up the dead walkers and compact the list.
- void update_energies ()

  Method for updating the DMC energy and calculating the new trial energy.
- bool move_autherized (double A)
- void **reset_parameters** ()
- void node_comm ()
- void save_distribution ()

  Method for storing positional data for the Distribtuon.
- void switch_souls (int root, int root_id, int dest, int dest_id)

Method for sending a walker between two nodes.

- void normalize_population ()

  Method for evening out the number of walkers on each node.

Protected Attributes

- int n_w_last

  The amount of walkers at the time the walker loop was initiated.
- int n_w_tot

  The total number of walkers across all nodes.
- arma::uvec n_w_list

  List of the number of walkers of each node.
- int **deaths**
- int **block_size**
- int **samples**
- unsigned long **tot_samples**
- double **E_tot**
- double dmc_E

  The DMC energy.
- double dmc_E_unscaled

  The accumulative DMC energy: The sum of all previous trial energies.
- double E_T

  The trial energy at the current cycle.
- double E

  The accumulative energy for each cycle.

Friends

- class **stdoutDMC**

3.10.1 Detailed Description

Implementation of the Diffusion Monte-Carlo Method. Very little needs to be added when the QMC superclass holds all the general functionality.

3.10.2 Member Function Documentation

3.10.2.1 void DMC::Evolve_walker (int *k*, double *GB*) [protected]

Method for the birth/death process of a walker.

Parameters

GB	The branching Green's Function.
k	The index of the walker.

3.10.2.2 void DMC::iterate_walker (int *k*, int *n_b* = 1) [protected]

Method for iterating a walker one time step.

Parameters

n_b	The number of block samples used in the iteration.
k	The index of the walker.

3.10.2.3 bool DMC::move_autherized (double *A*) [inline, protected, virtual]

In case of DMC, we must let the system have the possibility to override the metropolis test (fixed node approximation in case of a Fermion system)

Implements QMC.

3.10.2.4 void DMC::node_comm ( ) [protected, virtual]

For each process: -Calculates the total number of walkers. -Sums up the energies sampled. -Sums up the total number of samples made.

Implements QMC.

3.10.2.5 void DMC::save_distribution ( ) [protected, virtual]

Method for storing positional data for the Distribtuon.

Stores the position data from all currently alive DMC walkers every dist_tresh cycle.

Implements QMC.

3.10.2.6 void DMC::set_trial_positions ( ) [protected, virtual]

Method for setting the trial position of all DMC walkers.

In case VMC is not run prior to DMC, trial positions must be set.

Implements QMC.

3.10.2.7 void DMC::switch_souls (int *root*, int *root_id*, int *dest*, int *dest_id*) [protected]

Method for sending a walker between two nodes.

Parameters

root	The node from which the walker is sent.
root_id	The index of the walker being sent from root.
dest	The node which receives the walker.
dest_id	The index where the walker is to be received.

See also

Walker::send_soul(), Walker::recv_soul()

3.10.3 Member Data Documentation

3.10.3.1 const int DMC::K = 50 [static]

Factor of empty space for walkers over initial walkers.

See also

QMC::QMC()

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

Struct used to initialize DMC parameters.

Public Attributes

- int n_c

  The number of cycles.
- int therm

  Thermalization cycles.
- int n_b

  Number of block samples pr. walker pr. cycle.
- int n_w

  Number of walkers.
- double dt

  Time step.

3.11.1 Detailed Description

Struct used to initialize DMC parameters.

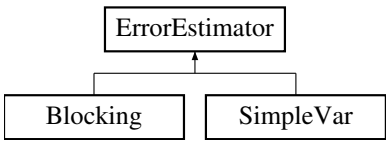
The documentation for this struct was generated from the following file:

- src/QMCheaders.h

3.12 ErrorEstimator Class Reference

Class handling error estimations of the QMC methods. The QMC class holds an object of this type, calling the update_data function in order to update the sampling pool. finalize() then either dumps the samples to file for later processing, or calulates an estimate.

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)

  Constructor.
- double combine_mean (double mean, int n, int n_tot=0)

  Calculates the combined mean of n_nodes means.
- double combine_variance (double var, double mean=0, int n=0)

  Calculates the combined variance of n_nodes variances.
- void finalize ()
- void node_comm_gather_data ()
- void node_comm_scatter_data ()
- void init_file ()

  Opens a file with filename at path supplied in constructor.
- virtual double estimate_error ()=0

  Estimates the error based on the subclass implementation.
- virtual void update_data (double val)

  Adds values to the data vector.

Public Attributes

- bool data_to_file

If true, the data vector are stored to file.

- bool output_to_file

  If init_file() method is called, this flag is true.

Protected Attributes

- int n_c

  Size of the data vector.

- int i

  Count variable for the data vector.

- bool **parallel**
- bool **is_master**
- int **node**
- int **n_nodes**
- bool rerun

  If false, data is assumed to already exist.

- std::string **filename**
- std::string **path**
- std::ofstream **file**
- arma::rowvec data

  The vector containing the samples used in error calculation.

3.12.1 Detailed Description

Class handling error estimations of the QMC methods. The QMC class holds an object of this type, calling the update_data function in order to update the sampling pool. finalize() then either dumps the samples to file for later processing, or calulates an estimate.

3.12.2 Constructor & Destructor Documentation

3.12.2.1 ErrorEstimator::ErrorEstimator (int *n_c*, std::string *filename*, std::string *path*, bool *parallel*, int *node*, int *n_nodes*, bool *rerun* = `false`)

Constructor.

Parameters

n_c	The expected number of samples to be stored.
filename	The name of the file. Only necessary if init_file() is called.
path	The path where the data and/or the file is stored (or read).

3.12.3 Member Function Documentation

3.12.3.1 double ErrorEstimator::combine_mean (double *mean*, int *n*, int *n_tot* = 0)

Calculates the combined mean of n_nodes means.

Only useful for parallel calls.

Parameters

mean	The local mean on an individual node
n	The number of samples used to calculate the local mean.
n_tot	The total number of samples on all nodes. Calculated if not supplied.

3.12.3.2 double ErrorEstimator::combine_variance (double *var*, double *mean* = 0, int *n* = 0)

Calculates the combined variance of n_nodes variances.

Only useful for parallel calls.

Parameters

var	The local variance on an individual node
mean	The local mean on an individual node
n_tot	The total number of samples used on all nodes.

3.12.3.3 void ErrorEstimator::finalize ( )

if [output_to_file]: Closes opened files if [data_to_file]: Stores accumulated data. if data vector was used, it's memory is freed.

3.12.3.4 void ErrorEstimator::init_file ( )

Opens a file with filename at path supplied in constructor.

Subclass implementations can call this function. Superclass does not.

3.12.3.5 void ErrorEstimator::node_comm_gather_data ( )

Gathers the data vectors from all processes into a single one on the master node.

3.12.3.6 void ErrorEstimator::node_comm_scatter_data ( )

Exact reverse of node_comm_gather_data()

3.12.3.7 void ErrorEstimator::update_data (double *val*) [virtual]

Adds values to the data vector.

Can be overridden if storage is not wanted.

Parameters

val	A local sample of the quantity of which the error is calculated

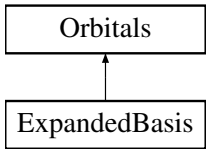
Reimplemented in SimpleVar.

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)
- double phi (const Walker *walker, int particle, int q_num)

  Calculates the single particle wave function for a given walker's particle.
- double del_phi (const Walker *walker, int particle, int q_num, int d)

  Calculates the single particle wave function derivative for a given walker's particle and dimension.
- double lapl_phi (const Walker *walker, int particle, int q_num)

  Calculates the single particle wave function for a given walker's particle.

Protected Attributes

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

3.13.1 Member Function Documentation

3.13.1.1 double ExpandedBasis::del_phi (const Walker * *walker,* int *particle,* int *q_num,* int *d*) [virtual]

Calculates the single particle wave function derivative for a given walker's particle and dimension.

Parameters

q_num	The quantum number index.
d	The dimension for which the derivative should be calculated (x,y,z).

Reimplemented from Orbitals.

3.13.1.2 double ExpandedBasis::lapl_phi (const Walker * *walker,* int *particle,* int *q_num*) [virtual]

Calculates the single particle wave function for a given walker's particle.

Parameters

q_num	The quantum number index.

Reimplemented from Orbitals.

3.13.1.3 double ExpandedBasis::phi (const Walker * *walker,* int *particle,* int *q_num*) [virtual]

Calculates the single particle wave function for a given walker's particle.

Parameters

q_num	The quantum number index.

Reimplemented from Orbitals.

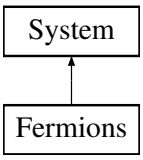
The documentation for this class was generated from the following files:

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

3.14 Fermions Class Reference

The Fermion system class.

Inheritance diagram for Fermions:



Public Member Functions

- **Fermions** (GeneralParams &, Orbitals ∗)
- void get_spatial_grad (Walker ∗walker, int particle) const

  Method for calculating the changed part of the spatial gradient.
- void get_spatial_grad_full (Walker ∗walker) const

  Method for calculating the full spatial gradient.
- double get_spatial_ratio (const Walker ∗walker_post, const Walker ∗walker_pre, int particle)

  Method for calculating the spatial wave function ratios between two subsequent time steps.
- double get_spatial_lapl_sum (const Walker ∗walker) const

  Method for calculating the sum of all Laplacians for a given walker.
- bool allow_transition ()

  Fixed node approximation.
- void copy_walker (const Walker ∗parent, Walker ∗child) const
- 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
- double get_spatial_wf (const Walker ∗walker)
- void initialize (Walker ∗walker)
- void calc_for_newpos (const Walker ∗walker_old, Walker ∗walker_new, int i)

Protected Member Functions

- void make_merged_inv (Walker ∗walker)

  Method for calculating the Slater matrix inverse.
- void update_inverse (const Walker ∗walker_old, Walker ∗walker_new, int particle)

  Method for updating the inverse given that we moved one particle.

Protected Attributes

- arma::rowvec l

  The diagonal of the new slater matrix times the old slater inverse.
- bool node_crossed

  True if the spatial ratio is negative.

3.14.1 Detailed Description

The Fermion system class.

3.14.2 Member Function Documentation

3.14.2.1 void Fermions::calc_for_newpos (const Walker * *walker_old,* Walker * *walker_new,* int *i*) [inline, virtual]

When a particle is moved, the inverse is updated.

Implements System.

3.14.2.2 void Fermions::copy_walker (const Walker * *parent,* Walker * *child*) const [inline, virtual]

Copies the inverse.

Implements System.

3.14.2.3 void Fermions::get_spatial_grad (Walker * *walker,* int *particle*) const [virtual]

Method for calculating the changed part of the spatial gradient.

Depending on which particle we moved, one of the spatial wave function parts (it is split) will be unchanged.

Implements System.

3.14.2.4 double Fermions::get_spatial_wf (const Walker * *walker*) [inline, virtual]

The determinant of each spin value multiplied.

Implements System.

3.14.2.5 void Fermions::initialize (Walker * *walker*) [inline, virtual]

Calculates the inverse.

Implements System.

3.14.2.6 void Fermions::make_merged_inv (Walker * *walker*) [protected]

Method for calculating the Slater matrix inverse.

The merged inverse is made by concatenating the two slater matrix inverses. This way we can sum freely over particles without having to if-test on the spin.

3.14.2.7 void Fermions::reset_walker (const Walker * *walker_pre*, Walker * *walker_post*, int *particle*) const [inline, virtual]

Resets the inverse.

Implements System.

3.14.2.8 void Fermions::update_walker (Walker * *walker_pre*, const Walker * *walker_post*, int *particle*) const [inline, virtual]

Updates the inverse.

Implements System.

3.14.3 Member Data Documentation

3.14.3.1 arma::rowvec Fermions::l [protected]

The diagonal of the new slater matrix times the old slater inverse.

Needed for updating the inverse. Stored because only half of the vector is changed when moving one particle.

See also

System::set_spin_state()

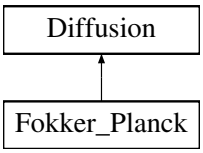
The documentation for this class was generated from the following files:

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

3.15 Fokker_Planck Class Reference

Anisotropic diffusion by the Fokker-Planck equation.

Inheritance diagram for Fokker_Planck:



Public Member Functions

- **Fokker_Planck** (int n_p, int dim, double timestep, seed_type random_seed, double D=0.5)
- double get_g_ratio (const Walker *walker_post, const Walker *walker_pre) const

  Calculates the Diffusion Green's function ratio needed by metropolis.
- double get_new_pos (const Walker *walker, int i, int j)

  Virtual function returning the new position.

3.15.1 Detailed Description

Anisotropic diffusion by the Fokker-Planck equation.

3.15.2 Member Function Documentation

3.15.2.1 double Fokker_Planck::get_g_ratio (const Walker * *walker_post,* const Walker * *walker_pre*) const [virtual]

Calculates the Diffusion Green's function ratio needed by metropolis.

Parameters

walker_post	Walker at current time step.
walker_pre	Walker at previous time step.

Returns

The Diffusion Green's function ratio.

Implements Diffusion.

3.15.2.2 double Fokker_Planck::get_new_pos (const Walker * *walker,* int *i,* int *j*) [inline, virtual]

Virtual function returning the new position.

Returns the simple diffusion step if not overridden.

Parameters

i	Particle number.
j	dimension (x,y,z).

Returns

The new position (relative to the old).

Reimplemented from Diffusion.

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

Struct used to initialize general parameters.

Public Attributes

- int n_p

  The number of particles.
- int dim

  The dimension.
- seed_type random_seed

  The random number generator's seed.
- double systemConstant

  The constant used in systems.
- bool **doMIN**
- bool **doVMC**
- bool **doDMC**
- bool **do_blocking**
- bool **use_jastrow**
- bool **use_coulomb**
- std::string system

  String specifing the system type, e.g. "Atoms".
- std::string sampling

  String specifing the sampling type, e.g. "IS".
- std::string runpath

  The directory which the simulation is set to run.

3.16.1 Detailed Description

Struct used to initialize general parameters.

3.16.2 Member Data Documentation

3.16.2.1 double GeneralParams::systemConstant

The constant used in systems.

e.g. charge for atoms and oscillator frequency for quantum dots.

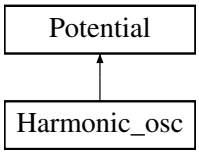
The documentation for this struct was generated from the following file:

- src/QMCheaders.h

3.17 Harmonic_osc Class Reference

Implementation of the Harmonic Oscillator potential. 0.5∗w∗∗2∗r∗∗2.

Inheritance diagram for Harmonic_osc:



Public Member Functions

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

  Method for calculating a walker's potential energy.

Protected Attributes

- double w

  The oscillator frequency.

3.17.1 Detailed Description

Implementation of the Harmonic Oscillator potential. 0.5∗w∗∗2∗r∗∗2.

3.17.2 Member Function Documentation

3.17.2.1 double Harmonic_osc::get_pot_E (const Walker ∗ *walker*) const [virtual]

Method for calculating a walker's potential energy.

Method overridden by subclasses.

Parameters

walker	The walker for which the potential energy should be calculated.

Returns

The potential energy.

Implements Potential.

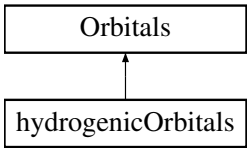
The documentation for this class was generated from the following files:

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

3.18 hydrogenicOrbitals Class Reference

Hyrogen-like single particle wave function class. Uses the hydrogenic BasisFunction subclasses auto-generated by SymPy through the orbitalsGenerator tool.

Inheritance diagram for hydrogenicOrbitals:



Public Member Functions

- **hydrogenicOrbitals** (GeneralParams &, VariationalParams &)
- **hydrogenicOrbitals** (GeneralParams &)
- void set_qnum_indie_terms (const Walker *walker, int i)

Protected Member Functions

- double get_variational_derivative (const Walker *walker, int n)

  ! Overridden superclass method implementing closed form expressions generated by SymPy.
- double get_dell_alpha_phi (const Walker *walker, int qnum, int i)

  Method for calculating a single particle wave functions variational derivative.
- double get_parameter (int n)
- void set_parameter (double parameter, int n)

Protected Attributes

- int Z

  The charge of the core.
- double * alpha

  Pointer to the variational parameter alpha. Shared address with all the BasisFunction subclasses.
- double * k

  *Pointer to alpha*Z. Shared address with all the BasisFunction subclasses.*
- double * k2

  *Pointer (alpha*Z)^2. Shared address with all the BasisFunction subclasses.*
- double * **r22d**
- double * **r2d**
- double * exp_factor_n1

  Pointer to a factor precalculated by set_qnum_indie_terms(). Shared address with all the BasisFunction subclasses.
- double * exp_factor_n2

  Pointer to a factor precalculated by set_qnum_indie_terms(). Shared address with all the BasisFunction subclasses.
- arma::Mat< int > **qnums**

Friends

- class **ExpandedBasis**

3.18.1 Detailed Description

Hyrogen-like single particle wave function class. Uses the hydrogenic BasisFunction subclasses auto-generated by SymPy through the orbitalsGenerator tool.

3.18.2 Member Function Documentation

3.18.2.1 double hydrogenicOrbitals::get_dell_alpha_phi (const Walker * *walker*, int *qnum*, int *i*) [protected]

Method for calculating a single particle wave functions variational derivative.

Parameters

i	The particle number.

3.18.2.2 double hydrogenicOrbitals::get_parameter (int *n*) [inline, protected, virtual]

Returns

The variational parameter alpha.

Implements Orbitals.

3.18.2.3 void hydrogenicOrbitals::set_parameter (double *parameter*, int *n*) [inline, protected, virtual]

Sets a new value for the alpha and updates all the pointer values.

Implements Orbitals.

3.18.2.4 void hydrogenicOrbitals::set_qnum_indie_terms (const Walker * *walker*, int *i*) [virtual]

Calculates the exponential terms exp(-r/n) for all needed n once pr. particle to save CPU-time.

See also

Orbitals::set_qnum_indie_terms()

Reimplemented from Orbitals.

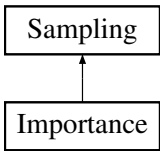
The documentation for this class was generated from the following files:

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

3.19 Importance Class Reference

Implementation of Importance sampled QMC. Using the Fokker-Planck diffusion class. Introduces the Quantum Force.

Inheritance diagram for Importance:



Public Member Functions

- **Importance** (GeneralParams &)

- 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 get_necessities (Walker ∗walker)
- void update_necessities (const Walker ∗walker_pre, Walker ∗walker_post, int particle) const
- void calculate_energy_necessities (Walker ∗walker) const
- void copy_walker (const Walker ∗parent, Walker ∗child) const

3.19.1 Detailed Description

Implementation of Importance sampled QMC. Using the Fokker-Planck diffusion class. Introduces the Quantum Force.

3.19.2 Member Function Documentation

3.19.2.1 void Importance::calculate_energy_necessities (Walker ∗ *walker*) const [inline, virtual]

No energy necessities (they are already calculated).

Implements Sampling.

3.19.2.2 void Importance::copy_walker (const Walker ∗ *parent*, Walker ∗ *child*) const [inline, virtual]

The gradients and the Quantum force is copied.

Implements Sampling.

3.19.2.3 void Importance::get_necessities (Walker ∗ *walker*) [inline, virtual]

The gradients and the Quantum force are calculated.

Implements Sampling.

3.19.2.4 void Importance::reset_walker (const Walker ∗ *walker_pre*, Walker ∗ *walker_post*, int *particle*) const [virtual]

The parts of the gradients with the same spin as the moved particle are reset.

Implements Sampling.

3.19.2.5 void Importance::update_necessities (const Walker * *walker_pre*, Walker * *walker_post*, int *particle*) const [inline, virtual]

The gradients are updated and the Quantum force is re-calculated.

Implements Sampling.

3.19.2.6 void Importance::update_walker (Walker * *walker_pre*, const Walker * *walker_post*, int *particle*) const [virtual]

The parts of the gradients with the same spin as the moved particle are updated.

Implements Sampling.

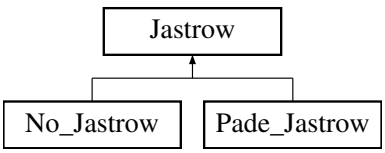
The documentation for this class was generated from the following files:

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

3.20 Jastrow Class Reference

The class representing the Jastrow correlation functions Holds all data concerning the Jastrow function and it's influence on the QMC algorithm.

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

  Calculates the ratio of the Jastrow factor needed by metropolis.
- virtual void get_grad (Walker *walker) const =0
- virtual void get_grad (const Walker *walker_pre, Walker *walker_post, int i) const =0

  Updates the gradient for a new particle move.
- virtual void get_dJ_matrix (Walker *walker, int i) const =0

  Updates the summation factors of Jastrow factors closed form expressions.

- void get_dJ_matrix (Walker ∗walker) const

  Calculates the summation factors of Jastrow factors closed form expressions.
- virtual double get_lapl_sum (Walker ∗walker) const =0

  Method for calculating the Laplacian.

Protected Member Functions

- virtual double get_parameter (int n)=0

  Returns variational parameters.
- virtual void set_parameter (double param, int n)=0

  Sets variational parameters.
- virtual double get_variational_derivative (const Walker ∗walker, int n)

  Calculates the derivative of the Jastrow factor with respect to a variational parameter.
- double get_derivative_num (Walker ∗walker, int i, int d) const

  Numerical Cartesian derivative.
- double get_laplaciansum_num (Walker ∗walker) const

  Numerical Cartesian Laplacian.

Protected Attributes

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

  Parameter false if No_Jastrow is loaded.

Friends

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

3.20.1 Detailed Description

The class representing the Jastrow correlation functions Holds all data concerning the Jastrow function and it's influence on the QMC algorithm.

3.20.2 Member Function Documentation

3.20.2.1 double Jastrow::get_derivative_num (Walker ∗ *walker,* int *i,* int *d*) const [protected]

Numerical Cartesian derivative.

For use in get_grad() when no closed form expression is implemented.

Parameters

i	Particle number.
d	Dimension (x,y,z).

3.20.2.2 virtual void Jastrow::get_dJ_matrix (Walker * *walker,* int *i*) const [pure virtual]

Updates the summation factors of Jastrow factors closed form expressions.

Used to optimize the calculations as few of these terms change as we move a particle.

Parameters

i	Particle number.

Implemented in Pade_Jastrow, and No_Jastrow.

3.20.2.3 void Jastrow::get_dJ_matrix (Walker * *walker*) const

Calculates the summation factors of Jastrow factors closed form expressions.

Used to optimize the calculations as few of these terms change as we move a particle.

3.20.2.4 virtual void Jastrow::get_grad (Walker * *walker*) const [pure virtual]

Calculates the entire Cartesian gradient.

Implemented in Pade_Jastrow, and No_Jastrow.

3.20.2.5 virtual void Jastrow::get_grad (const Walker * *walker_pre,* Walker * *walker_post,* int *i*) const [pure virtual]

Updates the gradient for a new particle move.

Parameters

walker_post	Walker at current time step
walker_pre	Walker at previous time step
i	Particle number.

Implemented in Pade_Jastrow, and No_Jastrow.

3.20.2.6 virtual double Jastrow::get_j_ratio (const Walker * *walker_new,* const Walker * *walker_old,* int *i*) const [pure virtual]

Calculates the ratio of the Jastrow factor needed by metropolis.

Parameters

walker_new	Walker at current time step
walker_old	Walker at previous time step
i	The particle number.

Implemented in Pade_Jastrow, and No_Jastrow.

3.20.2.7 virtual double Jastrow::get_lapl_sum (Walker * *walker*) const [pure virtual]

Method for calculating the Laplacian.

Calculates the sum of all particles Laplacians.

Implemented in No_Jastrow, and Pade_Jastrow.

3.20.2.8 double Jastrow::get_laplaciansum_num (Walker * *walker*) const [protected]

Numerical Cartesian Laplacian.

For use in get_lapl_sum() when no closed form expression is implemented.

3.20.2.9 virtual double Jastrow::get_parameter (int *n*) [protected, pure virtual]

Returns variational parameters.

Parameters

n	The index of the sought variational parameter

Returns

Variational parameter with index [n]

Implemented in Pade_Jastrow, and No_Jastrow.

3.20.2.10 virtual double Jastrow::get_val (const Walker * *walker*) const [pure virtual]

Calculates the value of the Jastrow Factor at the walker's position.

Implemented in Pade_Jastrow, and No_Jastrow.

3.20.2.11 double Jastrow::get_variational_derivative (const Walker * *walker*, int *n*) [protected, virtual]

Calculates the derivative of the Jastrow factor with respect to a variational parameter.

Parameters

n	The index of the variational parameter for which the derivative is to be taken
walker	The walker holds the positions etc. needed to evaluate the derivative

Reimplemented in No_Jastrow, and Pade_Jastrow.

3.20.2.12 virtual void Jastrow::initialize ( ) [pure virtual]

Initializes the non-variational parameters needed by the Jastrow Factor.

Implemented in Pade_Jastrow, and No_Jastrow.

3.20.2.13 virtual void Jastrow::set_parameter (double *param*, int *n*) [protected, pure virtual]

Sets variational parameters.

Parameters

n	The index of the sought variational parameter
param	The new value of parameter [n]

Implemented in No_Jastrow, and Pade_Jastrow.

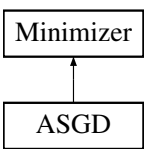
The documentation for this class was generated from the following files:

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

3.21 Minimizer Class Reference

Class for minimization methods used to obtain optimal variational parameters.

Inheritance diagram for Minimizer:



Public Member Functions

- Minimizer (VMC *vmc, const ParParams &, const arma::rowvec &alpha, const arma::rowvec &beta)

  Constructor.
- void add_output (OutputHandler *output_handler)

  Method used for loading the stdoutASGD object.
- Orbitals * **get_orbitals** ()
- Jastrow * **get_jastrow** ()
- virtual void minimize ()=0

  Method for executing the minimization main solver.
- void output (std::string message, double number=-1)

  Method for dumping variational parameter values to screen.
- void add_error_estimator (ErrorEstimator *error_estimator)

  Method used to add error estimators.

Protected Member Functions

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

  Method for updating the variational parameters based on the previous step.

Protected Attributes

- int **n_nodes**
- bool **is_master**
- VMC * vmc

  Uses VMC methods to calculate stochastic variational gradients.
- STDOUT * std_out

  Output object. Wraps and replaces std::cout.
- std::stringstream **s**
- int Nspatial_params

  The number of variational parameters in the spatial trial wave function.
- int Njastrow_params

  The number of variational parameters in the Jastrow factor.
- int Nparams

  The total number of variational parameters.
- std::vector< OutputHandler * > output_handler

  Either contains a stdoutASGD object or not.
- std::vector< ErrorEstimator * > error_estimators

  One ErrorEstimator object pr. variational parameter.

3.21.1 Detailed Description

Class for minimization methods used to obtain optimal variational parameters.

3.21.2 Constructor & Destructor Documentation

3.21.2.1 Minimizer::Minimizer (VMC * *vmc*, const ParParams & *pp*, const arma::rowvec & *alpha*, const arma::rowvec & *beta*)

Constructor.

Parameters

vmc	The VMC object used for storing variational parameters and calculating stochastic gradients.
alpha	Vector of initial conditions of spatial variational parameters
beta	Vector of initial conditions of Jastrow variational parameters

3.21.3 Member Function Documentation

3.21.3.1 void Minimizer::dump_output ( ) [protected]

Iterates over the output objects in the output_handler vector. No if-tests.

3.21.3.2 void Minimizer::error_output ( ) [protected]

Estimates and finalizes the ErrorEstimator objects initialized in the error_estimators vector.

3.21.3.3 void Minimizer::finalize_output ( ) [protected]

Calls the finalize function for the object in the output_handler vector.

3.21.3.4 virtual void Minimizer::update_parameters ( ) [protected, pure virtual]

Method for updating the variational parameters based on the previous step.

Needs to be implemented by a subclass.

Implemented in ASGD.

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

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

3.22 MinimizerParams Struct Reference

Struct used to initialize Minimization parameters.

Public Attributes

- double **max_step**
- double **f_max**
- double **f_min**
- double **omega**
- double **A**
- double **a**
- int **SGDsamples**
- int **n_w**
- int **therm**
- int **n_c**
- int **n_c_SGD**
- arma::rowvec alpha

  Initial condition for the spatial variational parameter(s).
- arma::rowvec beta

  Initial condition for the Jastrow variational parameter(s).

3.22.1 Detailed Description

Struct used to initialize Minimization parameters.

See also

ASGD

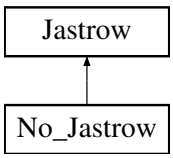
The documentation for this struct was generated from the following file:

- src/QMCheaders.h

3.23 No_Jastrow Class Reference

Class loaded when no correlation factor is used.

Inheritance diagram for No_Jastrow:



Public Member Functions

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

  Updates the gradient for a new particle move.
- void initialize ()
- void get_dJ_matrix (Walker ∗walker, int i) const

  Updates the summation factors of Jastrow factors closed form expressions.
- double get_j_ratio (const Walker ∗walker_post, const Walker ∗walker_pre, int i) const

  Calculates the ratio of the Jastrow factor needed by metropolis.
- double get_val (const Walker ∗walker) const
- double get_lapl_sum (Walker ∗walker) const

  Method for calculating the Laplacian.

Protected Member Functions

- double get_parameter (int n)

  Returns variational parameters.
- void set_parameter (double param, int n)

  Sets variational parameters.
- double get_variational_derivative (const Walker ∗walker, int n)

  Calculates the derivative of the Jastrow factor with respect to a variational parameter.

3.23.1 Detailed Description

Class loaded when no correlation factor is used.

3.23.2 Member Function Documentation

3.23.2.1 void No_Jastrow::get_dJ_matrix (Walker ∗ *walker,* int *i*) const [inline, virtual]

Updates the summation factors of Jastrow factors closed form expressions.

Used to optimize the calculations as few of these terms change as we move a particle.

Parameters

i	Particle number.

Implements Jastrow.

3.23.2.2 void No_Jastrow::get_grad (Walker * *walker*) const [inline, virtual]

Calculates the entire Cartesian gradient.

Implements Jastrow.

3.23.2.3 void No_Jastrow::get_grad (const Walker * *walker_pre*, Walker * *walker_post*, int *i*) const [inline, virtual]

Updates the gradient for a new particle move.

Parameters

walker_post	Walker at current time step
walker_pre	Walker at previous time step
i	Particle number.

Implements Jastrow.

3.23.2.4 double No_Jastrow::get_j_ratio (const Walker * *walker_new*, const Walker * *walker_old*, int *i*) const [inline, virtual]

Calculates the ratio of the Jastrow factor needed by metropolis.

Parameters

walker_new	Walker at current time step
walker_old	Walker at previous time step
i	The particle number.

Implements Jastrow.

3.23.2.5 double No_Jastrow::get_lapl_sum (Walker * *walker*) const [inline, virtual]

Method for calculating the Laplacian.

Calculates the sum of all particles Laplacians.

Implements Jastrow.

3.23.2.6 double No_Jastrow::get_parameter (int *n*) [inline, protected, virtual]

Returns variational parameters.

Parameters

n	The index of the sought variational parameter

Returns

Variational parameter with index [n]

Implements Jastrow.

3.23.2.7 double No_Jastrow::get_val (const Walker * *walker*) const [inline, virtual]

Calculates the value of the Jastrow Factor at the walker's position.

Implements Jastrow.

3.23.2.8 double No_Jastrow::get_variational_derivative (const Walker * *walker*, int *n*) [inline, protected, virtual]

Calculates the derivative of the Jastrow factor with respect to a variational parameter.

Parameters

n	The index of the variational parameter for which the derivative is to be taken
walker	The walker holds the positions etc. needed to evaluate the derivative

Reimplemented from Jastrow.

3.23.2.9 void No_Jastrow::initialize ( ) [inline, virtual]

Initializes the non-variational parameters needed by the Jastrow Factor.

Implements Jastrow.

3.23.2.10 void No_Jastrow::set_parameter (double *param*, int *n*) [inline, protected, virtual]

Sets variational parameters.

Parameters

n	The index of the sought variational parameter
param	The new value of parameter [n]

Implements Jastrow.

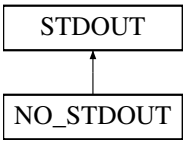
The documentation for this class was generated from the following files:

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

3.24 NO_STDOUT Class Reference

Class for suppressing standard output. Every node but the master has this. If-tests around cout is avoided.

Inheritance diagram for NO_STDOUT:



Public Member Functions

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

3.24.1 Detailed Description

Class for suppressing standard output. Every node but the master has this. If-tests around cout is avoided.

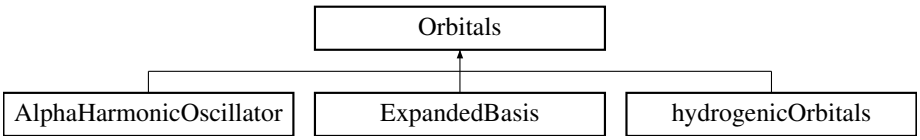
The documentation for this class was generated from the following file:

- src/QMCheaders.h

3.25 Orbitals Class Reference

Superclass for the single particle orbital classes. Handles everything specific regarding choice of single particle basis.

Inheritance diagram for Orbitals:



Public Member Functions

- **Orbitals** (int n_p, int dim)
- virtual void set_qnum_indie_terms (const Walker ∗walker, int i)

  Calculates single particle wave function terms which are independent of the quantum numbers.
- virtual double phi (const Walker ∗walker, int particle, int q_num)

  Calculates the single particle wave function for a given walker's particle.
- virtual double del_phi (const Walker ∗walker, int particle, int q_num, int d)

  Calculates the single particle wave function derivative for a given walker's particle and dimension.
- virtual double lapl_phi (const Walker ∗walker, int particle, int q_num)

  Calculates the single particle wave function for a given walker's particle.
- void **set_qmc_ptr** (QMC ∗qmc)

Protected Member Functions

- virtual double get_parameter (int n)=0

  A method for retrieving variational parameters.
- virtual void set_parameter (double parameter, int n)=0

  A method for setting variational parameters.
- virtual double get_variational_derivative (const Walker ∗walker, int n)

  A method for calculating the variational derivative.
- double num_diff (const Walker ∗walker, int particle, int q_num, int d)

  Method for calculating the single particle derivative using a finite difference scheme.
- double num_ddiff (const Walker ∗walker, int particle, int q_num)

  Method for calculating the single particle Laplacian using a finite difference scheme.
- void testLaplace (const Walker ∗walker, int particle, int q_num)

  Method for validating closed form expressions for laplacians by comparing them to numerical calculations.
- void testDell (const Walker ∗walker, int particle, int q_num, int d)

  Method for validating closed form expressions for derivatives by comparing them to numerical calculations.

Protected Attributes

- int **n_p**
- int **n2**
- int **dim**
- int max_implemented

  The maximum number basis size supported for any system ##RYDD OPP.
- QMC ∗ qmc

  A pointer to the QMC solver object. Needed for numerical variational derivatives.
- double h

The step length for finite difference schemes.

- double **h2**
- double **two_h**
- BasisFunctions ** basis_functions

  A vector maping a quantum number index to a single particle wave function.
- BasisFunctions *** dell_basis_functions

  A maxtrix maping a quantum number- and dimension index to a single particle wave function derivative.
- BasisFunctions ** lapl_basis_functions

  A vector maping a quantum number index to a single particle wave function Laplacian.

Friends

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

3.25.1 Detailed Description

Superclass for the single particle orbital classes. Handles everything specific regarding choice of single particle basis.

3.25.2 Member Function Documentation

3.25.2.1 double Orbitals::del_phi (const Walker * *walker*, int *particle*, int *q_num*, int *d*) [virtual]

Calculates the single particle wave function derivative for a given walker's particle and dimension.

Parameters

q_num	The quantum number index.
d	The dimension for which the derivative should be calculated (x,y,z).

Reimplemented in ExpandedBasis.

3.25.2.2 virtual double Orbitals::get_parameter (int *n*) [protected, pure virtual]

A method for retrieving variational parameters.

Parameters

n	Index of the sought variational parameter.

Implemented in AlphaHarmonicOscillator, and hydrogenicOrbitals.

3.25.2.3 double Orbitals::get_variational_derivative (const Walker * *walker,* int *n*) [protected, virtual]

A method for calculating the variational derivative.

By default uses a finite difference scheme. Can be overridden to evaluate a closed form expression.

Parameters

n	Index of the sought variational parameter.

Reimplemented in AlphaHarmonicOscillator, and hydrogenicOrbitals.

3.25.2.4 double Orbitals::lapl_phi (const Walker * *walker,* int *particle,* int *q_num*) [virtual]

Calculates the single particle wave function for a given walker's particle.

Parameters

q_num	The quantum number index.

Reimplemented in ExpandedBasis.

3.25.2.5 double Orbitals::num_ddiff (const Walker * *walker,* int *particle,* int *q_num*) [protected]

Method for calculating the single particle Laplacian using a finite difference scheme.

Method lapl_phi() can be overridden to use this method in case no closed form expressions are implemented.

Parameters

q_num	The quantum number index.

3.25.2.6 double Orbitals::num_diff (const Walker * *walker,* int *particle,* int *q_num,* int *d*) [protected]

Method for calculating the single particle derivative using a finite difference scheme.

Method del_phi() can be overridden to use this method in case no closed form expressions are implemented.

Parameters

d	The dimension for which the derivative should be calculated (x,y,z).

3.25.2.7 double Orbitals::phi (const Walker * *walker*, int *particle*, int *q_num*) [virtual]

Calculates the single particle wave function for a given walker's particle.

Parameters

q_num	The quantum number index.

Reimplemented in ExpandedBasis.

3.25.2.8 virtual void Orbitals::set_parameter (double *parameter*, int *n*) [protected, pure virtual]

A method for setting variational parameters.

Parameters

n	Index of the sought variational parameter.
parameter	The new value of the variational parameter.

Implemented in AlphaHarmonicOscillator, and hydrogenicOrbitals.

3.25.2.9 virtual void Orbitals::set_qnum_indie_terms (const Walker * *walker*, int *i*) [inline, virtual]

Calculates single particle wave function terms which are independent of the quantum numbers.

If a term in the single particle functions are independent of the quantum number, this function can be overridden to calculate them beforehand (for each particle), and rather extract the value instead of recalculating.

Parameters

i	Particle number.

Reimplemented in AlphaHarmonicOscillator, and hydrogenicOrbitals.

3.25.2.10 void Orbitals::testDell (const Walker * *walker*, int *particle*, int *q_num*, int *d*) [protected]

Method for validating closed form expressions for derivatives by comparing them to numerical calculations.

Parameters

q_num	The quantum number index.
d	The dimension for which the derivative should be calculated (x,y,z).

3.25.2.11 void Orbitals::testLaplace (const Walker * *walker,* int *particle,* int *q_num*) [protected]

Method for validating closed form expressions for laplacians by comparing them to numerical calculations.

Parameters

q_num	The quantum number index.

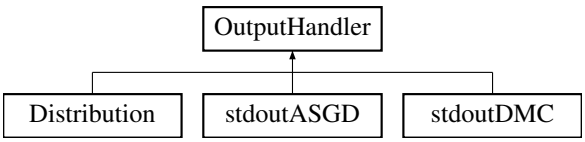
The documentation for this class was generated from the following files:

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

3.26 OutputHandler Class Reference

Class for handling output-methods. Designed to avoid rewriting code, as well as avoid if-tests if output is not desired.

Inheritance diagram for OutputHandler:



Public Member Functions

- OutputHandler (std::string filename, std::string path, bool parallel, int node, int n_nodes)

  Constructor.
- virtual void dump ()=0

  Methods for updating the output.
- virtual void finalize ()

  Finalizes the output.
- void set_qmc_ptr (QMC *qmc)
- void set_min_ptr (Minimizer *min)

Protected Member Functions

- void init_file ()
- virtual void post_pointer_init ()

  Method for initialization requires once the correct QMC/Min pointer type is set.

Protected Attributes

- bool is_vmc

  Switch used to typecast the QMC object to a VMC object.
- bool is_dmc

  Switch used to typecast the QMC object to a DMC object.
- bool is_ASGD

  Switch used to typecast the Min object to an ASGD object.
- bool **parallel**
- int **node**
- int **n_nodes**
- bool use_file

  If init_file() is called, this flag is set true. Assures correct finalization.
- std::stringstream **s**
- std::string **filename**
- std::string **path**
- std::ofstream **file**
- QMC ∗ **qmc**
- DMC ∗ **dmc**
- VMC ∗ **vmc**
- Minimizer ∗ **min**
- ASGD ∗ **asgd**

3.26.1 Detailed Description

Class for handling output-methods. Designed to avoid rewriting code, as well as avoid if-tests if output is not desired.

See also

QMC::output_handler, Minimizer::output_handler

3.26.2 Constructor & Destructor Documentation

3.26.2.1 OutputHandler::OutputHandler (std::string *filename*, std::string *path*, bool *parallel*, int *node*, int *n_nodes*)

Constructor.

Parameters

filename	The name of the output file.
path	The path of the output.

3.26.3 Member Function Documentation

3.26.3.1 virtual void OutputHandler::dump ( ) [pure virtual]

Methods for updating the output.

Typically retrieves information through the solver pointers (given correct accessibility levels/friend)

Implemented in Distribution, stdoutDMC, and stdoutASGD.

3.26.3.2 void OutputHandler::finalize ( ) [virtual]

Finalizes the output.

Closes file if use_file flag is true. Can be overridden if more complex tasks needs to be done, such as calculating histograms etc.

See also

Distribution::finalize()

Reimplemented in Distribution.

3.26.3.3 void OutputHandler::init_file ( ) [protected]

Opens a file with filename at path supplied in constructor. Subclass implementations can call this function. Superclass does not.

3.26.3.4 virtual void OutputHandler::post_pointer_init ( ) [inline, protected, virtual]

Method for initialization requires once the correct QMC/Min pointer type is set.

Defaults to nothing.

Reimplemented in stdoutASGD.

3.26.3.5 void OutputHandler::set_min_ptr (Minimizer * *min*)

Sets the Min pointer and typecasts it according to the minimizer flags.

3.26.3.6 void OutputHandler::set_qmc_ptr (QMC * *qmc*)

Sets the QMC pointer and typecasts it according to the solver flags.

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

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

3.27 OutputParams Struct Reference

Struct used to initialize output parameters.

Public Attributes

- bool dist_out

  If true, distributions are calculated for VMC/DMC.
- bool dmc_out

  If true, DMC outputs data to file each cycle.
- bool ASGD_out

  If true, ASGD outputs data to file each cycle.

3.27.1 Detailed Description

Struct used to initialize output parameters.

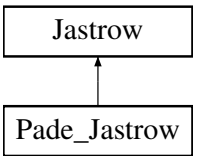
The documentation for this struct was generated from the following file:

- src/QMCheaders.h

3.28 Pade_Jastrow Class Reference

The Pade Jastrow factor with a single variational parameter.

Inheritance diagram for Pade_Jastrow:



Public Member Functions

- **Pade_Jastrow** (GeneralParams &, VariationalParams &)
- void initialize ()
- void get_grad (Walker ∗walker) const
- void get_grad (const Walker ∗walker_pre, Walker ∗walker_post, int i) const

  Updates the gradient for a new particle move.
- void get_dJ_matrix (Walker ∗walker, int i) const

  Updates the summation factors of Jastrow factors closed form expressions.
- double get_j_ratio (const Walker ∗walker_new, const Walker ∗walker_old, int i) const

  Calculates the ratio of the Jastrow factor needed by metropolis.
- double get_val (const Walker ∗walker) const
- double get_lapl_sum (Walker ∗walker) const

  Method for calculating the Laplacian.

Protected Member Functions

- double get_variational_derivative (const Walker ∗walker, int n)

  Calculates the derivative of the Jastrow factor with respect to a variational parameter.
- void set_parameter (double param, int n)

  Sets variational parameters.
- double get_parameter (int n)

  Returns variational parameters.

Protected Attributes

- double beta

  The variational parameter.
- arma::mat a

  The spin-dependent variables taking care of the cusp condition.

3.28.1 Detailed Description

The Pade Jastrow factor with a single variational parameter.

3.28.2 Member Function Documentation

3.28.2.1 void Pade_Jastrow::get_dJ_matrix (Walker ∗ *walker,* int *i*) const [virtual]

Updates the summation factors of Jastrow factors closed form expressions.

Used to optimize the calculations as few of these terms change as we move a particle.

Parameters

i	Particle number.

Implements Jastrow.

3.28.2.2 void Pade_Jastrow::get_grad (Walker * *walker*) const [virtual]

Calculates the entire Cartesian gradient.

Implements Jastrow.

3.28.2.3 void Pade_Jastrow::get_grad (const Walker * *walker_pre*, Walker * *walker_post*, int *i*) const [virtual]

Updates the gradient for a new particle move.

Parameters

walker_post	Walker at current time step
walker_pre	Walker at previous time step
i	Particle number.

Implements Jastrow.

3.28.2.4 double Pade_Jastrow::get_j_ratio (const Walker * *walker_new*, const Walker * *walker_old*, int *i*) const [virtual]

Calculates the ratio of the Jastrow factor needed by metropolis.

Parameters

walker_new	Walker at current time step
walker_old	Walker at previous time step
i	The particle number.

Implements Jastrow.

3.28.2.5 double Pade_Jastrow::get_lapl_sum (Walker * *walker*) const [virtual]

Method for calculating the Laplacian.

Calculates the sum of all particles Laplacians.

Implements Jastrow.

3.28.2.6 double Pade_Jastrow::get_parameter (int *n*) [inline, protected, virtual]

Returns variational parameters.

Parameters

n	The index of the sought variational parameter

Returns

Variational parameter with index [n]

Implements Jastrow.

3.28.2.7 double Pade_Jastrow::get_val (const Walker * *walker*) const [virtual]

Calculates the value of the Jastrow Factor at the walker's position.

Implements Jastrow.

3.28.2.8 double Pade_Jastrow::get_variational_derivative (const Walker * *walker,* int *n*) [protected, virtual]

Calculates the derivative of the Jastrow factor with respect to a variational parameter.

Parameters

n	The index of the variational parameter for which the derivative is to be taken
walker	The walker holds the positions etc. needed to evaluate the derivative

Reimplemented from Jastrow.

3.28.2.9 void Pade_Jastrow::initialize ( ) [virtual]

In case of Pade Jastrow, initializing means seting up the a matrix.

Implements Jastrow.

3.28.2.10 void Pade_Jastrow::set_parameter (double *param,* int *n*) [inline, protected, virtual]

Sets variational parameters.

Parameters

n	The index of the sought variational parameter
param	The new value of parameter [n]

Implements Jastrow.

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

3.29 ParParams Struct Reference

Struct used to initialize parallelization parameters.

Public Attributes

- bool is_master

  True for the master node.
- bool parallel

  True if n_nodes > 1.
- int node

  The process' rank.
- int n_nodes

  The total number of processes.

3.29.1 Detailed Description

Struct used to initialize parallelization parameters.

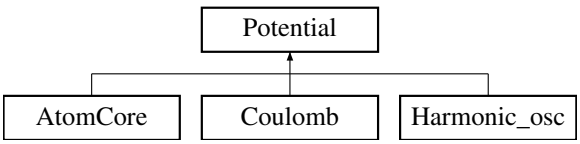
The documentation for this struct was generated from the following file:

- src/QMCheaders.h

3.30 Potential Class Reference

Superclass for potentials. Potentials are stores in a vector in the system object.

Inheritance diagram for Potential:



Public Member Functions

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

  Method for calculating a walker's potential energy.

Protected Attributes

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

3.30.1 Detailed Description

Superclass for potentials. Potentials are stores in a vector in the system object.

See also

System::potentials, System::get_potential_energy()

3.30.2 Member Function Documentation

3.30.2.1 virtual double Potential::get_pot_E (const Walker * *walker*) const [pure virtual]

Method for calculating a walker's potential energy.

Method overridden by subclasses.

Parameters

walker	The walker for which the potential energy should be calculated.

Returns

The potential energy.

Implemented in Harmonic_osc, AtomCore, and Coulomb.

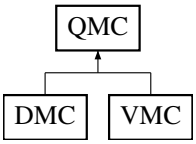
The documentation for this class was generated from the following files:

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

3.31 QMC Class Reference

The QMC superclass. Holds implementations of general functions for both VMC and DMC in order to avoid rewriting code and emphasize the similarities.

Inheritance diagram for QMC:



Public Member Functions

- QMC (GeneralParams &, int n_c, SystemObjects &, ParParams &, int n_w, int K=1)

  Constructor.
- virtual void run_method ()=0

  Method used for executing the solver.
- void get_QF (Walker *walker) const

  Method for calculating the Quantum Force.
- void get_gradients (const Walker *walker_pre, Walker *walker_post, int particle) const

  Method for calculating the gradients after moving a particle.
- void get_gradients (Walker *walker) const

  Method for calculating the full gradients.
- void get_laplsum (Walker *walker) const

  Method for calculating the Laplacian of all walkers.
- double get_wf_value (const Walker *walker) const

  Method for calculating the wave functions value at a given walker's position.
- double calculate_local_energy (const Walker *walker) const

  Method for calculating the local energy.
- void get_accepted_ratio ()

  Method for calculating the acceptance ratio.
- void add_output (OutputHandler *output_handler)

  Method used for loading the output_handler with objects.
- void set_error_estimator (ErrorEstimator *error_estimator)

  Method for setting the error estimator.
- virtual void output ()=0

  Method for standard output.
- System * **get_system_ptr** () const
- Sampling * **get_sampling_ptr** () const
- Jastrow * **get_jastrow_ptr** () const
- Orbitals * **get_orbitals_ptr** () const

Protected Member Functions

- virtual void set_trial_positions ()=0

  Method for setting the trial position of the QMC method's walkers.
- void diffuse_walker (Walker *original, Walker *trial)

  Method for diffusing a walker one time step.
- double get_acceptance_ratio (const Walker *walker_pre, const Walker *walker_post, int particle) const

  Method for calculating the acceptance ratio used in the Metropolis test.
- virtual bool move_autherized (double A)=0

  Method for deciding whether or not to accept a move.
- bool metropolis_test (double A)

  Method for performing the metropolis test after when diffusing a walker.
- void update_walker (Walker *walker_pre, const Walker *walker_post, int particle) const

  Method for updating the walker after an accepted step.
- void reset_walker (const Walker *walker_pre, Walker *walker_post, int particle) const

  Method for reseting the walker after a rejected step.
- void copy_walker (const Walker *parent, Walker *child) const

  Method for (hard) copying a walker object.
- void calculate_energy_necessities (Walker *walker) const

  Method for calculating the necessary quantities needed in order to calculate the local energy.
- double get_KE (const Walker *walker) const

  Method for storing positional data.
- virtual void **save_distribution** ()=0
- virtual void node_comm ()=0

  Method for performing node communication.
- void dump_output ()
- void finalize_output ()
- void estimate_error () const
- void set_spin_state (int particle) const
- void test_ratios (const Walker *walker_pre, const Walker *walker_post, int particle, double R_qmc) const

  Method used for testing the optimized ratio calculation.
- void test_gradients (Walker *walker)

  Method for testing the optimized gradients calculation.

Protected Attributes

- STDOUT * std_out

  Output object. Wraps and replaces std::cout.
- std::stringstream **s**

- std::string runpath

  The directory which the simulation is set to run.
- std::string dist_path

  The path where the distribution are saved.
- arma::mat dist

  Matrix holding positional data for the distribution.
- int last_inserted

  Index of last inserted positional data.
- int dist_tresh

  Amount of cycles to skip in between storing position data.
- bool **is_master**
- bool **parallel**
- int **node**
- int **n_nodes**
- int n_c

  The number of Monte-Carlo cycles.
- int thermalization

  The number of thermalization steps.
- int cycle
- int n_w

  The number of walkers.
- int **n_p**
- int **n2**
- int **dim**
- unsigned long int accepted

  Number of accepted moves.
- unsigned long int total_samples

  Total number of moves.
- double local_E

  The last calculated local energy.
- Walker * trial_walker

  The trial walker used to test a move.
- Walker ** original_walkers

  A list of n_w walkers used in DMC.
- Jastrow * jastrow

  The Jastrow object.
- Sampling * sampling

  The Sampling object.
- System * system

  The system object.
- ErrorEstimator * error_estimator

  The error estimator.
- std::vector< OutputHandler * > output_handler

  Can hold stdoutDMC (in case of DMC), Distribution, both or none.

Friends

- class **Distribution**

3.31.1 Detailed Description

The QMC superclass. Holds implementations of general functions for both VMC and DMC in order to avoid rewriting code and emphasize the similarities.

3.31.2 Constructor & Destructor Documentation

3.31.2.1 QMC::QMC (GeneralParams & *gP,* int *n_c,* SystemObjects & *sO,* ParParams & *pp,* int *n_w,* int *K* = 1)

Constructor.

K K times n_w walkers are initialized. K != 0 only sensible in DMC.

3.31.3 Member Function Documentation

3.31.3.1 void QMC::calculate_energy_necessities (Walker * *walker*) const [protected]

Method for calculating the necessary quantities needed in order to calculate the local energy.

See also

Sampling::calculate_energy_necessities()

3.31.3.2 double QMC::calculate_local_energy (const Walker * *walker*) const

Method for calculating the local energy.

See also

get_KE(), System::get_potential_energy()

3.31.3.3 void QMC::copy_walker (const Walker * *parent,* Walker * *child*) const [protected]

Method for (hard) copying a walker object.

Parameters

parent,child	The parent is copied to the child.

3.31.3.4 void QMC::diffuse_walker (Walker * *original*, Walker * *trial*) [protected]

Method for diffusing a walker one time step.

The trial walker must equal the original walker in input. The original walker is updated on output.

3.31.3.5 void QMC::dump_output ( ) [protected]

Iterates over the output objects in the output_handler vector. No if-tests.

3.31.3.6 void QMC::estimate_error ( ) const [protected]

Estimates and finalizes the ErrorEstimator object initialized in the error_estimator vector.

3.31.3.7 void QMC::finalize_output ( ) [protected]

Calls the finalize function for the object in the output_handler vector.

3.31.3.8 void QMC::get_gradients (const Walker * *walker_pre*, Walker * *walker_post*, int *particle*) const

Method for calculating the gradients after moving a particle.

See also

Jastrow::get_grad(), System::get_spatial_grad()

3.31.3.9 void QMC::get_gradients (Walker * *walker*) const

Method for calculating the full gradients.

See also

Jastrow::get_grad(), System::get_spatial_grad()

3.31.3.10 double QMC::get_KE (const Walker * *walker*) const [protected]

Method for storing positional data.

Stored in the dist matrix. Used by OutputHandler::Distribution.

See also

Distribution::dump() Method for calculating the kinetic energy of a walker.

3.31.3.11 void QMC::get_laplsum (Walker * *walker*) const [inline]

Method for calculating the Laplacian of all walkers.

See also

System::get_spatial_lapl_sum(), Jastrow::get_lapl_sum()

3.31.3.12 double QMC::get_wf_value (const Walker * *walker*) const [inline]

Method for calculating the wave functions value at a given walker's position.

See also

System::get_spatial_wf(), Jastrow::get_val()

3.31.3.13 bool QMC::metropolis_test (double *A*) [protected]

Method for performing the metropolis test after when diffusing a walker.

Parameters

A	The acceptance ratio calulated by get_acceptance_ratio().

3.31.3.14 virtual bool QMC::move_autherized (double *A*) [protected, pure virtual]

Method for deciding whether or not to accept a move.

Wraps the metropolis sampling with possibilities of overriding.

See also

System::allow_transition()

Implemented in DMC, and VMC.

3.31.3.15 void QMC::reset_walker (const Walker * *walker_pre*, Walker * *walker_post*, int *particle*) const [protected]

Method for reseting the walker after a rejected step.

Given a particle number, the method only resets the changed values.

Parameters

walker_post	Walker at current time step
walker_pre	Walker at previous time step

3.31.3.16 void QMC::set_spin_state (int *particle*) const [protected]

Since the spatial wave function is split, certain values are unchanged if the moved particle has opposite spin. Assuming a two-level system, the first half of the particles are assumed to have one spin value, and the second half the other.

This method sets the start and end position of the block that needs to be changed.

See also

System::start, System::end

3.31.3.17 virtual void QMC::set_trial_positions ( ) [protected, pure virtual]

Method for setting the trial position of the QMC method's walkers.

See also

Sampling::set_trial_pos()

Implemented in DMC, and VMC.

3.31.3.18 void QMC::test_gradients (Walker * *walker*) [protected]

Method for testing the optimized gradients calculation.

Compares with finite difference calculation.

3.31.3.19 void QMC::test_ratios (const Walker * *walker_pre*, const Walker * *walker_post*, int *particle*, double *R_qmc*) const [protected]

Method used for testing the optimized ratio calculation.

Compares to brute force computation of the wave function values. R_qmc The optimized trial wave function ratio (spatial and Jastrow).

3.31.3.20 void QMC::update_walker (Walker * *walker_pre*, const Walker * *walker_post*, int *particle*) const [protected]

Method for updating the walker after an accepted step.

Given a particle number, the method only updates the changed values.

Parameters

walker_post	Walker at current time step
walker_pre	Walker at previous time step

3.31.4 Member Data Documentation

3.31.4.1 int QMC::cycle [protected]

The current Monte-Carlo cycle.

3.31.4.2 int QMC::n_w [protected]

The number of walkers.

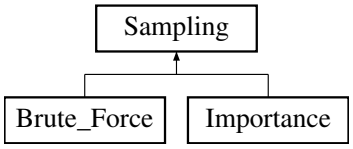
VMC stores this many cycles in case of DMC

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

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

3.32 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

  Method for updating the position of a walker's particle.
- virtual void update_necessities (const Walker ∗walker_pre, Walker ∗walker_post, int particle) const =0

  Method for updating the sampling specific necessary values.
- virtual void update_walker (Walker ∗walker_pre, const Walker ∗walker_post, int particle) const =0
- virtual void reset_walker (const Walker ∗walker_pre, Walker ∗walker_post, int particle) const =0
- void set_trial_pos (Walker ∗walker, bool set_pos=true)

  Method for setting the trial position for a given walker.
- void set_trial_states (Walker ∗walker)

  Method for setting up the single particle orbitals and it's derivatives for a given walker.
- virtual void get_necessities (Walker ∗walker)=0

Method for calculating the sampling specific necessary values.

- virtual void calculate_energy_necessities (Walker ∗walker) const =0

  Method for calculating the sampling specific necessary values in order to compute the local energy.

- virtual void copy_walker (const Walker ∗parent, Walker ∗child) const =0

  Method for copying the sampling specific parts of a walker.

- virtual double get_g_ratio (const Walker ∗walker_post, const Walker ∗walker_pre) const

  Method for calculating the diffusion Green's function ratios.

- 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 **get_std** () const
- double call_RNG ()

  Calls a uniform random number generator.

- void set_spin_state (int start, int end)

Protected Attributes

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

  The Diffusion object.

- QMC ∗ qmc

  The QMC main solver object. Needed to access e.g. the system object.

3.32.1 Member Function Documentation

3.32.1.1 double Sampling::call_RNG ( ) [inline]

Calls a uniform random number generator.

Returns a random uniform number on [0,1).

3.32.1.2 virtual void Sampling::copy_walker (const Walker ∗ *parent*, Walker ∗ *child*) const [pure virtual]

Method for copying the sampling specific parts of a walker.

See also

QMC::copy_walker()

Implemented in Importance, and Brute_Force.

3.32.1.3 virtual double Sampling::get_g_ratio (const Walker * *walker_post,* const Walker * *walker_pre*) const [inline, virtual]

Method for calculating the diffusion Green's function ratios.

See the Diffusion class for documentation.

3.32.1.4 virtual void Sampling::get_necessities (Walker * *walker*) [pure virtual]

Method for calculating the sampling specific necessary values.

Called after a trial position is set.

Implemented in Importance, and Brute_Force.

3.32.1.5 virtual void Sampling::reset_walker (const Walker * *walker_pre,* Walker * *walker_post,* int *particle*) const [pure virtual]

See also

QMC::reset_walker()

Implemented in Brute_Force, and Importance.

3.32.1.6 void Sampling::set_spin_state (int *start,* int *end*) [inline]

See also

QMC::set_spin_state()

3.32.1.7 void Sampling::update_pos (const Walker * *walker_pre,* Walker * *walker_post,* int *particle*) const

Method for updating the position of a walker's particle.

Sets a new position according to the diffusion rules, and calls all the functions necessary to get all the values updates, e.g. System::calc_for_new_pos()

3.32.1.8 virtual void Sampling::update_walker (Walker * *walker_pre,* const Walker * *walker_post,* int *particle*) const [pure virtual]

See also

QMC::update_walker()

Implemented in Importance, and Brute_Force.

3.32.2 Member Data Documentation

3.32.2.1 Diffusion* Sampling::diffusion [protected]

The Diffusion object.

See also

Diffusion

3.32.2.2 int Sampling::end [protected]

See also

System::end

3.32.2.3 int Sampling::start [protected]

See also

System::start

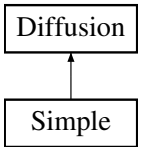
The documentation for this class was generated from the following files:

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

3.33 Simple Class Reference

Simple Isotropic diffusion model.

Inheritance diagram for Simple:



Public Member Functions

- **Simple** (int n_p, int dim, double timestep, seed_type random_seed, double D=0.-5)
- double get_new_pos (const Walker *walker, int i, int j)

  Virtual function returning the new position.
- double get_g_ratio (const Walker *walker_post, const Walker *walker_pre) const

  Calculates the Diffusion Green's function ratio needed by metropolis.

3.33.1 Detailed Description

Simple Isotropic diffusion model.

3.33.2 Member Function Documentation

3.33.2.1 double Simple::get_g_ratio (const Walker * *walker_post*, const Walker * *walker_pre*) const [inline, virtual]

Calculates the Diffusion Green's function ratio needed by metropolis.

Parameters

walker_post	Walker at current time step.
walker_pre	Walker at previous time step.

Returns

The Diffusion Green's function ratio.

Implements Diffusion.

3.33.2.2 double Simple::get_new_pos (const Walker * *walker*, int *i*, int *j*) [inline, virtual]

Virtual function returning the new position.

Returns the simple diffusion step if not overridden.

Parameters

i	Particle number.
j	dimension (x,y,z).

Returns

The new position (relative to the old).

Reimplemented from Diffusion.

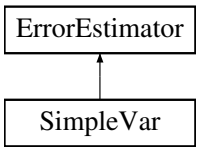
The documentation for this class was generated from the following files:

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

3.34 SimpleVar Class Reference

Calculates the simple variance of the sampled values.

Inheritance diagram for SimpleVar:



Public Member Functions

- **SimpleVar** (ParParams &)
- double estimate_error ()

  Estimates the error based on the subclass implementation.
- void update_data (double val)
- void **normalize** ()

Protected Attributes

- double f

  sum variable used to calculate the mean
- double f2

  sum variable used to calulate the mean of squares.

3.34.1 Detailed Description

Calculates the simple variance of the sampled values.

3.34.2 Member Function Documentation

3.34.2.1 void SimpleVar::update_data (double *val*) [virtual]

Overrides the default described in the superclass. Does not store values in memory, but rather use sum variables.

Reimplemented from ErrorEstimator.

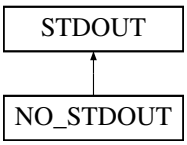
The documentation for this class was generated from the following files:

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

3.35 STDOUT Class Reference

Class for handling standard output. Only the master node has this object.

Inheritance diagram for STDOUT:



Public Member Functions

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

3.35.1 Detailed Description

Class for handling standard output. Only the master node has this object.

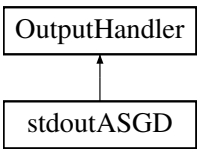
The documentation for this class was generated from the following file:

- src/QMCheaders.h

3.36 stdoutASGD Class Reference

Class for handling the output of ASGD. Ouputs values such as the variational gradients, step length, variational parameters, etc.

Inheritance diagram for stdoutASGD:



Public Member Functions

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

  Methods for updating the output.
- void post_pointer_init ()

3.36.1 Detailed Description

Class for handling the output of ASGD. Ouputs values such as the variational gradients, step length, variational parameters, etc.

3.36.2 Member Function Documentation

3.36.2.1 void stdoutASGD::dump ( ) [virtual]

Methods for updating the output.

Typically retrieves information through the solver pointers (given correct accessibility levels/friend)

Implements OutputHandler.

3.36.2.2 void stdoutASGD::post_pointer_init ( ) [inline, virtual]

Initializes the correct size of the variational gradient once the min pointer has been cast to ASGD.

Reimplemented from OutputHandler.

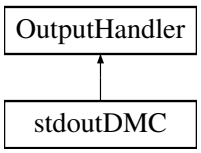
The documentation for this class was generated from the following files:

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

3.37 stdoutDMC Class Reference

Class for handling the output of DMC. Outputs values such as the trial energy, dmc energy, number of walkers, etc.

Inheritance diagram for stdoutDMC:



Public Member Functions

- **stdoutDMC** (std::string path, std::string filename="DMC_out")
- void dump ()

  Methods for updating the output.

Protected Attributes

- int n

  Number of times the dump() method has been called.
- double sumE

  Sum of the DMC energy used to calculate the trailing average.
- double sumN

  Sum of the number of walkers used to calculate the trailing average.

3.37.1 Detailed Description

Class for handling the output of DMC. Outputs values such as the trial energy, dmc energy, number of walkers, etc.

3.37.2 Member Function Documentation

3.37.2.1 void stdoutDMC::dump ( ) [virtual]

Methods for updating the output.

Typically retrieves information through the solver pointers (given correct accessibility levels/friend)

Implements OutputHandler.

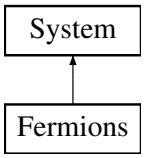
The documentation for this class was generated from the following files:

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

3.38 System Class Reference

The system class separating Fermions and Bosons. Designed to generalize the solver in terms of particle species.

Inheritance diagram for System:



Public Member Functions

- **System** (int n_p, int dim, Orbitals *orbital)
- virtual void initialize (Walker *walker)=0

  Initializes the system before the main solver loop starts.
- void add_potential (Potential *pot)

  Method for adding a potential to the system.
- double get_potential_energy (const Walker *walker)

  Method for calculating the total potential energy.
- virtual void update_walker (Walker *walker_pre, const Walker *walker_post, int particle) const =0
- virtual void reset_walker (const Walker *walker_pre, Walker *walker_post, int particle) const =0
- virtual void calc_for_newpos (const Walker *walker_old, Walker *walker_new, int particle)=0

  Method for calculating the necessary values needed by the walker after a new step is made.
- virtual double get_spatial_ratio (const Walker *walker_pre, const Walker *walker_post, int particle)=0

  Method for calculating the spatial wave function ratios between two subsequent time steps.
- virtual double get_spatial_wf (const Walker *walker)=0

  Method for calculating the spatial wave function's value at a given walkers position.
- virtual void get_spatial_grad (Walker *walker, int particle) const =0

  Method for calculating the changed part of the spatial gradient.
- virtual void get_spatial_grad_full (Walker *walker) const =0

  Method for calculating the full spatial gradient.
- virtual double get_spatial_lapl_sum (const Walker *walker) const =0

  Method for calculating the sum of all Laplacians for a given walker.
- virtual void copy_walker (const Walker *parent, Walker *child) const =0

  Method for copying the system specific parts of a walker.
- virtual bool allow_transition ()=0

Method allowing the system to override the Metropolis test.

- Orbitals * **get_orbital_ptr** ()
- void set_spin_state (int start, int end)

Protected Attributes

- int **n_p**
- int **n2**
- int **dim**
- int start

  The start point of separable calculations.
- int end

  The end point of separable calculations.
- std::vector< Potential * > potentials

  A vector of potentials.
- Orbitals * orbital

  The single particle wave function object.

3.38.1 Detailed Description

The system class separating Fermions and Bosons. Designed to generalize the solver in terms of particle species.

3.38.2 Member Function Documentation

3.38.2.1 virtual void System::calc_for_newpos (const Walker * *walker_old*, Walker * *walker_new*, int *particle*) [pure virtual]

Method for calculating the necessary values needed by the walker after a new step is made.

Given a particle number, the method does not recompute unchanged values.

Parameters

walker_old	Walker at current time step.
walker_new	Walker at previous time step.

Implemented in Fermions.

3.38.2.2 virtual void System::copy_walker (const Walker * *parent*, Walker * *child*) const [pure virtual]

Method for copying the system specific parts of a walker.

See also

QMC::copy_walker()

Implemented in Fermions.

3.38.2.3 double System::get_potential_energy (const Walker * *walker*)

Method for calculating the total potential energy.

Iterates over all objects in the potentials vector and accumulates their potential energies for the given walker.

3.38.2.4 virtual void System::get_spatial_grad (Walker * *walker,* int *particle*) const [pure virtual]

Method for calculating the changed part of the spatial gradient.

Depending on which particle we moved, one of the spatial wave function parts (it is split) will be unchanged.

Implemented in Fermions.

3.38.2.5 virtual void System::initialize (Walker * *walker*) [pure virtual]

Initializes the system before the main solver loop starts.

Called by the Sampling class when trial positions are set.

Implemented in Fermions.

3.38.2.6 virtual void System::reset_walker (const Walker * *walker_pre,* Walker * *walker_post,* int *particle*) const [pure virtual]

See also

QMC::reset_walker()

Implemented in Fermions.

3.38.2.7 void System::set_spin_state (int *start,* int *end*) [inline]

See also

QMC::set_spin_state()

3.38.2.8 virtual void System::update_walker (Walker * *walker_pre,* const Walker * *walker_post,* int *particle*) const [pure virtual]

See also

QMC::update_walker()

Implemented in Fermions.

3.38.3 Member Data Documentation

3.38.3.1 int System::end [protected]

The end point of separable calculations.

Either N/2 or N. Since the spatial wave function is split, particles with spin not equal that of the moved particle is unchanged and does not need to be recalculated.

3.38.3.2 int System::start [protected]

The start point of separable calculations.

Either 0 or N/2. Since the spatial wave function is split, particles with spin not equal that of the moved particle is unchanged and does not need to be recalculated.

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

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

3.39 SystemObjects Struct Reference

Struct used to initialize system objects.

Public Attributes

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

3.39.1 Detailed Description

Struct used to initialize system objects.

The memory addresses allocated here will not change throughout the run.

See also

Orbitals, Potential, System, Sampling, Jastrow

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

- src/QMCheaders.h

3.40 VariationalParams Struct Reference

Struct used to initialize the varational parameters.

Public Attributes

- double alpha

  The spatial variational parameter.
- double beta

  The Jastrow variational parameter.

3.40.1 Detailed Description

Struct used to initialize the varational parameters.

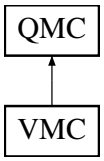
The documentation for this struct was generated from the following file:

- src/QMCheaders.h

3.41 VMC Class Reference

Implementation of the Variational Monte-Carlo Method. Very little needs to be added when the QMC superclass holds all the general functionality.

Inheritance diagram for VMC:



Public Member Functions

- VMC (GeneralParams &, VMCparams &, SystemObjects &, ParParams &, int n_w, bool dist_out)

Constructor.

- void **set_e** (double E)
- double **get_energy** () const
- void run_method ()

  Method used for executing the solver.
- void output ()

  Method for standard output.

Protected Member Functions

- void set_trial_positions ()
- void store_walkers ()

  Method for storing walkers for DMC.
- void save_distribution ()

  Method for storing positional data for the Distribtuon.
- bool move_autherized (double A)
- void **scale_values** ()
- void node_comm ()

  Method for performing node communication.

Protected Attributes

- int pop_tresh

  The amount of cycles between storing walkers for DMC.
- int offset

  The amount of cycles before starting to store walkers for DMC.
- int last_walker

  Count variable for the last walker stores for DMC.
- double vmc_E

  The VMC energy.
- Walker * original_walker

  The VMC walker.

Friends

- class **DMC**
- class **Minimizer**
- class **ASGD**
- class **BlockingData**

3.41.1 Detailed Description

Implementation of the Variational Monte-Carlo Method. Very little needs to be added when the QMC superclass holds all the general functionality.

3.41.2 Member Function Documentation

3.41.2.1 bool VMC::move_autherized (double *A*) [inline, protected, virtual]

In VMC, only the metropolis test is performed.

Implements QMC.

3.41.2.2 void VMC::save_distribution ( ) [protected, virtual]

Method for storing positional data for the Distribtuon.

Stores the position data of the single VMC walker every dist_tresh cycle after thermalization.

Implements QMC.

3.41.2.3 void VMC::set_trial_positions ( ) [protected, virtual]

Sets the trial position for the single walker.

Implements QMC.

3.41.2.4 void VMC::store_walkers ( ) [protected]

Method for storing walkers for DMC.

Stores the single VMC walker every pop_thresh cycle after offset cycles.

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

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

3.42 VMCparams Struct Reference

Struct used to initialize VMC parameters.

Public Attributes

- int n_c

  The number of cycles.
- double dt

  The time step.

3.42.1 Detailed Description

Struct used to initialize VMC parameters.

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

- src/QMCheaders.h

3.43 Walker Class Reference

Class representing a Random Walker. Holds position data, alive state, etc. Designed to lighten function arguments, and ease implementation of QMC methods involving multiple walkers. Alot of values are stored to avoid calculating the same value twice.

Public Member Functions

- **Walker** (int n_p, int dim, bool do_init=true)
- void calc_r_i2 (int i)

  Method for calculating the radius squared for one particle.
- void calc_r_i2 ()

  Method for calculating the radius squared for all particles.
- double calc_r_rel (int i, int j) const

  Method for calculating the relative distance between two particles.
- void make_rel_matrix ()
- void send_soul (int source)
- void recv_soul (int root)
- double get_r_i2 (int i) const

  Method for fetching the squared radius of a particle.
- double get_r_i (int i) const

  Method for calculating the radius of a particle.
- void kill ()
- bool **is_dead** ()
- bool **is_alive** ()
- void ressurect ()
- void **set_E** (double E)
- double **get_E** () const
- void print (std::string header="----") const

  Prints out all the walkers information.

Public Attributes

- double spatial_ratio

  The ratio of the spatial wave function (stored in the newest walker).
- double lapl_sum

The sum of the Laplacians of all particles.

- double E

  The energy of the given configuration (stored to speed up DMC).

- arma::mat r

  The positions of all particles.

- arma::mat r_rel

  The relative positions of all particles.

- arma::mat qforce

  The Quantum Force for all particles.

- arma::mat spatial_grad

  The gradient of the Spatial Wave function for all particles.

- arma::mat jast_grad

  The gradient of the Jastrow Factor for all particles.

- arma::mat inv

  The inverse of the Slater matrix (given fermion system)

- arma::mat phi

  The single particle wave functions for all particles and quantum numbers.

- arma::field< arma::mat > dell_phi

  The derivatives of the single particle wave functions for all particles and quantum numbers.

- arma::cube dJ

  Cube used for storing sum terms for the Jastrow Factor's closed form expressions.

- arma::rowvec r2

  The radius squared for all particles.

Protected Attributes

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

  If true, the walker will be deleted and removed (DMC only).

3.43.1 Detailed Description

Class representing a Random Walker. Holds position data, alive state, etc. Designed to lighten function arguments, and ease implementation of QMC methods involving multiple walkers. Alot of values are stored to avoid calculating the same value twice.

3.43.2 Member Function Documentation

3.43.2.1 void Walker::calc_r_i2 (int *i*)

Method for calculating the radius squared for one particle.

Parameters

i	The particle number.

3.43.2.2 double Walker::calc_r_rel (int *i*, int *j*) const

Method for calculating the relative distance between two particles.

Parameters

i,j	The particle numbers.

3.43.2.3 double Walker::get_r_i (int *i*) const [inline]

Method for calculating the radius of a particle.

Parameters

i	Particle number.

3.43.2.4 double Walker::get_r_i2 (int *i*) const [inline]

Method for fetching the squared radius of a particle.

Used in order to avoid calculating the same radius twice.

Parameters

i	Particle number.

3.43.2.5 void Walker::kill ( ) [inline]

Flags the walker for destruction.

See also

DMC::bury_the_dead()

3.43.2.6 void Walker::make_rel_matrix ( )

Creates the relative position matrix.

3.43.2.7 void Walker::print (std::string *header* = "----") const

Prints out all the walkers information.

Extremely handy for debugging.

Parameters

header	A header for the printout in order to distinguish several printouts easily.

3.43.2.8 void Walker::recv_soul (int *root*)

Receives a walker from a different node.

Parameters

root	The rank of the node from which the walker was sent.

3.43.2.9 void Walker::ressurect ( ) [inline]

Sets the destruction flag to false.

3.43.2.10 void Walker::send_soul (int *source*)

Send a walker to a different node.

Parameters

source	The receiving node's rank.

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

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