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# HANDE Documentation

*Release git*

**HANDE developers**

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## Contents

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<b>1</b>	<b>User's guide</b>	<b>1</b>
1.1	Introduction	1
1.2	Some geography...	1
1.3	Prerequisites	2
1.4	Compilation	5
1.5	Test suite	15
1.6	Usage	17
1.7	Input file	17
1.8	Interacting with running calculations	77
1.9	Analysis	78
1.10	Generating integrals	81
1.11	Tips	84
1.12	Old (removed) functionality	85
1.13	Tutorials	86
<b>2</b>	<b>pyhande</b>	<b>133</b>
2.1	pyhande.analysis	133
2.2	pyhande.canonical	137
2.3	pyhande.extract	137
2.4	pyhande.lazy	138
2.5	pyhande.utils	144
2.6	pyhande.weight	144
2.7	pyhande.data_preparing	145
2.8	pyhande.error_analysing	146
2.9	pyhande.extracting	152
2.10	pyhande.helpers	153
2.11	pyhande.results_viewer	154
<b>3</b>	<b>Developers' Guide</b>	<b>159</b>
3.1	Git	159
3.2	Adding a new test	163
3.3	Debugging options	165
3.4	FAQ	166
<b>4</b>	<b>Notes on Releases</b>	<b>171</b>
4.1	Release notes for v1.6	171
4.2	Release notes for v1.5	172

4.3	Release notes for v1.4 . . . . .	173
4.4	Release notes for v1.3 . . . . .	174
4.5	What’s new in version 1.2? (not an exhaustive list) . . . . .	174
<b>5</b>	<b>Bibliography</b>	<b>177</b>
	<b>Bibliography</b>	<b>179</b>
	<b>Python Module Index</b>	<b>183</b>
	<b>Index</b>	<b>185</b>

## 1.1 Introduction

HANDE [Spencer19] contains optimised, highly parallel implementations of the full configuration interaction quantum Monte Carlo (FCIQMC) [Booth09], coupled cluster Monte Carlo (CCMC) [Thom10] and Density Matrix Quantum Monte Carlo (DMQMC) [Blunt14], [Malone15] algorithms for a variety of systems. Development work continues to add new features and investigate the algorithms and new applications.

HANDE can perform calculations on generic systems such as molecules via an externally generated integral file. The integral file is in the FCIDUMP format [Knowles89], which can be generated by several quantum chemistry codes such as MOLPRO, Q-Chem (with patches from Alex Thom) and PSI4. HANDE can also perform calculations on model Hamiltonians, for which no additional integrals are required. The model Hamiltonians currently available are the Hubbard model, Heisenberg model and uniform electron gas.

Configuration interaction (CI) is also implemented using an external library (lapack/scalapack) and can be performed in both serial and parallel. Note that this is rather slow and intended for debugging purposes only. Most quantum chemistry codes (e.g. PSI4) contain a substantially more powerful and optimised CI implementation.

## 1.2 Some geography...

Files are organised in the HANDE repository as follows:

**./** Root directory of the program.

**bin/** Directory containing the compiled program, hande.x. Created during compilation.

**cmake/** Directory containing the configuration used by the cmake build system.

**config/** Directory containing the configuration input files used to generate makefiles.

**dest/** Directory containing the compiled object files and dependency files. Created during compilation.

**documentation/** Directory containing documentation on the HANDE program. The documentation is written in reStructured Text and can be converted into a wide range of output formats.

**src/** Directory containing the main source files.

**lib/** Directory containing “library” source files. These are procedures which are not specific to the HANDE code but are generally useful. Some are written by the authors, some are freely available (as noted in the source files).

**tools/** Directory containing scripts and tools for compiling, running and analysing output from HANDE.

**test\_suite/** Directory containing a set of tests which HANDE should agree with.

## 1.3 Prerequisites

HANDE builds upon several well-written, efficient libraries to aid portability, efficiency and sustainability.

### 1.3.1 Dependencies

**Fortran and C compilers** HANDE is written in (mostly) Fortran 2003 with some C code. We have tested HANDE most recently (as of 2021) using GCC, and Intel compilers and are interested in hearing of use with other compilers.

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**Note:** HANDE is relatively aggressive in adopting new language features and hence requires a fairly modern Fortran compiler. In particular, gfortran 5.5 or earlier is unlikely to successfully compile HANDE. We regularly test with gfortran 7 and Intel 19.

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**LAPACK and BLAS** Available from <http://www.netlib.org/lapack/> and <http://www.netlib.org/blas/> and vendor implementations. Typically installed on HPC systems and available from package manager. This is only required for the FCI functionality in HANDE; the performance of the QMC algorithms do not depend upon the quality of the LAPACK and BLAS libraries used.

**lua 5.3 or 5.4** Lua (available from <http://www.lua.org>) is required. HANDE links to the lua library, which is used for parsing the input file. No performance critical code is written in lua.

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**Note:** A different version of the AOTUS library (which is included with HANDE) is needed to use lua 5.2 due to API changes. This is also provided with HANDE (in the lib/aotus-5.2 directory). To use it, set the variable lua\_52 to any non-empty value in the config file.

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**MPI (parallel compilation only)** MPI 2 is required. We have used a variety of implementations (including OpenMPI and various vendor implementations). MPI 3 is **highly** recommended and is used by default. MPI 3 shared memory functionality is used if detected.

**python 3.6+** Almost all tools packaged with HANDE are written in python.

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**Note:** python 3 versions **may** be sufficient but will probably require additional work. In particular, the argparse module (included from 2.7 and 3.2 onwards) is required and installing (especially recent versions of) pandas may be problematic. Using a recent version of python is highly recommended.

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**pandas 0.14.1+** The HANDE data analysis tools build heavily upon the python scientific stack. In particular, pandas (available from <http://pandas.pydata.org>) is required for the pyhande module and analysis scripts, almost all of which build upon pyhande. pandas is not required for running HANDE but is highly recommended for data analysis (though strictly speaking is only required if pyhande is used, either directly or via analysis scripts). It has been tested up to pandas 1.2.2

**statsmodels 0.11.0+** Required from the latest version (1.5) for the `pyhande` module. It has been tested up to 0.12.2.

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**Note:** statsmodels 0.13.0+ will not work due to a change in the namespace of various functions. This will be addressed in a later version.

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### 1.3.2 Bundled dependencies

**AOTUS** AOTUS provides a nice Fortran wrapper to Lua's C-API. For convenience (given that module files are Fortran-specific), AOTUS is included in the HANDE source distribution.

**cephes** Mathematical functions. Only the minimal subset required for the digamma ( $\psi$ ) function are included.

**dSFMT and dSFMT\_F03\_interface** dSFMT (double precision SIMD-oriented Fast Mersenne Twister) is a fast and high quality pseudo-random number generator; dSFMT\_F03\_interface is a Fortran 2003 wrapper to it.

**pyblock** python module for performing blocking analyses.

### 1.3.3 Optional dependencies

The following are optional dependencies which add useful (in some cases almost critical) functionality. However, they are less likely to be compiled on HPC systems so for ease of testing the functionality which depends upon them can be disabled at compile-time.

**HDF5** HDF5 is a library for storing scientific data and is used in HANDE for checkpointing (i.e. writing and reading restart files) in QMC calculations.

Highly recommended. Disabling HDF5 removes the ability to perform any checkpointing. It has been tested with up to version 1.12.0

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**Note:** HANDE requires the Fortran 2003 interface to HDF5, which is not compiled by default (see below), as this offers substantial advantages when working with dynamically sized arrays containing variables of arbitrary kinds/precision.

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**libuuid** Provenance of a calculation, and the output file(s) produced by it, is an important topic, currently the subject of much debate in computational science. HANDE generates a universally unique identifier (UUID), which is included in all files it produces.

Highly recommended but can be disabled without impacting on performance (but perhaps not on the user's sanity).

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**Note:** Some Linux distributions install libuuid but require an additional package (e.g. `uuid-dev`) to be installed in order for libuuid to exist on default search paths. Some luck may be found by looking under `/lib` or `/lib64` instead of `/usr/lib` and `/usr/lib64`.

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**scalapack (parallel compilation only)** Available from <http://www.netlib.org/scalapack/> and vendor implementations. Often already installed on HPC systems, included in Intel Maths Kernel Library and can be installed from most package managers.

### 1.3.4 Compilation and installation notes

Some notes on compiling the less common dependencies.

**Note:** The following are guidelines and the links provided are not necessarily the latest version of each package. Checking for the latest version is highly recommended.

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### lua

Lua is straightforward to compile. For example:

```
$ wget -O - http://www.lua.org/ftp/lua-5.3.5.tar.gz | tar xvfz -
$ cd lua-5.3.5
$ make linux
$ make install INSTALL_TOP=$HOME/local
```

will install the lua program and library to subdirectories in \$HOME/local. It is usually fine to compile lua using the GCC compiler and link HANDE against it using another compiler family (e.g. Intel).

### HDF5

HDF5 uses the GNU autotools build system, so is also straightforward to compile. For example:

```
$ wget -O - https://support.hdfgroup.org/ftp/HDF5/releases/hdf5-1.12/hdf5-1.12.0/src/
↳ hdf5-1.12.0.tar.gz | tar xvfz -
$ cd hdf5-1.12.0
$ ./configure --prefix=$HOME/local --enable-fortran
$ make
$ make install
```

will compile HDF5 and install it to subdirectories in \$HOME/local. By default this will use the GCC compiler suite; other compilers can be used by setting the CC, CXX and F77 environment variables. Note that for versions of HDF5 prior to 1.10.0 it is necessary to use the additional flag `--enable-fortran2003` to include the Fortran 2003 interface which is required by HANDE.

### pandas

Pandas can be installed by

```
$ pip install pandas
```

If you do not have root access, you can install the library locally with:

```
$ pip install pandas --user
```

Alternatively, where pip is not available, one can install it locally:

```
$ wget -O - https://github.com/pandas-dev/pandas/releases/download/v0.21.0/pandas-0.
↳ 21.0.tar.gz | tar -xvfz -
$ cd pandas-0.21.0
$ python setup.py build
$ python setup.py install
```

Again, pandas can be installed locally by replacing the final command with:



```
$ python setup.py install --user
```

## 1.4 Compilation

It is possible to configure and build HANDE using CMake or using bare make.

The former requires CMake 3.6 (or newer). It will generate Makefile-s based on the given configuration parameters and the detected tools and libraries on your system. It will, in most cases, work out of the box.

The bare make build offers a higher degree of customisation. Also in this case a Makefile will be generated based on a configuration file, of which you can find examples in the `config` folder.

### 1.4.1 Compilation using CMake

It is possible to configure and build HANDE using CMake. At least version 3.6 of CMake is required. You can get CMake either *via* your package manager or by downloading an executable tarball from [here](#) Unpacking and adding to your PATH will do the trick:

```
$ curl -L https://cmake.org/files/v3.10/cmake-3.10.2-Linux-x86_64.tar.gz | tar -xz
$ export PATH=$HOME/Software/cmake-3.10.2-Linux-x86_64/bin${PATH:+:$PATH}
```

where we have assumed the tarball was downloaded in the `$HOME/Software` directory.

Once dependencies are installed, you can configure HANDE either by running the `cmake` executable directly:

```
$ cmake -H. -Bbuild
```

or by using the frontend Python script `cmakeconfig.py`:

```
$ ./cmakeconfig.py build
```

The result of using the two methods is exactly the same: a subdirectory `build` will be created containing the build system. Using the frontend script however results in more compact configure lines.

### Configuration options

Building of HANDE can be tweaked in various ways passing options to the frontend script (or CMake directly). The help menu for the `cmakeconfig.py` script shows the available options:

```
Usage:
  ./cmakeconfig.py [options] [<builddir>]
  ./cmakeconfig.py (-h | --help)

Options:
  --fc=<FC>                               Fortran compiler [default: gfortran].
  --extra-fc-flags=<EXTRA_FCFLAGS>         Extra Fortran compiler flags [default: ''].
  --cc=<CC>                                C compiler [default: gcc].
  --extra-cc-flags=<EXTRA_CFLAGS>          Extra C compiler flags [default: ''].
  --python=<PYTHON_INTERPRETER>           The Python interpreter (development version)
  ↪to use. [default: ''].
  --add-definitions=<STRING>              Add preprocessor definitions [default: ''].
  --lua=<LUA_ROOT>                        Specify the path to the Lua installation to
  ↪use [default: ''].

```

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<code>--mpi</code>	Enable MPI parallelization [default: False].
<code>--mpi-with-scalapack</code>	Enable ScaLAPACK usage with MPI [default: <code>False</code> ].
<code>--omp</code>	Enable OpenMP parallelization [default: <code>False</code> ].
<code>--blas=&lt;BLAS&gt;</code>	Detect and link BLAS library (auto or off) <code>[default: auto]</code> .
<code>--lapack=&lt;LAPACK&gt;</code>	Detect and link LAPACK library (auto or off) <code>[default: auto]</code> .
<code>--mkl=&lt;MKL&gt;</code>	Pass MKL flag to the Intel compiler and linker and skip BLAS/LAPACK detection (sequential, parallel, cluster, or off) <code>[default: off]</code> .
<code>--scalapack=&lt;SCALAPACK_LIBRARIES&gt;</code>	Link line <b>for</b> ScaLAPACK libraries [default: <code>'</code>
<code>--blacs=&lt;BLACS_IMPLEMENTATION&gt;</code>	Implementation of BLACS <b>for</b> MKL ScaLAPACK <code>(openmpi, intelmpi, sgimpt) [default: openmpi]</code>
<code>--explicit-libs=&lt;EXPLICIT_LIBS&gt;</code>	Explicit linker options <b>for</b> extra libraries <code>to be linked in [default: '']</code> .
<code>--dsfmt-mexp=&lt;HANDE_DSfmt_MEXP&gt;</code>	An integer among 521, 1279, 2203, 4253, 11213, 19937, 44497, 86243, 1322049, 216091 [default: 19937].
<code>--det-size=&lt;HANDE_DET_SIZE&gt;</code>	An integer among 32 or 64 [default: 32].
<code>--pop-size=&lt;HANDE_POP_SIZE&gt;</code>	An integer among 32 or 64 [default: 32].
<code>--exe-name=&lt;HANDE_EXE_NAME&gt;</code>	[default: <code>"hande.cmake.x"</code> ].
<code>--hdf5=&lt;HDF5_ROOT&gt;</code>	Specify the path to the HDF5 installation to <code>use [default: '']</code> .
<code>--uuid=&lt;UUID&gt;</code>	Whether to activate UUID generation <code>[default: True]</code> .
<code>--single</code>	Enable usage of single precision, where <code>appropriate [default: False]</code> .
<code>--backtrace</code>	Enable backtrace functionality [default: <code>False</code> ].
<code>--popcnt</code>	Enable use of intrinsic popcnt [default: <code>False</code> ].
<code>--type=&lt;TYPE&gt;</code>	Set the CMake build <b>type</b> (debug, release, <code>relwithdebinfo, minsizerel) [default: release]</code> .
<code>--generator=&lt;STRING&gt;</code>	Set the CMake build system generator <code>[default: Unix Makefiles]</code> .
<code>--show</code>	Show CMake <b>command</b> and exit.
<code>--cmake-executable=&lt;CMAKE_EXECUTABLE&gt;</code>	Set the CMake executable [default: <code>cmake</code> ].
<code>--cmake-options=&lt;STRING&gt;</code>	Define options to CMake [default: <code>'</code> ].
<code>--prefix=&lt;PATH&gt;</code>	Set the install path <b>for</b> make install.
<code>&lt;builddir&gt;</code>	Build directory.
<code>-h --help</code>	Show this screen.

These options are translated to CMake native options. For more detailed information on HANDE-specific compile-time settings, see [Compile-time settings](#). The following list is a translation guide between the frontend script and “bare” CMake:

- `--fc=FC/-DCMAKE_Fortran_COMPILER=FC`. To set the Fortran compiler. Default is `gfortran`.
- `--extra-fc-flags="list-of-flags"/-DEXTRA_FCFLAGS="list-of-flags"`. To set additional flags for the Fortran compiler.
- `--cc=CC/-DCMAKE_C_COMPILER=CC`. To set the C compiler. Default is `gcc`.
- `--extra-cc-flags="list-of-flags"/-DEXTRA_CFLAGS="list-of-flags"`. To set additional flags for the C compiler.
- `--python=INTERP/-DPYTHON_INTERPRETER=INTERP`. To set the Python interpreter. The default is

empty, so that CMake will attempt to find a suitable version.

- `--lua=LUA/-DLUA_ROOT=LUA`. To set the Lua installation to use. Minimum required version of Lua is 5.3. The default is empty, so that CMake will attempt to find a suitable version. See below for Lua detection issues.

**Warning:** CMake will not pick up Lua from a nonstandard location, even though it is on path (any or all of `CPATH`, `LIBRARY_PATH`, `LD_LIBRARY_PATH`, `PATH`)

- `--mpi/-DENABLE_MPI=ON`. Enables MPI parallelization. CMake will attempt to find a suitable implementation of MPI and set the compilers accordingly.

**Warning:** To use a specific MPI implementation, pass the appropriate MPI compiler wrappers as arguments to `--fc` (`-DCMAKE_Fortran_COMPILER`) and `--cc` (`-DCMAKE_C_COMPILER`) For example, for the Intel MPI compiler wrappers `mpiifort` and `mpiicc` use `./cmakeconfig.py --mpi --fc=mpiifort --cc=mpiicc`.

- `--mpi-with-scalapack/-DENABLE_SCALAPACK=OFF`. Enables linking to ScaLAPACK. This requires that MPI is enabled and that a ScaLAPACK implementation is available.
- `--omp/-DENABLE_OPENMP=ON`. Enables OpenMP parallelization. CMake will check which flags are supported by your choice of compilers and add them to the compiler flags.
- `--blas=auto/-DENABLE_BLAS=auto`. Triggers autodetection of BLAS libraries. See below for math libraries detection issues.
- `--lapack=auto/-DENABLE_LAPACK=auto`. Triggers autodetection of BLAS libraries. See below for math libraries detection issues.
- `--mkl=VALUE/-DMKL_FLAG=VALUE`. Sets the `-mkl=VALUE` flag for the Intel compiler and linker. Valid values are `sequential`, `parallel`, `cluster`, or `off`, with `off` being the default.

**Warning:** Passing this option overrides automatic detection of math libraries

- `--scalapack="link-line"/-DSCALAPACK_LIBRARIES="link-line"`. Link line for ScaLAPACK libraries. If using Intel MKL, CMake will be able to correctly locate and set these for you. Use this option in case you run into trouble with detecting ScaLAPACK and prefer setting the link line explicitly.
- `--blacs=openmpi/-DBLACS_IMPLEMENTATION=openmpi`. Sets the implementation of BLACS for the Intel MKL ScaLAPACK libraries. Valid values are `openmpi`, `intelmpi` and `sgimpt`, with `openmpi` being the default.
- `--explicit-libs="link-line"/-DEXPLICIT_LIBS="link-line"`. Sets explicit linker options for extra libraries to be linked in. See below for math libraries detection issues.
- `--dsfmt-mexp=VALUE/-DHANDE_DSFMT_MEXP=VALUE`. Set exponent for the period of the Mersenne Twister (MT) random number generator (RNG). Valid values are 521, 1279, 2203, 4253, 11213, 19937, 44497, 86243, 1322049, and 216091. with 19937 being the default.
- `--det-size=VALUE/-DHANDE_DET_SIZE=VALUE`. Set the integer length for representing Slater determinants as bit strings. Valid values are 32 and 64, with 32 being the default.
- `--pop-size=VALUE/-DHANDE_POP_SIZE=VALUE`. Set the integer length for storing walker populations. Valid values are 32 and 64, with 32 being the default.

- `--exe-name=NAME/-DHANDE_EXE_NAME=NAME`. Set the name for the generated HANDE executable. The default is `hande.cmake.x`. The executable is copied to the `bin` directory in the root of the project and symlinked to `hande.x`. Passing the executable name will let you preserve executables generated with different configuration settings.
- `--hdf5=<HDF5>/-DENABLE_HDF5=<ON/OFF> -DHDF5_ROOT=<HDF5>`. Enables use of HDF5 and specifies the path to the HDF5 installation to use. By default, use of HDF5 is turned on. At least HDF5 1.8.15 is required and with Fortran 2003 bindings enabled. CMake will search for a suitable version of HDF5 and check that all necessary components are available. In addition, CMake will check the compatibility of the chosen HDF5 implementation and Fortran compiler. See below for HDF5 detection issues.
- `--uuid=<ON/OFF>/-DENABLE_UUID=<ON/OFF>`. Enables use of the UUID library. By default, this is turned on.
- `--single/-DENABLE_SINGLE_PRECISION=ON`. Enables use of single precision, where appropriate.
- `--backtrace/-DENABLE_BACKTRACE=ON`. Enables backtrace functionality.
- `--popcnt/-DENABLE_INTRINSIC_POPCNT=ON`. Enables usage of popcnt intrinsic (requires hardware support)
- `--type=debug/-DCMAKE_BUILD_TYPE=Debug`. Switches build type. Valid values are `debug`, `release`, `releasewithdebinfo` and `minsizerel`. The default is a debug build.
- `--cmake-options="-DTHIS -DTHAT"`. Sets options to be forwarded as-is to CMake.

## Installation

It is possible to install HANDE either running outside the build directory:

```
$ cmake --build build --target install
```

or from within the build directory:

```
$ make install
```

By default, CMake will set the install prefix to `/usr/local` and you might hence not have permissions to successfully install. The install prefix can be set *via* the `--prefix` option to the frontend script or, equivalently, passing the desired path to CMake *via* the `CMAKE_INSTALL_PREFIX` variable. The HANDE executable and static library will be installed to the `bin` and `lib` (`lib64` on 64-bit systems) subdirectories of the install prefix.

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**Note:** It might be advisable to install `pyhande` to the same prefix as the HANDE executable. Refer to `pyhande's README` for detailed instructions.

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Assuming the install prefix to have been set to `$HOME/Software/hande`, the install tree will thus look as follows:

```
$HOME/Software/hande/
├── bin
│   └── hande.cmake.x
├── lib64
│   └── libhande.a
```

The ``DESTDIR` mechanism <[https://www.gnu.org/prep/standards/html\\_node/DESTDIR.html](https://www.gnu.org/prep/standards/html_node/DESTDIR.html)>‘ can be used to adjust the install location:

```
$ env DESTDIR=/tmp/local make install
```

will result in the following install tree:

```
/tmp/local/$HOME/Software/hande
├── bin
│   └── hande.cmake.x
└── lib64
    └── libhande.a
```

## CMake compilation issues

When dependencies are not in standard search paths, CMake needs to be nudged and pointed in the right direction. This can be done directly using either `cmake` or `cmakeconfig.py`; the equivalent commands for both are given below but only one should be used.

- Detection of math libraries is usually the trickiest part. The CMake math detection scripts shipped with HANDE rely on the `MATH_ROOT` environment variable being set to point to the root of the math libraries installation you want to use. The detection scripts will attempt to provide a link line for math libraries based on the search order in the CMake variable `MATH_LIB_SEARCH_ORDER`. By default, Intel MKL is searched for first, using the `MKLROOT` environment variable. If math detection fails, libraries can be set manually:

```
$ ./cmakeconfig.py --blas=off --lapack=off --explicit-libs="-L/usr/lib -lblas -
↳llapack"
$ cmake -H. -DENABLE_BLAS=OFF -DENABLE_LAPACK=OFF -DEXPLICIT_LIBS="-L/usr/lib -
↳lblas -llapack"
```

- Lua in a non-standard directory. Exporting the root directory of the Lua installation as `LUA_ROOT` (or `LUA_DIR`) or directly passing it as an option:

```
$ ./cmakeconfig.py --lua=/install/dir/for/Lua build
$ cmake -H. -Bbuild -DLUA_ROOT=/install/dir/for/Lua
```

- HDF5 in a non-standard directory. Exporting the root directory of the HDF5 installation as `HDF5_ROOT` or directly passing it as an option:

```
$ ./cmakeconfig.py --hdf5=/install/dir/for/HDF5 build
$ cmake -H. -Bbuild -DENABLE_HDF5=ON -DHDF5_ROOT=/install/dir/for/HDF5
```

CMake will check that the chosen HDF5 library and Fortran compiler are compatible. If this test fails, configuration will abort. The output from the compatibility file will be saved to the log file `HDF5_HAS_Fortran2003-test.log` in the build directory. Note that it is possible to completely deactivate usage of HDF5:

```
$ ./cmakeconfig.py --hdf5=False
$ cmake -H. -Bbuild -DENABLE_HDF5=OFF
```

For compiler- and library-specific issues, see [Compiler and library issues](#).

## Compiling with MPI

To compile with MPI it is necessary to pass **both** the `--mpi` option **and** the correct compiler wrappers with the `--cc` and `--fc`:

```
$ ./cmakeconfig.py --mpi --fc=mpif90 --cc=mpicc
$ cmake -H. -Bbuild -DCMAKE_Fortran_COMPILER=mpif90 -DCMAKE_C_COMPILER=mpicc -DENABLE_
↳MPI=ON
```

CMake can in fact botch the identification of the compiler wrappers and MPI libraries, a mismatch that will result in linker errors. Here are some examples of configuration lines. In all cases, remember to set the `MATH_ROOT` variable to point to the location of the math libraries:

- OpenMPI with GNU compilers.

```
$ ./cmakeconfig.py --mpi --fc=mpif90 --cc=mpicc
$ cmake -H. -Bbuild -DCMAKE_Fortran_COMPILER=mpif90 -DCMAKE_C_COMPILER=mpicc -
  ↪DENABLE_MPI=ON
```

- OpenMPI with Intel compilers.

```
$ ./cmakeconfig.py --mpi --fc=mpif90 --cc=mpicc
$ cmake -H. -Bbuild -DCMAKE_Fortran_COMPILER=mpif90 -DCMAKE_C_COMPILER=mpicc -
  ↪DENABLE_MPI=ON
```

- IntelMPI with Intel compiler.

```
$ ./cmakeconfig.py --mpi --fc=mpiifort --cc=mpiicc
$ cmake -H. -Bbuild -DCMAKE_Fortran_COMPILER=mpiifort -DCMAKE_C_COMPILER=mpiicc -
  ↪DENABLE_MPI=ON
```

- OpenMPI with GNU compilers and OpenBLAS ScaLAPACK.

```
$ ./cmakeconfig.py --mpi --fc=mpif90 --cc=mpicc --mpi-with-scalapack --scalapack=
  ↪"-L/location/of/scalapack -lscalapack"
$ cmake -H. -Bbuild -DCMAKE_Fortran_COMPILER=mpif90 -DCMAKE_C_COMPILER=mpicc -
  ↪DENABLE_MPI=ON -DENABLE_SCALAPACK=ON -DSCALAPACK_LIBRARIES="-L/location/of/
  ↪scalapack -lscalapack"
```

- OpenMPI with Intel compilers and MKL ScaLAPACK. The math detection script will use the OpenMPI implementation of BLACS by default.

```
$ ./cmakeconfig.py --mpi --fc=mpif90 --cc=mpicc --mpi-with-scalapack
$ cmake -H. -Bbuild -DCMAKE_Fortran_COMPILER=mpif90 -DCMAKE_C_COMPILER=mpicc -
  ↪DENABLE_MPI=ON -DENABLE_SCALAPACK=ON
```

- IntelMPI with Intel compiler and MKL ScaLAPACK. In this case we need to tell CMake what BLACS implementation to use with ScaLAPACK.

```
$ ./cmakeconfig.py --mpi --fc=mpiifort --cc=mpiicc --mpi-with-scalapack --
  ↪blacs=intelmpi
$ cmake -H. -Bbuild -DCMAKE_Fortran_COMPILER=mpiifort
  -DCMAKE_C_COMPILER=mpiicc -DENABLE_MPI=ON -DENABLE_SCALAPACK=ON
  -DBLACS_IMPLEMENTATION=intelmpi
```

## 1.4.2 Compilation

After ensuring HANDE's dependencies are installed, produce a makefile by running the `mkconfig.py` (residing in the `tools` subdirectory) script in the root directory:

```
$ tools/mkconfig.py config/conf
```

where `conf` is one of the platforms available and is simply the name of the relevant file residing in the `config/` directory. Various configurations are provided and it is simple to adapt one to the local environment (e.g. changing compiler or library paths).

**Warning:** If any *prereq* have been installed to non-default (e.g. to \$HOME/local) paths, then these paths must be made available to the compiler via `ldflags` (see below) – e.g. using `-L $HOME/local` – and, for dynamic libraries added to the environment by setting the `LD_LIBRARY_PATH` environment variable.

Run

```
$ tools/mkconfig.py --help
```

to see the options available, including inspecting available configurations.

A configuration is defined using a simple ini file, consisting of three sections: main, opt and dbg. For instance:

```
.. [todo] - minimal working example
```

```
[main] fc = gfortran ld = gfortran libs = -llapack -lblas
```

```
[opt] fflags = -O3
```

```
[dbg] fflags = -g
```

Any option not specified in the ‘opt’ and ‘dbg’ sections is inherited from the ‘main’ section. The settings in ‘opt’ are used by default; the debug options can be selected by passing the `-g` option to `mkconfig`.

All options are strings unless otherwise specified. Available options are:

**fc** Set the fortran compiler.

**fflags** Set flags to be passed to the fortran compiler during compilation.

**f90\_module\_flag** Set the flag used by the compiler which is used to specify the directory where module (.mod) files are placed when created and where they should be searched for.

**f90\_module\_flag\_pad [boolean]** True if a space needs to be inserted between the defined `f90_module_flag` and the corresponding directory argument. Default: true.

**cc** Set the C compiler.

**cflags** Set flags to be passed to the C compiler during compilation.

**ccd** Set the C compiler used to generate the C dependency files. Only required if `cc` doesn’t support `-MM` and `-MT` flags. Default: use `cc`.

**cdflags** Set the flags for the c++ compiler used to generate the C++ dependency files. Default: `$CFLAGS -MM -MT`

**cxx** Set the C++ compiler.

**cxxflags** Set flags to be passed to the C++ compiler during compilation.

**cxxd** Set the C compiler used to generate the C++ dependency files. Only required if `cc` doesn’t support `-MM` and `-MT` flags. Default: use `cxx`.

**cxxdflags** Set the flags for the c++ compiler used to generate the C++ dependency files. Default: `$CXXFLAGS -MM -MT`

**cpp** Set the C preprocessor to be used on Fortran source files. If not defined then the Fortran compiler is used to do the preprocessing.

**cppflags** Set flags to be used in the C preprocessing step. C preprocessing is applied to .F90, .F, .c and .cpp files (and not .f90 files).

**ld** Set the linker program.

**ldflags** Set flags to be passed to the linker during linking of the compiled objects.

**libs** Set libraries to be used during the linking step.

**ar** Set the archive program. Default: ar.

**arflags** Set the flags to be passed to the archive program. Default: -rcs.

To compile the code run

```
$ make
```

HANDE's build system uses the `sfmakedepend` script (<http://people.arsc.edu/~kate/Perl/>, supplied in `tools/`) by Kate Hedstrom to generate the list of dependencies for each Fortran source file. These are generated automatically when `make` is run if the dependency files do not exist.

The executable, `hande.x`, is placed in the `bin` subdirectory. Note that this is actually a symbolic link: a unique executable is produced for each platform and optimisation level and `hande.x` merely points to the most recently compiled executable for convenience. This makes testing against multiple platforms particularly easy.

There are various goals in the makefile. Run

```
$ make help
```

to see the available goals.

### Compile-time settings

The behaviour of the program can be changed in various ways by some choices at compile-time by using C pre-processing. These choices largely influence the speed, memory usage, inclusion of parallel code and workarounds for certain compilers.

The pre-processing options which accept a value are set by:

```
-DOPTION=VAL
```

which defines the pre-processing definition `OPTION` to have value `VAL`. Similarly, the options which just need to be defined to be used are set by:

```
-DOPTION
```

These should be added to the `cppflags` or `cppdefs` lines in the configuration files or in the Makefile, as desired.

**Warning:** Certain options, for technical reasons, change the Markov chain of QMC calculations. Results should be in statistical agreement but the precise data produced by the calculation (even using the same random number seed) may well be changed.

This currently applies to the following options: `POP_SIZE` and `SINGLE_PRECISION`.

**DET\_SIZE** Default: 32.

HANDE uses bit strings to store Slater determinants, where each bit corresponds to an occupied spin-orbital if the bit is set and an unoccupied spin orbital otherwise. As Fortran does not include a type for a single bit, integers are used. Note that this does lead to some wasted memory when the number of spin-orbitals is not a multiple of the size of the integer used. An array of integers is used to store the determinant bit string if a single integer is not sufficient.

This option sets the integer length to be used. Allowed values are 32 and 64, corresponding to using 32-bit and 64-bit integers respectively. As bit operations on a 64-bit integer are faster than those on two 32-bit integers, using `DET_SIZE=64` is recommended for production calculations. (Note, however, that this will use more



memory than DET\_SIZE=32 if the number of basis functions is closer to a multiple of 32 rather than 64. This is rarely a concern in practice.)

**POP\_SIZE** Default: 32

This option is used to specify whether 32 or 64-bit integers are used to store walker populations in HANDE. It is unlikely that 64-bit integers will be needed when using the integer code but this option is more critical when the **real\_amplitudes** option is being used. When using the **real\_amplitudes** option with POP\_SIZE=32, the largest walker amplitude that can be stored is  $2^{20} = 1048576$ , while the smallest fractional part that can be represented is  $2^{-11} = 0.00049$ . When using this option and POP\_SIZE=64 the largest amplitude is  $2^{32} = 4.3 \times 10^9$  and the smallest fractional part is  $2^{-31} = 4.66 \times 10^{-10}$ .

**DEBUG** Default: not defined.

If defined then add additional information in output (e.g. stack traces) that might be useful for debugging. Recommended for developers only. The format and content of the additional debug output should not be relied upon.

**DISABLE\_MPI3** Default: not defined. Only relevant when PARALLEL is defined.

If defined then additional functionality provided by the MPI 3 standard is not used. This disables some functionality (e.g. exploiting MPI 3 shared memory to store large integral arrays only once per node rather than once per processor) and causes slower fallback communication procedures to be used in some cases.

**DISABLE\_HDF5** Default: not defined.

If defined then the QMC restart functionality is disabled and the dependency on HDF5 (which can be tricky to compile on some machines) is removed. Note that restart functionality is extremely useful in production simulations so this option should only be used during initial porting efforts.

**DISABLE\_UUID** Default: not defined.

If defined then each calculation will not print universally unique identifier. This removes the dependency on libuuid.

**DISABLE\_SCALAPACK** Default: not defined

If defined then FCI calculations in parallel are disabled, and the dependency on ScaLAPACK is removed.

**DISABLE\_BACKTRACE** Default: not defined

If defined then the backtrace is disabled. The backtrace functionality is a GNU extension and not available on all POSIX architectures. No working functionality is lost.

**DSFMT\_MEXP** Default: 19937.

HANDE uses the dSFMT random number generator (RNG). It is based on a Mersenne Twister algorithm, is extremely fast and produces high quality random numbers. See <http://www.math.sci.hiroshima-u.ac.jp/~m-mat/MT/SFMT/index.html> for more details.

DSFMT\_EXP sets the exponent of the period of the RNG. Allowed values are 521, 1279, 2203, 4253, 11213, 19937, 44497, 86243, 132049 and 216091 and lead to, for example, random numbers with a period of a Mersenne Prime such as  $2^{521} - 1$ .

**ENABLE\_SHMEM\_POSIX** Default: not defined. Only relevant when PARALLEL is defined.

If defined, then use POSIX functions to allocate large arrays using shared memory (i.e. once per node rather than once per processor). This depends upon having access to various system-level functionality and so, depending upon local configuration, may not work when run as a non-privileged user (and hande should **not** be run by privileged users!). As a result, we recommend using MPI 3 instead of this where possible. This may require the rt library to be added to the link line.

**NAGF95** Default: not defined.

If defined then code specific to, and necessary for compilation using, the NAG Fortran compiler is included.

**PARALLEL** Default: not defined.

Include source code required for running in parallel.

**SINGLE\_PRECISION** Default: not defined.

Set the precision (where possible) to be single precision. The default is double precision. This is faster, but (of course) can change results significantly. Use with care.

**USE\_POPCNT** Default: not defined.

Use the intrinsic popcnt function instead of the version implemented in HANDE.

An important procedure involves counting the number of set bits in an integer. HANDE includes a very efficient, branchless procedure to do this. However, the Fortran 2008 standard includes an intrinsic function, `popcnt`, for this exact operation. The performance of this intrinsic will be implementation-dependent and, with standard compilation flags, we expect the HANDE version to be competitive or more performant, based upon some simple tests. The key difference is on modern processors containing the `popcnt` instruction: the `popcnt` intrinsic can then make use of this instruction and will be much faster than the implementation in HANDE. The existence of the `popcnt` instruction can be found, on Unix and Linux platforms, by inspecting the flags field in `/proc/cpuinfo`: if it contains `popcnt`, then the processor contains the `popcnt` instruction.

Using the `popcnt` instruction often involves a compiler-specific flag to tell the compiler to use that instruction set; often compilers include the `popcnt` instruction with the flag that specifies the use of the SSE4.2 instruction set. The use of the `popcnt` instruction can be tested using `objdump`. For example:

```
$ objdump -d bin/hande.x | grep popc
000000000400790 <__popcountdi2@plt>:
    400931:e8 5a fe ff ff      callq  400790 <__popcountdi2@plt>
```

indicates that HANDE is using a compiler-supplied function for `popcnt`. Exact output (especially the function name) is compiler dependent. In contrast:

```
$ objdump -d bin/hande.x | grep popc
4008ac:f3 0f b8 c0      popcnt %eax,%eax
```

indicates HANDE is using the `popcnt` instruction. If the above command does not give any output, then `USE_POPCNT` has most likely not been defined.

## Compiler and library issues

We attempt to work round any compiler and library issues we encounter but sometimes this is not possible. Issues and, where known, workarounds we have found are:

- gcc 6.3.0 has a code generation bug which causes incorrect energies for all molecular QMC calculations. Please use either a later version of gcc (either 6.4.0 or 7.1.0 do not have this problem) or a different compiler or an optimisation level no higher than `-O0`. Warning: the latter is **very** slow! See <https://gcc.gnu.org/ml/fortran/2017-05/msg00074.html> and the subsequent discussion for more details.
- gcc 7.1.0 has a bug that prevents reading in molecular integrals correctly and instead causes HANDE to exit with an error. See [https://gcc.gnu.org/bugzilla/show\\_bug.cgi?id=80741](https://gcc.gnu.org/bugzilla/show_bug.cgi?id=80741) for details. A mitigation has been implemented to avoid this.
- gcc 7.1.0 and 7.2.0 have a bug that causes `c_associated` to sometimes return incorrect values. This might affect the error reporting from reading a restart file but should not cause any problems under normal usage. If affected, the only workaround is to use a later version of gcc or a different compiler. See [https://gcc.gnu.org/bugzilla/show\\_bug.cgi?id=82869](https://gcc.gnu.org/bugzilla/show_bug.cgi?id=82869) for more details.

- gcc 7.3.0 (and possibly earlier) has a bug affecting inquire on internal units. A workaround is in place for gcc 7.3.0. See [https://gcc.gnu.org/bugzilla/show\\_bug.cgi?id=84412](https://gcc.gnu.org/bugzilla/show_bug.cgi?id=84412) for more details.
- HDF5 1.8.14 (and possibly 1.8.13) has a bug revealed by Intel compilers v15 onwards. This results in unusual error messages and/or segmentation faults when writing out restart files. Possibly workarounds:
  - use HDF5 1.8.15 (best).
  - recompile HDF5 with `-assume nostd_value`.
  - recompile HDF5 with an earlier version of the Intel compilers.
  - recompile HANDE with HDF5 support disabled.
- Compiling with GCC and linking the Intel MKL library leads to segmentation faults or incorrect answers for FCI calculation on systems with complex-valued integrals when run in parallel. Either use a different ScaLAPACK library, or use the Intel compilers.
- Recent versions of Intel MKL do not support recent versions of OpenMPI (including OpenMPI 1.10 and 2.x families), and OpenMPI has a long-standing issue with certain datatypes. This results in `MPI_ERR_TRUNCATE` in parallel FCI calculations. Either use a different ScaLAPACK library or a different MPI implementation or use `--mca coll ^tuned` as an argument to `mpirun/mpiexec`. See <https://github.com/open-mpi/ompi/issues/3937> for more details.
- Using some versions of Intel MPI 5.1 with very large molecular systems (more than 2GB of integrals) causes crashes due to an overflow in a broadcast operation. This is fixed in 5.1.3.
- Intel 2017 compilers, MKL 2017 and OpenMPI 1.10 or later cause segmentation faults in FCI calculations in parallel (see <https://software.intel.com/en-us/forums/intel-math-kernel-library/topic/734559> for more details). QMC calculations are unaffected. Either use MKL 2016 or an alternative MPI library (MPICH is not affected by this issue) or only perform QMC calculations.
- Linking lua depends on how it was compiled. Errors of the type

```
liblua.a(loadlib.o): undefined reference to symbol dlclose@@GLIBC_2.2.5
```

indicate that lua requires dynamic loading and requires `-ldl` to be added to the link line (`libs` in the config file).

A Docker image is also available to try out our code. After installing Docker (<https://docs.docker.com/install/>) you can run the following command:

```
docker run -it handeqmc/hande_ubuntu18.04:latest
```

to start an Ubuntu 18.04 container with the latest version of HANDE installed. The Python dependencies of HANDE are also installed in a virtual environment, which you can access with `pipenv shell`.

To mount your local directory in common with the virtual machine use

```
docker run -it -v "$PWD":/home/mightybuilder/work handeqmc/hande_ubuntu18.04:latest
```

## 1.5 Test suite

HANDE has an extensive test suite covering all core functionality. The tests are run using the `testcode` package (<https://github.com/jsspencer/testcode>). Note that the data extraction scripts for HANDE require the `pandas` python library.

`testcode` can be run from the `test_suite` subdirectory:

```
$ testcode.py
```

As the full test suite is extensive, it can take a long time to run, so the `quick` and even shorter `vquick` categories are provided that aim to test most functionality but run in a few minutes. By default the only the `quick` tests are run. The entire test suite is run every week in a mirrored GitLab repository (<https://gitlab.developers.cam.ac.uk/ch/thom/hande-public-testing>), using the latest GNU and Intel compilers. The `quick` tests are also run on every push to the master branch.

Selected data from the HANDE output is compared to known ‘good’ results (‘benchmarks’).

testcode is quite flexible and it’s easy to run subsets of tests, check against different benchmarks, compare previously run tests, run tests concurrently for speed, etc. Please see the testcode documentation for more details.

---

**Note:** For algorithmic reasons, certain compilation and runtime options (principally `POP_SIZE` and processor/thread count) result in different Markov chains and hence different exact results (but same results on average). The tests should therefore be run using the same compilation options and the same parallel distribution as was used for the benchmarks. The latter for MPI parallelisation is done automatically by testcode. Separate tests exist for both `POP_SIZE=32` and `POP_SIZE=64`.

Similarly, the tests will not pass to default accuracy if using `SINGLE_PRECISION`. There is a `single_precision` category, consisting of the tests which will pass with a tolerance set to  $10^{-5}$ .

Currently there are no QMC tests suitable for OpenMP parallelisation due to difficulties with making the scheduler behave deterministically without affecting performance of production simulations. It is advised that you make sure to set the shell variable `OMP_NUM_THREADS` to 1 when running the test suite - otherwise these will all be marked `SKIPPED`.

---

### 1.5.1 What if the tests fail?

A common cause for tests failing is that the configuration causes a different Markov Chain to be run, or part of the code has been disabled in your build. testcode should determine that some tests are inappropriate and skip them. To force testcode to skip some tests, see below.

A second cause of failure is that some floating point values have rounded differently on different architectures. The tolerances used for the tests can also be adjusted as specified below:

### 1.5.2 Skipping Tests

If there is a unique line printed out in the output for jobs which are to be skipped, this can be used to tell testcode this, by modifying the `skip_args` line in the `test_suite/userconfig` file. See the testcode documentation for more details

### 1.5.3 Adjusting Test Tolerances

The tolerance for an individual job can be modified as specified in the testcode documentation. As an example, to modify the tolerance because of the following failure:

```
dmqmc/np1/heisenberg_1d - replica.in: **FAILED**.  
\sum\rho_{ij}M2{ji}  
  ERROR: absolute error 1.00e-06 greater than 1.00e-10. (Test: 17.378583.   
↪Benchmark: 17.378584.)
```

The follow section can be inserted into `test_suite/jobconfig`. Note the backslash-quoting of the backslashes, as the tolerance value is interpreted as a python tuple containing a python string.

```
#Job specific tolerances:
[dmqmc/np1/heisenberg_1d/]
tolerance = (1e-5,1e-5,'\\sum\\rho_{ij}M2{ji}')
```

## 1.6 Usage

```
$ hande.x [input_filename]
```

Output is sent to STDOUT and can be redirected as desired.

### 1.6.1 Parallel Usage

Using MPI only:

```
$ mpirun -np n hande.x [input_filename]
```

where *n* is the number of processors to run on in parallel. On an HPC system this may differ (for example `mpirun -np n` may be replaced with `mpiexec`), depending on how the environment has been set up.

Using OpenMP parallelism:

```
$ export OMP_NUM_THREADS=n
$ hande.x [input_filename]
```

OpenMP parallelism is currently only implemented for CCMC.

Using OpenMP and MPI parallelism:

```
$ export OMP_NUM_THREADS=n
$ mpirun -np m hande.x [input_filename]
```

where *m* is the number of MPI processes and *n* is the number of OpenMP threads per MPI process. HANDE prints this information at the top of the output, so one can easily check their environment is set up correctly.

HANDE only performs I/O operations on the root processor when run on multiple processors.

---

**Note:** Due to the implementation of efficient Monte Carlo algorithms, running the Monte Carlo algorithms in HANDE on different numbers of processors (or using OpenMP) results in different Markov chains and hence such calculations will not agree exactly but instead statistically.

---

## 1.7 Input file

HANDE is controlled via an input file which is a simple lua script. This has the advantage of creating a clean, simple interface to HANDE whilst allowing advanced users to perform complex simulations without requiring parsing complicated (and perhaps bespoke) logic in a custom input parser. Future work will include exposing more of HANDE via the lua API, thus increasing the flexibility available.

Running a simulation typically involves creating a quantum system (i.e. a collection of spins/fermions/etc acting under a specified Hamiltonian) and then performing one or more calculations on that system. Both tasks involve calling functions from the input file.

The following sections detail options available in each system and calculation function. Variables can be required (i.e. must be specified if a function is called) or optional (in which case the default is stated). The type (e.g. float, such as 1.234; integer, such as 1; boolean, either `true` or `false`) of each variable is also given.

## 1.7.1 Systems

All functions which create a system return a pointer to a `system` object (which currently cannot be manipulated or inspected from lua). All calculation functions take this variable as an argument.

### Model lattice systems

#### Hubbard model (momentum-space)

```
hubbard_k {
    -- options,
}
```

**Returns:** a system object.

`hubbard_k` creates a system object for the Hubbard model:

$$H = -t \sum_{\langle r, r' \rangle, \sigma} c_{r, \sigma}^\dagger c_{r', \sigma} + U \sum_r n_{r, \uparrow} n_{r, \downarrow}$$

using a single-particle basis of Bloch functions,  $\psi_k$ :

$$\psi_k(r) = e^{ik \cdot r} \sum_i \phi_i(r)$$

where  $\phi_i(r)$  is a single-particle basis function centred on site  $i$  in real space.

### Options

**sys** type: system object produced by a previous call.

Optional.

If provided, a previously created system object is updated with the new settings supplied, otherwise a new system object is created.

**electrons** type: integer.

Required.

Number of electrons in the unit cell.

**lattice** type:  $N$   $N$ -dimensional vectors of floats.

Required.

Unit cell on which periodic boundary conditions are placed. See below.

**ms** type: integer.

Required.

Set the spin polarisation of the system in units of electron spin (i.e. a single electron can take values 1 or -1).

**sym** type: integer or string.

Optional. Default: `aufbau`.

Set the symmetry (i.e. crystal momentum) of the system if a reference determinant is not provided. This can be set to:

- An integer specifying the index of a specific wavevector; see the output produced by creating a system for possible values and their corresponding wavevectors.
- `aufbau`. Uses the symmetry of a determinant selected using the Aufbau principle.
- `tot_sym`. Uses the totally symmetric representation, whatever its index may be.

**U** type: float.

Optional. Default: 1.

Specifies the  $U$  parameter in the Hamiltonian.

**t** type: float.

Optional. Default: 1.

Specifies the  $t$  parameter in the Hamiltonian.

**twist** type:  $N$ -dimensional vector

Optional. Default: 0 in each dimension.

Apply a twist to the wavevector grid. The twist is an  $ndim$ -dimensional vector in terms of the reciprocal lattice vectors. The twist angle is chosen to be within the primitive reciprocal cell, and hence the components should be between -0.5 and +0.5.

**verbose** type: boolean.

Optional. Default: `true`.

Print out the single-particle basis set.

## Hubbard model (real-space)

```
hubbard_real {
    -- options,
}
```

**Returns:** a system object.

`hubbard_real` creates a system object for the Hubbard model:

$$H = -t \sum_{\langle r, r' \rangle, \sigma} c_{r, \sigma}^{\dagger} c_{r', \sigma} + U \sum_r n_{r, \uparrow} n_{r, \downarrow}$$

using a single-particle basis of functions in real-space.

## Options

**sys** type: system object produced by a previous call.

Optional.

If provided, a previously created system object is updated with the new settings supplied, otherwise a new system object is created.

**electrons** type: integer.

Required.

Number of electrons in the unit cell.

**lattice** type:  $N$   $N$ -dimensional vectors of floats.

Required.

Unit cell on which periodic boundary conditions are placed. See below.

**ms** type: integer.

Required.

Set the spin polarisation of the system in units of electron spin.

**U** type: float.

Optional. Default: 1.

Specifies the  $U$  parameter in the Hamiltonian.

**t** type: float.

Optional. Default: 1.

Specifies the  $t$  parameter in the Hamiltonian.

**finite** type: boolean.

Optional. Default: false.

If false then periodic boundary conditions are applied to the unit cell, otherwise the system specified by the lattice is treated as an isolated set of sites.

**verbose** type: boolean.

Optional. Default: true.

Print out the single-particle basis set.

## Heisenberg model

```
heisenberg {
    -- options,
}
```

**Returns:** a system object.

`heisenberg` creates a system object for the Heisenberg model, which models a set of spin 1/2 particles on a lattice:

$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j - h_z \sum_i \hat{S}_{iz} - h'_z \sum_i \hat{S}_{iz}^\xi,$$

where  $h_z$  and  $h'_z$  denote the magnetic field strength and staggered magnetic field strength, respectively, and  $\xi$  is equal to +1 for sites on sublattice 1 and is equal to -1 for sites on sublattice 2.



## Options

**sys** type: system object produced by a previous call.

Optional.

If provided, a previously created system object is updated with the new settings supplied, otherwise a new system object is created.

**lattice** type:  $N$   $N$ -dimensional vectors of floats.

Required.

Unit cell on which periodic boundary conditions are placed. See below.

**Warning:** For efficiency reasons it is assumed that the smallest dimension lattice vector is greater than 2 if periodic boundary conditions are used.

**ms** type: integer.

Required.

Set the spin polarisation of the system in units of 1/2.

**J** type: float.

Optional. Default: 1.

Set the coupling constant for the Heisenberg model.

**magnetic\_field** type: float.

Optional. Default: 0.

**staggered\_magnetic\_field** type: float.

Optional. Default: 0.

---

**Note:** Specifying non-zero values for both `magnetic_field` and `staggered_magnetic_field` is not currently possible.

---

**finite** type: boolean.

Optional. Default: false.

If false then periodic boundary conditions are applied to the unit cell, otherwise the system specified by the lattice is treated as an isolated set of sites.

**triangular** type: boolean.

Optional. Default: false.

If true, then a triangular lattice of sites on which the spins reside is used, requiring a 2D lattice. The default is to use a  $N$ -dimensional cubic arrangement of sites.

**verbose** type: boolean.

Optional. Default: true.

Print out the single-particle basis set.

## Chung-Landau model

```
chung_landau {
    -- options,
}
```

**Returns:** a system object.

`chung_landau` creates a system object for the system of spinless fermions proposed by Chung and Landau:

$$H = -t \sum_{\langle r, r' \rangle} c_r^\dagger c_{r'} + U \sum_{\langle r, r' \rangle} n_r n_{r'}$$

using a single-particle basis of functions in real-space.

## Options

**sys** type: system object produced by a previous call.

Optional.

If provided, a previously created system object is updated with the new settings supplied, otherwise a new system object is created.

**electrons** type: integer.

Required.

Number of fermions in the unit cell.

**lattice** type:  $N$   $N$ -dimensional vectors of floats.

Required.

Unit cell on which periodic boundary conditions are placed. See below.

**U** type: float.

Optional. Default: 1.

Specifies the  $U$  parameter in the Hamiltonian.

**t** type: float.

Optional. Default: 1.

Specifies the  $t$  parameter in the Hamiltonian.

**finite** type: boolean.

Optional. Default: false.

If false then periodic boundary conditions are applied to the unit cell, otherwise the system specified by the lattice is treated as an isolated set of sites.

**verbose** type: boolean.

Optional. Default: true.

Print out the single-particle basis set.

## Specifying the lattice

The lattice is specified as a table of vectors. Sites (on which a spin or electron resides) are at unit locations on the grid. The unit cell (or, if periodic boundary conditions are not used, the geometry of the ‘flake’ essentially cut out of the infinite lattice) are given in this basis. The lattice variable hence requires  $N$  vectors, each of dimension  $N$ . This is specified in lua by a nested table. For example:

```
lattice = { { 10 } }
```

sets a 1D system, with the unit cell containing 10 sites;

```
lattice = { { 2, 0 }, { 0, 2 } }
```

sets a 2D system, with the unit cell containing 4 sites; and

```
lattice = { { 3, 3 }, { 3, -3 } }
```

sets a 2D system, with the (square) unit cell containing 18 sites and rotated by  $45^\circ$  relative to the primitive lattice.

HANDE supports 1-, 2- and 3-dimensional lattices. Lattice vectors must be orthogonal.

## Electron gases

An electron gas contains interacting electrons in some geometry with a constant compensating positive charge.

### Uniform electron gas

```
ueg {  
    -- options,  
}
```

**Returns:** a system object.

ueg creates a system object for the (conventional) electron gas:

$$H = -\frac{1}{2} \sum_i \nabla_i^2 + \sum_{i<j} \frac{1}{r_{ij}}$$

(including an appropriate uniform background potential to counteract the charge), using a single-particle basis of plane waves,  $\psi_{\mathbf{k}} = e^{i\mathbf{k}\cdot\mathbf{r}}$ .

## Options

**sys** type: system object produced by a previous call.

Optional.

If provided, a previously created system object is updated with the new settings supplied, otherwise a new system object is created.

**electrons** type: integer.

Required.

Number of electrons in the unit cell.

**ms** type: integer.

Required.

Set the spin polarisation of the system in units of electron spin (i.e. a single electron can take values 1 or -1).

**sym** type: integer or string.

Optional. Default: `aufbau`.

Set the symmetry (i.e. crystal momentum) of the system if a reference determinant is not provided. This can be set to:

- An integer specifying the index of a specific wavevector; see the output produced by creating a system for possible values and their corresponding wavevectors.
- `aufbau`. Uses the symmetry of a determinant selected using the Aufbau principle.
- `tot_sym`. Uses the totally symmetric representation, whatever its index may be.

**rs** type: float.

Optional. Default: 1.

Set the density,  $r_s$ , of the UEG.

**cutoff** type: float.

Optional. Default: 3.

Set the maximum kinetic energy of the orbitals included in the basis set.

Note that this is in scaled units of  $(2\pi/L)^2$ , where  $L$  is the dimension of simulation cell defined by *electrons* and *rs* and is compared to the kinetic energy of each plane-wave without the twist angle included. In this way the cutoff can be kept constant whilst the twist is varied and the basis set used will remain consistent.

**dim** type: integer.

Optional. Default: 3.

Set the dimension of the electron gas. 2- and 3-dimensional gases are implemented.

**twist** type:  $N$ -dimensional vector

Optional. Default: 0 in each dimension.

Apply a twist to the wavevector grid. The twist is an  $ndim$ -dimensional vector in terms of the reciprocal lattice vectors. The twist angle is chosen to be within the primitive reciprocal cell, and hence the components should be between -0.5 and +0.5.

**verbose** type: boolean.

Optional. Default: true.

Print out the single-particle basis set.

## Ringium

```
ringium {
    -- options,
}
```

**Returns:** a system object.

Ringium [Loos13], is a 1D system of electrons confined to a ring of radius  $R$ :

$$H = -\frac{1}{2R^2} \sum_i \frac{\partial^2}{\partial \theta_i^2} + \sum_{i < j} \frac{1}{r_{ij}}$$

where  $r_{ij} = R\sqrt{2 - 2\cos(\theta_i - \theta_j)}$ , using a single-particle basis of functions  $\psi_n = e^{in\theta}$ . As it is 1D, the different spin polarisations are degenerate, so without loss of generality all electrons are forced to be spin up.

## Options

**sys** type: system object produced by a previous call.

Optional.

If provided, a previously created system object is updated with the new settings supplied, otherwise a new system object is created.

**electrons** type: integer

Required.

Number of electrons in the system.

**radius** type: float

Required.

The radius of the ring.

**maxlz** type: integer

Required.

The maximum angular momentum of the orbitals used in the basis set.

Note that this is in units of  $\frac{\hbar}{2}$  and must have opposite parity to the number of electrons.

**verbose** type: boolean.

Optional. Default: true.

Print out the single-particle basis set.

## Generic systems

```
read_in {
    -- options
}
```

**Returns:** a system object.

A generic system, including atoms and molecules, can be specified by providing a file containing information about the single-particle basis set and the one- and two-body integrals between these basis functions. This file is in FCIDUMP format [Knowles89], which can be produced by several quantum chemistry packages including MOLPRO, Q-Chem (via additions from Alex Thom) and PSI4 (via a plugin from James Spencer). See *Generating integrals* for more details.

## Options

**sys** type: system object produced by a previous call.

Optional.

If provided, a previously created system object is updated with the new settings supplied, otherwise a new system object is created.

**electrons** type: integer.

Optional. If specified, then **ms** **must** be specified.

Number of electrons in the unit cell. If not provided, the value in the FCIDUMP file is used.

**ms** type: integer.

Optional. If specified, then **electrons** **must** be specified.

Set the spin polarisation of the system in units of electron spin (i.e. a single electron can take values 1 or -1). If not provided, the value in the FCIDUMP file is used.

**sym** type: integer or string.

Optional. Default: `aufbau`.

Set the symmetry of the system if a reference determinant is not provided. This can be set to:

- An integer specifying the index of a specific irreducible representation from the FCIDUMP file; see the output produced by creating a system for possible values.
- `aufbau`. Uses the symmetry of a determinant selected using the Aufbau principle.
- `tot_sym`. Uses the totally symmetric representation, whatever its index may be.;

**Lz** type: boolean.

Optional. Default: `false`.

If true, enable  $L_z$  symmetry. See below for details.

**int\_file** type: string.

Optional. Default: `'FCIDUMP'`.

Specify the FCIDUMP file containing the integrals and information relating to the single-particle basis. For details of the format see [FCIDUMP format](#). This can also be an HDF5 file previously produced by HANDE from a FCIDUMP via the `write_read_in_system` function (see [Write HDF5 system file](#)), which is both more compact in size and considerably faster to process.

**dipole\_int\_file** type: string.

Optional. No default.

Specify a FCIDUMP-like file containing the dipole integrals, i.e.  $\langle i|x|i \rangle$ , in a given direction.

Not currently used.

**CAS** type: 2D-vector of integers.

Optional. No default.

If specified, then the basis set is restricted to a given complete active space, whereby `CAS = {N,M}` corresponds to allowing only  $N$  electrons to be distributed among  $2M$  spin orbitals. Any additional electrons are 'frozen' (i.e. forced to be in the lowest spin orbitals) and any additional high-energy spin orbitals are removed from the basis set.

**Warning:** This functionality is not compatible with reading from an HDF5 file; to use a CAS in combination with HDF5 initialisation, create the HDF5 file using a system with the desired CAS.

**verbose** type: boolean.

Optional. Default: true.

Print out the single-particle basis set.

**complex** type: boolean.

Optional. Default: false.

Specify if the calculation should use complex dynamics in any calculation performed, and if the FCIDUMP supplied is complex-formatted. Currently compatible with fci, fciqmc, ccmc and dmqmc (including ip-dmqmc) calculations.

**max\_integral\_chunk** type: integer

Optional. Default  $2^{31} - 1$ .

Maximum number of MPI objects to broadcast in a single call for two body integrals. Above this value a contiguous MPI type is used instead.

**Warning:** This functionality is included only for ease of testing. It should not be used for production calculations.

## $L_z$ symmetry

For cylindrically symmetrical systems, the  $L_z$  (z-component of orbital angular momentum) operator commutes with the Hamiltonian, and this can be a convenient symmetry to conserve.  $L_z$  is measured in units of  $\hbar$ . Normal FCIDUMP files do not contain orbitals which are eigenfunctions of the  $L_z$  operator, so they must be transformed using post-processing.

SYMLZ give the eigenvalue of  $L_z$  (the  $m_l$  value). Orbitals with defined values of  $L_z$  are likely to be complex-valued, but luckily the integrals involving them are not, so although the FCIDUMP file must be translated, it still retains the same format (see comments in `src/read_in.F90`, `src/molecular_integrals.F90` and [FCIDUMP format](#) for details if you wish to create FCIDUMP files by other means).

The FCIDUMP file header format has been modified to include additional parameters: SYML, and SYMLZ which have a list of values, one for each orbital.

SYML gives the magnitude of L for the orbital if known (or -20 if not) but is not used.

**Note:** There is a tool provided in `tools/fcidump/lz_fcidump.py` that can generate  $L_z$ -transformed FCIDUMPs from PySCF calculations. To run this script, you need to:

- compile the `lz_transform.f90` Fortran script,
- have PySCF,
- install a Python package called `f90nml`.

See the comments within the Python script for further help.

**Warning:** These transformed integral files require you to enforce  $L_z$  symmetry and will produce incorrect results if you do not.

## 1.7.2 Calculations

All QMC methods (FCIQMC, CCMC, UCCMC, DMQMC and the simple FCIQMC implementation) return a pointer to a `qmc_state` object (which cannot be directly manipulated or inspected from lua) as the first return value. They also accept such an object as an optional argument to resume a previous QMC calculation. Additional, calculation-specific, values are returned in some cases, as described in the relevant section.

### Full Configuration Interaction

Calculate the ground state of a system via a full diagonalisation of the Hamiltonian matrix [Knowles89], or the Davidson iterative diagonalisation scheme [Davidson75] if only a few lowest eigenpairs are sought.

```
fci {  
  sys = system,  
  fci = { ... },  
  reference = { ... },  
  davidson = { ... },  
}
```

---

**Note:** The FCI engine in HANDE is particularly simple (i.e. slow, dumb, memory hungry) and is designed mainly for testing. A conventional quantum chemistry package, such as MOLPRO, or PSI4, is highly recommended for production FCI calculations as these implement substantially more efficient algorithms.

---

### Options

**sys** type: system object.

Required.

The system on which to perform the calculation. Must be created via a system function.

**fci** type: lua table.

Optional. No default.

Further FCI options. See below.

**reference** type: lua table.

Optional. No default.

If not specified, the entire Hilbert space is used. See *reference options*.

**davidson** type: lua table.

Optional. No default.

Davidson diagonalisation options. See below.



## fcf options

The `fcf` table can take the following options:

**write\_hamiltonian** type: boolean.

Optional. Default: false.

Write out the diagonal and the non-zero off-diagonal elements of the Hamiltonian matrix.

**hamiltonian\_file** type: string.

Optional. Default: 'HAMIL'.

Filename to which the Hamiltonian matrix is written.

**hamiltonian\_diagonal\_only** type: boolean.

Optional. Default: false.

Overrides traditional exact diagonalization of the full system Hamiltonian and instead prints out the diagonal elements of the Hamiltonian matrix. The diagonal eigenspectrum can be used for generating exact THF comparison data for the grand canonical initialization in IP-DMQMC by performing a sum over thermal weights (See "propagate\_fcf.py" within the `hande tools` folder) [Malone15].

**write\_determinants** type: boolean.

Optional. Default: false.

Write out the enumerated list of determinants in the FCI Hilbert space.

**determinant\_file** type: string.

Optional. Default: 'DETS'.

Filename to which the list of determinants (or, more generally, many-body basis functions) is written.

**write\_nwfns** type: integer.

Optional. Default: 0.

Number of wavefunctions to write out (in the basis of Slater determinants). A negative value indicates all wavefunctions are to be written out.

**wfn\_file** type: string.

Optional. Default: 'FCF\_WFN'.

Filename to which the wavefunctions are written.

**nanalyse** type: integer.

Optional. Default: 0.

Calculate properties of the first *nwfn* FCI wavefunctions from each spin and symmetry block. If *nwfn* is negative (default) then all wavefunctions are analysed. This is slow, and uses a very simple algorithm. It is only designed for debugging purposes. The properties evaluated depend upon the system and are liable to change without warning.

**blacs\_block\_size** type: integer.

Optional. Default: 64.

The block size used by BLACS to distribute the Hamiltonian matrix across the processors with MPI parallelism. The Hamiltonian matrix is divided into  $n \times n$  sub-matrices, where  $n$  is the block size, which are the distributed over the processors in a cyclic fashion.

**rdm** type: table of integers.

Optional. No default.

If present, calculate the eigenvalues for the reduced density matrix consisting of the specified list of sites, with a trace performed over all other sites.

---

**Note:** The `rdm` option is only currently available for Heisenberg systems.

---

---

**Note:** The `write_wfn`, `nanalyse` and `rdm` options require the eigenvectors to be calculated in addition to the eigenvalues, which requires additional computational time.

---

### davidson options

---

**Note:** Davidson diagonalisation currently only supports real Hamiltonians on a single node. Although multi-threaded BLAS/LAPACK libraries (MKL, OpenBLAS, etc.) are supported.

---

The `davidson` table can take the following options (specifying the table automatically enables Davidson diagonalisation):

`ndavidson_eigv` type: integer.

Optional. Default: 4.

Number of eigenpairs to solve for.

`ndavidson_trialvec` type: integer.

Optional. Default: 8.

Number of trial vectors to use, usually double `ndavidson_eigv`.

`davidson_maxsize` type: integer.

Optional. Default: 50.

Maximum number of guess vectors held at the same time. This should be very small compared to the dimensions of the full Hamiltonian you're trying to diagonalise. If larger an error will be thrown. It also has to be at least double `ndavidson_trialvec`, as the first iteration after each subspace collapse produces a very small change in eigenvalues and hence cannot be used for convergence testing.

`davidson_tol` type: float.

Optional. Default: 1e-7.

Tolerance in the norm of the changes in all eigenvalues.

`davidson_maxiter` type: integer.

Optional. Default: 100.

Maximum number of iterations to run, if convergence is not reached a warning will be thrown, and the results will still be printed.

## Monte Carlo estimate of size of the Hilbert space

Whilst calculating the size of an entire Hilbert space is straightforward via combinatorics, calculating the size of a specific part of the Hilbert space meeting a given set of quantum numbers (e.g. spin and symmetry) is more challenging. Instead, the size of this subspace can be estimated via a simple Monte Carlo approach [[Booth10](#)].

```
hilbert_space {
  sys = system,
  hilbert = { ... },
  output = { ... },
}
```

**Returns:** a table containing the mean (key: `mean`) and associated standard error (key: `std. err.`) of the Monte Carlo estimate of the size of the Hilbert space.

## Options

All options should be in the `hilbert` table bar the `sys` option.

**sys** type: system object.

Required.

The system on which to perform the calculation. Must be created via a system function.

**hilbert** type: lua table.

Required.

Further options to control the Monte Carlo estimation of the Hilbert space. See below.

**output** type: lua\_table.

Optional.

Further options to enable direction of calculation output to a different file. See [output options](#) for more information.

## hilbert options

The `hilbert` table can take the following options:

**nattempts** type: integer.

Required.

Number of random attempts (i.e. the number of random determinants to generate) to perform per Monte Carlo cycle.

**ncycles** type: integer

Optional. Default: 20.

Number of Monte Carlo cycles to perform. Each cycle produces an independent estimate of the Hilbert space size. Estimates of the mean and standard error are automatically calculated from each independent value.

**rng\_seed** type: integer.

Optional. Default: generate a seed based upon the time and UUID (if available).

Seed for initialising the random number generator.

**reference** type: vector of integers.

Optional. Default: attempt to make a good guess based upon the spin and symmetry quantum numbers of the system.

The reference determinant as a list of occupied spin-orbitals. The reference determinant is used in the generation of truncated Hilbert spaces only.

**ex\_level** type: integer.

Optional. Default: set to the number of electrons in the system (i.e. generate the FCI space).

Maximum excitation level to consider relative to the reference determinant.

## Canonical total energy

```
canonical_estimates {
  sys = system,
  canonical_estimates = { ... },
}
```

`canonical_estimates` calculates various estimates for properties of a system in the canonical ensemble at a given temperature, using knowledge of the grand canonical ensemble and the single-particle eigenvalues of the underlying non-interacting system. See [Malone15] for details. Currently only implemented for the UEG and `read_in`.

## Options

**sys** type: system object.

Required.

The system on which to perform the calculation. Must be created via a system function.

**canonical\_estimates** type: lua table.

Required.

Further options controlling the calculation.

## kinetic options

**ncycles** type: integer.

Required.

The number of Monte Carlo iterations to perform. Each iteration produces independent estimates based upon the `nattempts` made.

**nattempts** type: integer.

Required.

Number of determinants within the canonical ensemble we attempt to generate each Monte Carlo cycle.

**beta** type: float.

Required.

The temperature of the system.

**fermi\_temperature** type: boolean.

Optional. Default: false.

If true, rescale `beta` as the inverse reduced temperature:  $\tilde{\beta} = 1/\Theta = T_F/T$ , where  $T_F$  is the Fermi temperature. If false, `beta` is taken to be in atomic units.

**rng\_seed** type: integer.

Optional. Default: generate a seed from a hash of the time and calculation UUID.

The seed used to initialise the random number generator.

## Full Configuration Interaction Quantum Monte Carlo

```
fciqmc {
  sys = system,
  qmc = { ... },
  fciqmc = { ... },
  semi_stoch = { ... },
  restart = { ... },
  reference = { ... },
  load_bal = { ... },
  logging = { ... },
  output = { ... },
  blocking = { ... },
  qmc_state = qmc_state,
}
```

**Returns:** a `qmc_state` object.

`fciqmc` performs a full configuration interaction quantum Monte Carlo (FCIQMC) calculation [Booth09] on a system.

## Options

**sys** type: system object.

Required.

The system on which to perform the calculation. Must be created via a system function.

**qmc** type: lua table.

Required.

Further options that are common to all implemented QMC algorithms. See [qmc options](#).

**fciqmc** type: lua table.

Optional.

Further options to control the FCIQMC algorithm. See [fciqmc options](#).

**semi\_stoch** type: lua table.

Optional.

Further options to control using a semi-stochastic projection of the Hamiltonian operator instead of a purely stochastic projection. Note that some options in the `semi_stoch` table are required to be set if the table is given. See [semi\\_stoch options](#).

**restart** type: lua table.

Optional.

Further options to control restarting the calculation from a previous calculation. See [restart options](#).

**reference** type: lua table.

Optional.

Further options to select the reference state used. See [reference options](#).

**load\_bal** type: lua table.

Optional.

Further options to improve the parallel load balancing of an FCIQMC simulation. If present (even if empty) an advanced load-balancing algorithm is used [Malone16a]. See [load\\_bal options](#) for more details.

**logging** type: lua table.

Optional.

Further options to enable various logging outputs from a FCIQMC simulation. Only available when compiled in debug mode. See [logging options](#) for information on current options.

**output** type: lua\_table.

Optional.

Further options to enable direction of calculation output to a different file. See [output options](#) for more information.

**blocking** type: lua table.

Optional.

Further options to switch on and control blocking on the fly. See [blocking options](#).

**qmc\_state** type: qmc\_state object.

Optional.

Output of a previous calculation to resume.

**Warning:** The qmc\_state object must have been returned by a previous FCIQMC calculation. The validity of this is not checked. The system must also be unchanged.

**Warning:** This destroys the qmc\_state object and so it cannot be re-used in subsequent QMC calculations.

## fcirqmc options

**select\_reference\_det** type: boolean or Lua table.

Optional. Default: false.

If true or if a lua table is provided, attempt to automatically set the reference state to be the state with the greatest population. A lua table can contain the following options and need only be provided in order to modify the defaults.

---

**Note:** Care should be taken when analysing the projected estimator to ensure that all quantities averaged have the same reference state.

---

**Warning:** Excitation levels are relative to the reference state and hence this should **not** be used with a truncated CI calculation.

**update\_every** type: integer

Optional. Default: 20.

The number of report loops between attempts to update the reference state.

**pop\_factor** type: float.

Optional. Default: 1.5.

The factor of the reference population another state must have in order for the reference to be changed. This helps prevent continually switching between states with similar or degenerate populations.

**non\_blocking\_comm** type: boolean.

Optional. Default: false.

Use non-blocking MPI communications instead of blocking MPI communications.

---

**Note:** This is an experimental option and may or may not improve performance. In particular, its efficiency is highly dependent upon architecture and MPI implementation. For expert use only!

---

**load\_balancing** type: boolean.

Optional. Default: false.

Enable dynamic load balancing of determinants among processors. This will move determinants to try and keep the number of walkers on each processor roughly constant. See [load\\_bal options](#) for more details.

**init\_spin\_inverse\_reference\_det** type: boolean.

Optional. Default: false.

In addition to initialising the reference determinant with an initial population, initialise the spin-inversed determinant (if different) with the same population. Overridden by a restart file.

**trial\_function** type: string.

Optional. Default: 'single\_basis'.

Possible values: 'single\_basis', 'neel\_singlet' (Heisenberg model only).

The trial function to use in the projected energy estimator. 'single\_basis' uses the single reference state as the trial function. 'neel\_singlet' uses the Neel singlet state,  $|NS\rangle = \sum_i a_i |D_i\rangle$ , where the amplitudes  $a_i$  are defined in K. Runge, Phys. Rev. B 45, 7229 (1992).

Using a multi-reference trial function can substantially reduce stochastic noise.

**guiding\_function** type: string.

Optional. Default: 'none'.

Possible values: 'none', 'neel\_singlet' (Heisenberg model only).

The importance sampling transformation to apply to the Hamiltonian.

'neel\_singlet' uses the Neel singlet state (K. Runge, Phys. Rev. B 45, 7229 (1992)) to transform the Hamiltonian such that the matrix elements,  $H_{ij}$ , are replaced with  $a_i H_{ij} / a_j$ . Using 'neel\_singlet' automatically sets `trial_function` to 'neel\_singlet'.

**replica\_tricks** type: boolean.

Optional. Default: false.

Perform replica simulations (i.e. evolve two independent FCIQMC simulations concurrently).

**density\_matrices** type: boolean.

Optional. Default: false.

Samples the 2-RDM and reports the trace and numerator of the energy estimate. Prints the Hermitian part of the 2-RDM once the calculation has completed.

Requires `replica_tricks` to be enabled.

---

**Note:** Both replicas must be in variable shift mode in order for the 2-RDM to be calculated.

---

**density\_matrix\_file** type: string.

Optional. Default: RDM

The name of the output file that the final 2-RDM is printed to. The (normalised, Hermitian part of) the 2-RDM is given in physical notation.

**density\_matrix\_report** type: int.

Optional. Default: 3000

The minimum report cycle the 2-RDM statistics are collected after.

## load\_bal options

The default values are usually sufficient if load balancing is enabled. It is highly recommended to only attempt to improve load balancing for large calculations and once the population has been stabilised by the shift. It may be easiest to do this by monitoring a calculation carefully until this condition is reached, producing a restart file and then running a production calculation with load balancing enabled.

**nslots** type: integer.

Optional. Default: 20.

The average number of slots per processor used to distribute the list of occupied states via a hashing of the states. A large value will affect performance but could potentially result in a better distribution of walkers.

**min\_pop** type: integer.

Optional. Default: 1000.

The minimum total population required before load balancing is attempted. This is a system dependent value and, in order to maximise performance improvements, should be set such that the population is roughly stable.

**target** type: float.

Optional. Default: 0.05.

Desired imbalance (as a percentage of the average population per processor) between the most and least populated processors. Note that the workload on a processor is not entirely determined by its population and that, due to the algorithms used, an arbitrary small population imbalance is not usually possible.



**max\_attempts** type: integer.

Optional. Default: 2.

The number of attempts to make to improve load balancing. Often multiple attempts can improve the balancing but each attempt may be non-negligible and there are usually diminishing returns.

**write** type: boolean.

Optional. Default: false.

Write out the population of the most and least heavily populated processor before and after load balancing is carried out. Also print out the minimum slot population on the most populated processor which will indicate if load balancing is possible.

## Coupled Cluster Monte Carlo

```
ccmc {
  sys = system,
  qmc = { ... },
  ccmc = { ... },
  restart = { ... },
  reference = { ... },
  logging = { ... },
  output = { ... },
  blocking = { ... },
  qmc_state = qmc_state,
  psip_list = psip_list,
}
```

**Returns:** a qmc\_state object.

`ccmc` performs a coupled cluster Monte Carlo (CCMC) calculation [Thom10] on a system.

## Options

**sys** type: system object.

Required.

The system on which to perform the calculation. Must be created via a system function.

**qmc** type: lua table.

Required.

Further options that are common to all implemented QMC algorithms. See *qmc options*.

**ccmc** type: lua table.

Required.

Further options to control the CCMC algorithm. See *ccmc options*.

**restart** type: lua table.

Optional.

Further options to control restarting the calculation from a previous calculation. See *restart options*.

**reference** type: lua table.

Optional.

Further options to select the reference state used. See [reference options](#).

**logging** type: lua table.

Optional.

Further options to enable various logging outputs from a CCMC simulation. Only available when compiled in debug mode. See [logging options](#) for information on current options.

**output** type: lua\_table.

Optional.

Further options to enable direction of calculation output to a different file. See [output options](#) for more information.

**blocking** type: lua table.

Optional.

Further options to switch on and control blocking on the fly. See [blocking options](#).

**qmc\_state** type: qmc\_state object.

Optional.

Output of a previous calculation to resume.

**Warning:** The qmc\_state object must have been returned by a previous CCMC calculation. The validity of this is not checked. The system must also be unchanged and must not have a different even selection setting. To switch between using even selection and not a written restart file must be used.

**Warning:** This destroys the qmc\_state object and so it cannot be re-used in subsequent QMC calculations.

**psip\_list** type: particle\_t object.

Optional.

Output wavefunction of a previous calculation to initialise the current CCMC calculation. Currently only the [MPI wavefunction](#) calculation can generate a psip\_list.

**Warning:** The contents of the psip\_list directly writes over the initial CCMC wavefunction, so make sure the settings that were used to generate it are identical with those provided for the CCMC table, otherwise undefined behaviour may result. The easiest way to ensure this is outlined in [MPI wavefunction](#).

## ccmc options

**move\_frequency** type: integer

Optional. Default: 5.

Allow excitors to move processors every  $2^x$  iterations, where  $x$  is the value of move\_frequency, in order to allow all composite excitors to be correctly sampled. Relevant only when performing CCMC with MPI

parallelisation. A large value may introduce a bias. Modify with caution. Can be changed when restarting calculations (and/or when *redistributing restart files*) but may impose some initialisation overhead whilst excitors are reassigned to different processors.

**cluster\_multispawn\_threshold** type: float.

Optional. Default:  $2^{31} - 1$ .

Set the maximum value of  $A_C/p_C$ , where  $A_C$  is the cluster amplitude and  $p_C$  is the probability of selecting the cluster. A cluster with a value above this is split into multiple spawning attempts. The default value essentially disables this but a smaller option can substantially reduce population blooms, albeit potentially at a significant computational cost.

---

**Note:** This is an experimental option and feedback is most welcome. The current recommendation is to use the smallest setting such that large blooms do not occur.

---

**full\_non\_composite** type: boolean.

Optional. Default: false.

If true, allow all non-composite clusters to attempt to spawn each iteration. The original CCMC algorithm involves randomly selecting a cluster of arbitrary size consisting of any set of excitors and then making spawning attempts from it. The full non-composite algorithm is a simple modification in which all occupied non-composite clusters (i.e. those consisting of the reference or just a single excitor) are (deterministically) selected and composite clusters (involving two or more excitors) are randomly selected to make spawning attempts. This has been shown to give substantially more stable dynamics and reduce the plateau height in several systems.

**linked** type: boolean.

Optional. Default: false.

If true, sample the linked coupled cluster equations instead of the unlinked coupled cluster equations [Franklin16]. The original CCMC algorithm solves the equations

$$\langle D_m | \hat{H} - E | \psi_{CC} \rangle = 0.$$

It is possible to instead sample the equivalent equations

$$\langle D_m | e^{-\hat{T}} (\hat{H} - E) | \psi_{CC} \rangle = 0.$$

Using the Hausdorff expansion of the Hamiltonian and the linked cluster theorem means that the only clusters which contribute are those with at most four excitors and where the excitation sampled from the Hamiltonian has an orbital in common with each excitor in the cluster operator. Using this option can give substantial reductions in the plateau height.

**vary\_shift\_reference** type: boolean.

Optional. Default: false.

Vary the shift to keep the population at the reference,  $N_0$ , constant, rather than the total population  $N_p$ . If `target_population` is below the plateau (or an equivalently low `reference_target` is specified) then, whilst the reference population will be controlled, the total population will continue to grow until a stable distribution is reached.

**density\_matrices** type: boolean.

Optional. Default: false.

Calculate the (unrelaxed) two-electron coupled cluster density matrix, given by:

$$d_{PQRS} = \langle \psi_{HF} | P^\dagger R^\dagger S Q | \psi_{CC} \rangle$$

**density\_matrix\_file** type: string.

Optional. Default: 'RDM'.

Filename to which the reduced density matrix is written.

**even\_selection** type: boolean

Optional. Default: false.

If true, use selection probabilities for composite clusters such that the probability of selecting a cluster of any size is proportional to its contribution to the overall amplitude of the instantaneous wavefunction representation.

**Warning:** This algorithm gives drastically different behaviour and is a subject of current research. As such, the situations in which this is the optimal approach are not yet entirely clear (benchmarking is underway). In addition, it is not currently confirmed to be compatible with propagation of the linked coupled cluster equations.

**multiref** type: boolean.

Optional. Default: false.

If true, perform a coupled cluster calculation using multiple references [Filip19]. `n_secondary_ref` and `secondary_refX` must then be defined.

**n\_secondary\_ref** type: integer.

Optional.

Number of secondary references used. Must be in the range 1-999.

**secondary\_refX** type: lua table.

Describes the X-th secondary reference state used. See [reference options](#). Must include at least `det` and `ex_level`. One table must be included for each secondary reference.

**mr\_acceptance\_search** type: string.

Optional. Default: 'linear'.

Possible values are 'linear' and 'bk\_tree'.

Specifies the acceptance algorithm for multireference excitation generation.

Linear search iterates through the list of `secondary_refX` provided and accepts a proposed excitation upon the first secondary reference that is within `ex_level` of it. This is more suitable for when `n_secondary_ref` is small (< 100).

BK tree search first builds a tree made of specified secondary references, and descends into the tree to search. A good explanation can be found [here](#). It should achieve sublinear time complexity, and the advantage over linear search will be more evident the larger the secondary reference space and the smaller the coupled cluster truncation (meaning a smaller subspace of the tree needs to be searched).

---

**Note:** The BK tree search algorithm is currently being benchmarked and optimised.

---

**mr\_read\_in** type: boolean.

Whether to read in the secondary references from a file. If set to `true`, then `mr_secref_file` must also be specified.

**mr\_secref\_file** type: string.

The name of the file with the list of secondary references. Can be generated with `tools/ccmc/generate_mr_input_file.py`, to see the available options, run

```
$ generate_mr_input_file.py -h
```

When the `compress` flag is specified, only necessary references (those that are necessary to span the active space uniquely) are generated, without the flag every single determinant in the active space is generated.

The `--nfrozen` option is used to minimize the size of the `secref` file, where the frozen core electrons are not included in the bitstrings, and instead the `mr_n_frozen` option is written into the Lua input file and passed to HANDE, to be added back in when secondary references are initialised.

The `-l` option is related to the size of the active space, such that a 1-fold excitation can reach the ‘middle’ determinant (for a  $(6e, 6o)$  active space for nitrogen molecule, this would be a three-fold excitation from the ground into all six orbitals being singly occupied ( $M_s = 0$  of course).

**mr\_n\_frozen** type: integer.

Optional. Default: 0.

Number of frozen core electrons, i.e., number of electrons that never move in the secondary references.

**mr\_excit\_lvl** type: integer.

Required if `mr_read_in` is true.

The excitation level allowable from every secondary reference.

---

**Note:** This essentially disables the ability to set excitation levels separately for each secondary reference.

---

**mr\_secref\_sym\_only** type: boolean.

Optional. Default: false.

Whether to include only secondary references that belong to the symmetry sector specified in `sys`.

---

**Note:** This is only compatible with `mr_read_in` being set to true.

---

**discard\_threshold** type: float.

Optional. Default:  $2^{31} - 1$ .

The threshold of  $A_C/p_C$ , where  $A_C$  is the cluster amplitude and  $p_C$  is the probability of selecting the cluster (exactly like `cluster_multispawn_threshold`), beyond which a cluster is discarded. This should be bigger than `cluster_multispawn_threshold` if both are specified.

## Unitary Coupled Cluster Monte Carlo

```
uccmc {
  sys = system,
  qmc = { ... },
  ccmc = { ... },
  uccmc = { ... },
  restart = { ... },
  reference = { ... },
  logging = { ... },
```

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(continued from previous page)

```
output = { ... },  
blocking = { ... },  
qmc_state = qmc_state,  
}
```

**Returns:** a `qmc_state` object.

`uccmc` performs a coupled cluster Monte Carlo (CCMC) calculation [Filip20] on a system.

## Options

**sys** type: system object.

Required.

The system on which to perform the calculation. Must be created via a system function.

**qmc** type: lua table.

Required.

Further options that are common to all implemented QMC algorithms. See [qmc options](#).

**ccmc** type: lua table.

Required.

Further options to control the CCMC algorithm. See [ccmc options](#).

**uccmc** type: lua table.

Required.

Further options to control the UCCMC algorithm. See [uccmc options](#).

**restart** type: lua table.

Optional.

Further options to control restarting the calculation from a previous calculation. See [restart options](#).

**reference** type: lua table.

Optional.

Further options to select the reference state used. See [reference options](#).

**logging** type: lua table.

Optional.

Further options to enable various logging outputs from a UCCMC simulation. Only available when compiled in debug mode. See [logging options](#) for information on current options.

**output** type: lua\_table.

Optional.

Further options to enable direction of calculation output to a different file. See [output options](#) for more information.

## uccmc options

**pow\_trunc** type: integer.

Optional. Default: 12.

Polynomial order at which to truncate UCCMC Taylor expansion.

**average\_wfn** type: logical.

Optional. Default: false.

Whether to print out the average wavefunction sampled over the course of the UCCMC calculation.

**trot** type: logical.

Optional. Default: false.

Whether to run a trotterized UCCMC calculation, rather than using the full exponential ansatz.

**threshold** type: float.

Optional. Default:  $2^{31} - 1$ .

The threshold of  $A_C/p_C$ , where  $A_C$  is the cluster amplitude and  $p_C$  is the probability of selecting the cluster (exactly like `cluster_multispawn_threshold`), beyond which a cluster is discarded. This should be bigger than `cluster_multispawn_threshold` if both are specified.

## Density Matrix Quantum Monte Carlo

```
dmqmc {
  sys = system,
  qmc = { ... },
  dmqmc = { ... },
  ipdmqmc = { ... },
  operators = { ... },
  rdm = { ... },
  restart = { ... },
  reference = { ... },
  qmc_state = qmc_state,
}
```

**Returns:** a `qmc_state` object. a lua table containing the sampling probabilities found if `find_weights` is set to `true`. This can be passed directly to the `weights` option of a subsequent DMQMC calculation and/or manipulated inside the lua script. If `find_weights` is `false`, only the `qmc_state` object is returned.

`dmqmc` performs a density matrix quantum Monte Carlo (DMQMC) calculation on a system.

Unlike *Coupled Cluster Monte Carlo* and *Full Configuration Interaction Quantum Monte Carlo*, where quantities are averaged inside each report loop, any quantities in DMQMC are evaluated at the **first** iteration of the report loop only. This is because different iterations represent different temperatures in DMQMC, and so averaging over a report loop would average over different temperatures, which is not the desired behaviour.

**Note:** Density Matrix Quantum Monte Carlo is currently rather experimental. In particular, it is not implemented for all systems yet and some options are only implemented for specific systems. In particular, DMQMC is only implemented for the Heisenberg model, the UEG, the real and momentum-space Hubbard model, and for molecular systems. The evaluation of operators other than the total energy, such as correlation functions and entanglement measures, is currently only possible for the Heisenberg model. The calculation of the reduced density matrices from

DMQMC is also only supported for the Heisenberg model (for both temperature-dependent and ground state RDM calculations).

---

## Options

**sys** type: system object.

Required.

The system on which to perform the calculation. Must be created via a system function.

**qmc** type: lua table.

Required.

Further options that are common to all implemented QMC algorithms. See [qmc options](#).

**dmqmc** type: lua table.

Optional.

Further options to control the DMQMC algorithm. See [dmqmc options](#).

**ipdmqmc** type: lua table.

Optional.

If set, even to an empty table, then interaction picture DMQMC [Malone15] is performed. The table can contain further options to control the IP-DMQMC algorithm. See [ipdmqmc options](#).

**operators** type: lua table.

Optional.

Further options to select the operators for which expectation values are evaluated. See [operators options](#).

**rdm** type: lua table.

Optional.

Further options to select which (if any) reduced density matrices and corresponding operators are to be evaluated. See [rdm options](#).

**restart** type: lua table.

Optional.

Further options to control restarting the calculation from a previous calculation. See [restart options](#).

**reference** type: lua table.

Optional.

Further options to select the reference state used. See [reference options](#).

**qmc\_state** type: qmc\_state object.

Optional.

Output of a previous calculation to resume.

**Warning:** The qmc\_state object must have been returned by a previous DMQMC calculation. The validity of this is not checked. The system must also be unchanged.



**Warning:** This destroys the `qmc_state` object and so it cannot be re-used in subsequent QMC calculations.

## dmqmc options

**symmetric\_bloch** type: boolean.

Optional. Default: true.

Use the symmetrized form of the Bloch equation,  $\frac{d\hat{\rho}}{d\beta} = -\frac{1}{2}\{\hat{H}, \hat{\rho}\}$ , to propagate the density matrix when true. Otherwise the non-symmetrized form,  $\frac{d\hat{\rho}}{d\beta} = -\hat{\rho}\hat{H}$  of the Bloch equation is used. The **symmetrize** option only works with the symmetric version of the Bloch equation.

---

**Note:** The use of symmetric or asymmetric propagation in the DMQMC methods can impact the behavior of the sign problem as well the convergence with respect to beta loops. For more information see [Petras21].

---

**replica\_tricks** type: boolean.

Optional. Default: false.

Perform replica simulations (i.e. evolve two independent DMQMC simulations concurrently) if true. This allows calculation of unbiased estimators that are quadratic in the density matrix.

**fermi\_temperature** type: boolean.

Optional. Default: false.

Rescale tau so that the simulation runs in timesteps of  $\Delta\tau/T_F$  where  $T_F$  is the Fermi temperature. This is so results are at dimensionless inverse temperatures of  $\Theta^{-1} = T_F/T$ . This option is only valid for systems with a well defined Fermi energy.

**all\_sym\_sectors** type: boolean.

Optional. Default: false.

Sample states with all symmetries of the system instead of just those which conserve the symmetry of the reference state.

**all\_spin\_sectors** type: boolean.

Optional. Default: false.

Sample states with all spin polarisations of the system instead of just those which conserve the spin polarisation of the reference state.

**beta\_loops** type: integer.

Optional. Default: 100.

The number of loops over the desired temperature range (each starting from  $T = \infty$  and performing the desired number of iterations) to perform. Each beta loop samples the initial conditions independently.

---

**Note:** Estimators must be averaged at each temperature from different beta loops. As each beta loop is independent, this can be done in separate calculations in an embararassingly parallel fashion.

---

**final\_beta** type: float.

Optional. Default: 0.0.

Sets the final inverse temperature the density matrix is propagated to. When not provided in the input, the number of reports and Monte Carlo cycles controls the final temperature instead. If specified while using the interaction picture, the interaction picture and Bloch equation are used in a piecewise fashion to sample a range of temperatures from **target\_beta** to **final\_beta**. [VanBenschoten22]

**sampling\_weights** type: vector of floats.

Optional. Default: none.

Specify factors used to alter the spawning probabilities in the DMQMC importance sampling procedure. See PRB, 89, 245124 (2014) for an explanation, in particular section IV and appendix B.

The length of the vector of floats should be equal to the maximum number of excitations from any determinant in the space. For a chemical system with  $N$  electrons and more than  $2N$  spin orbitals, this would be equal to  $N$ . For a Heisenberg model with  $N$  spins in the  $M_s = 0$  spin sector, this should be equal to  $N/2$  (each pair of opposite spins flipped is one excitation).

**vary\_weights** type: integer.

Optional. Default: 0

The number of iterations over which to introduce the weights in the importance sampling scheme (see PRB, 89, 245124 (2014)). If not set then the full weights will be used from the first iteration. Otherwise, the weights will be increased by a factor of  $(W_\gamma)^{\beta/\beta_{target}}$  each iteration, where  $W_\gamma$  is the final weight of excitation level  $\gamma$  and  $\beta_{target}$  is the beta value to vary the weights until (equal to the value specified by this option, multiplied by the time step size).

**find\_weights** type: boolean.

Optional. Default: false.

Run a simulation to attempt to find appropriate weights for use in the DMQMC importance sampling procedure. This algorithm will attempt to find weights such that the population of psips is evenly distributed among the various excitation levels when the ground state is reached (at large beta values). The algorithm should be run for several beta loops until the weights settle down to a roughly constant value.

The weights are output at the end of each beta loop.

This option should be used together with the **find\_weights\_start** option, which is used to specify at which iteration the ground state is reached and therefore when averaging of the excitation distribution begins.

This option cannot be used together with the **excit\_dist** option. The **find\_weights** option averages the excitation distribution in the ground state, whereas the **excit\_dist** option accumulates and prints out the excitation distribution at every report loop.

**Warning:** This feature is found to be unsuccessful for some larger lattices (for example, 6x6x6, for the Heisenberg model). The weights output should be checked. Increasing the number of psips used may improve the weights calculated.

**find\_weights\_start** type: integer.

Optional. Default: 0.

The iteration number at which averaging of the excitation distribution begins, when using the **find\_weights** option.

**symmetrize** type: boolean.

Optional. Default: false.

Explicitly symmetrize the density matrix, thus only sampling one triangle of the matrix. This can yield significant improvements in stochastic error in some cases.

**initiator\_level** type: integer.

Optional. Default: -1.

Set all density matrix elements at excitation level **initiator\_level** and below to be initiator determinants. An **initiator\_level** of -1 indicates that no preferential treatment is given to density matrix elements and the usual initiator approximation is imposed, 0 indicates that the diagonal elements are initiators, etc.

This is experimental and the user should identify when convergence has been reached.

**piecewise\_shift** type: float.

Optional. Default: 0.

Sets the value of the simulation shift when the propagator change occurs at the **target\_beta** when running the piecewise interaction picture method.

**walker\_scale\_factor** type: integer.

Optional. Default: 1.

Scales the walker population on the initial trial density matrix by a constant factor. The simulations target population is scaled as well.

**Warning:** This feature is experimental, and results should be tested for accuracy.

## ipdmqmc options

**target\_beta** type: float.

Optional. Default: 1.0.

The inverse temperature to propagate the density matrix to. If **fermi\_temperature** is set to True then **target\_beta** is interpreted as the inverse reduced temperature  $\tilde{\beta} = 1/\Theta = T_F/T$ , where  $T_F$  is the Fermi temperature. Otherwise **target\_beta** is taken to be in atomic units.

---

**Note:** If **final\_beta** is set to a value greater than **target\_beta**, the interaction picture will be used until the **target\_beta** has been reached. Thereafter, the Bloch equation will be used to sample continuously until the **final\_beta** has been reached.

---

**initial\_matrix** type: string.

Optional. Default: 'hartree\_fock'.

Possible values: 'free\_electron', 'hartree\_fock'.

Initialisation of the density matrix at  $\tau = 0$ . 'free\_electron' samples the free electron density matrix, i.e.  $\hat{\rho} = \sum_i e^{-\beta \sum_j \varepsilon_j \hat{n}_j} |D_i\rangle \langle D_i|$ , where  $\varepsilon_j$  is the single-particle eigenvalue and  $\hat{n}_j$  the corresponding number operator. 'hartree\_fock' samples a 'Hartree-Fock' density matrix defined by  $\hat{\rho} = \sum e^{-\beta H_{ii}} |D_i\rangle \langle D_i|$ , where  $H_{ii} = \langle D_i | \hat{H} | D_i \rangle$ .

It is normally best to use the hartree-fock option as this removes cloning/death on the diagonal if the shift is fixed at zero. This requires slightly more work when also using the **grand\_canonical\_initialisation**, but this is negligible.

**grand\_canonical\_initialisation** type: boolean.

Optional. Default: false.

Use the grand canonical partition function to initialise the psip distribution. The default behaviour will randomly distribute particles among the determinants requiring a non-zero value of `metropolis_attempts` to be set for the correct distribution to be reached.

**skip\_gci\_reference\_check** type: boolean.

Optional. Default: false.

When performing **grand\_canonical\_initialisation**, we check that  $H_{ii}$  is not lower in energy than  $H_{00}$ . If a lower energy  $H_{ii}$  is found this can cause many spawns to occur with a weight lower than 1.0 which is undesirable, and so the simulation exits with information to update the reference. Setting this flag to true will ignore the lower energy  $H_{ii}$ .

**Warning:** It is recommended that the orbital single particle eigenvalues in the FCIDUMP are recalculated with the new reference.

**metropolis\_attempts** type: integer.

Optional. Default: 0.

Number of Metropolis moves to perform (per particle) on the initial distribution. It is up to the user to determine if the desired distribution has been reached, i.e. by checking if results are independent of `metropolis_attempts`.

**symmetric\_interaction\_picture** type: boolean.

Optional. Default: true.

Use symmetric version of ip-dmcmc where now  $\hat{f}(\tau) = e^{-\frac{1}{2}(\beta-\tau)\hat{H}^0} e^{-\tau\hat{H}} e^{-\frac{1}{2}(\beta-\tau)\hat{H}^0}$ .

**Warning:** This feature is experimental and only tested for the 3D uniform electron gas.

**count\_diagonal\_occupations** type: boolean.

Optional. Default: false.

When performing **grand\_canonical\_initialisation**, instead of accumulating the number of walkers being added to the trace count the number of diagonal elements that are occupied. The original **grand\_canonical\_initialisation** would count the number of successful occupations which could lead to substantially more particles being added than the provided initial population. Generally only applicable when **initial\_matrix** is set to 'hartree\_fock'.

## operators options

**renyi2** type: boolean.

Optional. Default: false.

Calculate the Renyi-2 entropy of the entire system. Requires `replica_tricks` to be enabled.

**energy** type: boolean.

Optional. Default: false.

Calculate the thermal expectation value of the Hamiltonian operator.

**energy2** type: boolean.

Optional. Default: false.

Calculate the thermal expectation value of the Hamiltonian operator squared. Only available for the Heisenberg model.

**staggered\_magnetisation** type: boolean.

Optional. Default: false.

Calculate the thermal expectation value of the staggered magnetisation operator. Only available for the Heisenberg model and with bipartite lattices.

**excit\_dist** type: boolean.

Optional. Default: false.

Calculate the fraction of psips at each excitation level, where the excitation level is the number of excitations separating the two states labelling a given density matrix element. This fraction is then output to the data table at each report loop, and so the temperature-dependent excitation distribution is printed out.

This option should not be used with the **find\_weights** option, which averages the excitation distribution within the ground state.

**correlation** type: 2D vector of integers.

Optional. Default: false.

Calculate the spin-spin correlation function between the two specified lattice sites,  $i$  and  $j$ , which is defined as the thermal expectation value of:

$$\hat{C}_{ij} = \hat{S}_{xi}\hat{S}_{xj} + \hat{S}_{yi}\hat{S}_{yj} + \hat{S}_{zi}\hat{S}_{zj}.$$

Only available for the Heisenberg model.

**potential\_energy** type: boolean

Optional. Default: false

Evaluate the bare Coulomb energy. Only available for the UEG.

**kinetic\_energy** type: boolean

Optional. Default: false

Evaluate the kinetic energy. Only available for the UEG.

**H0\_energy** type: boolean

Optional. Default: false

Evaluate the thermal expectation value of the zeroth order Hamiltonian where  $\hat{H} = \hat{H}^0 + \hat{V}$ . See **initial\_matrix** option. Only available when using the ip-dmqlmc algorithm.

**HI\_energy** Evaluate the expectation value of the interaction picture Hamiltonian where

$$\hat{H}_I \left( \frac{1}{2}(\beta - \tau) \right) = e^{\frac{1}{2}(\beta - \tau)\hat{H}^0} \hat{H} e^{-\frac{1}{2}(\beta - \tau)\hat{H}^0}.$$

**mom\_dist** type: float

Optional. Default: 0.0

Evaluate the (spin averaged) momentum distribution in kspace, i.e.,  $\langle \hat{n}_{\mathbf{k}} \rangle$ , up to a maximum wavevector defined by kmax which is a multiple of the Fermi wavevector. The momentum distribution will be printed out at unique kpoints which have the same kinetic energy. Results can be extracted from the analysed (i.e. by using the finite\_temp\_analysis script in the tools/dmqlmc (see tutorial for more information)) dmqlmc output using the extract\_momentum\_correlation.py script in the tools/dmqlmc directory.

Only currently implemented for the UEG.

**structure\_factor** type: float

Optional. Default: 0.0

Evaluate the static structure factor:

$$S_{\sigma\sigma'}(q) = \frac{N_{\sigma}\delta_{\sigma\sigma'}}{N} + \frac{1}{N} \sum_{kp} \left\langle c_{k+q\sigma}^{\dagger} c_{p-q\sigma'}^{\dagger} c_{p\sigma'} c_{k\sigma} \right\rangle$$

up to a maximum wavevector defined by `qmax` which is a multiple of the Fermi wavevector. The static structure factor will be printed out at unique kpoints which have the same kinetic energy. Note that in the output file we actually print out  $S(q) - 1$ ,  $S_{\uparrow\uparrow}(q) + S_{\downarrow\downarrow}(q) - 1$  and  $S_{\uparrow\downarrow}(q) + S_{\downarrow\uparrow}(q)$ , where  $S(q) = \sum_{\sigma\sigma'} S_{\sigma\sigma'}$ . Results can be extracted from the analysed (i.e. by using the `finite_temp_analysis` script in the `tools/dmqmc` (see tutorial for more information)) `dmqmc` output using the `extract_momentum_correlation.py` script in the `tools/dmqmc` directory. The extraction script takes care of the factors of 1.

Currently only implemented for the UEG.

## rdm options

Note that the use of RDMs is currently only available with the Heisenberg model.

**rdms** type: table of 1D vectors.

Required.

Each vector corresponds to the subsystem of a reduced density matrix as a list of the basis function indices in the subsystem. For example:

```
rdms = { { 1, 2 } }
```

specifies one RDM containing basis functions with indices 1 and 2, and

```
rdms = { { 1, 2 }, { 3, 4 } }
```

specifies two RDMs, with the first containing basis functions with indices 1 and 2, and the second basis functions 3 and 4.

Either `instantaneous` or `ground_state` must be enabled to set the desired mode of evaluating the RDM (but both options cannot be used together).

**instantaneous** type: boolean.

Optional. Default: false.

Calculate the RDMs at each temperature based upon the instantaneous `psip` distribution.

Cannot be used with the `ground_state` option (either `ground_state` or `instantaneous` RDMs can be calculated, but not both concurrently).

**ground\_state** type: boolean.

Optional. Default: false.

Accumulate the RDM once the ground state (as specified by `ground_state_start`) is reached. This has two limitations: only one RDM can be accumulated in a calculation and the subsystem should be at most half the size of the system (which is always sufficient for ground-state calculations).

Cannot be used with the `instantaneous` option (either `ground_state` or `instantaneous` RDMs can be calculated, but not both concurrently).

**spawned\_state\_size** type: integer.

Required if `instantaneous` is true. Ignored otherwise.

Maximum number of states (i.e. reduced density matrix elements) to store in the “spawned” list, which limits the number of unique RDM elements that each processor can set. Should be a sizeable fraction of `state_size` (see *qmc options*) and depends on the size of the subsystem compared to the full space.

---

**Note:** This is a **per processor** quantity. It is usually safe to assume that each processor has approximately the same number of states.

---

**ground\_state\_start** type: integer.

Optional. Default: 0.

Monte Carlo cycle from which the RDM is to be accumulated in each beta loop. Relevant only if `ground_state` is set to true and, as such, should be set to an iteration (which is a measure of temperature) such that the system has reached the ground state.

**concurrency** type: boolean.

Optional. Default: false.

Calculate the unnormalised concurrency and the trace of the reduced density matrix at the end of each beta loop. The normalised concurrency can be calculated from this using the `average_entropy.py` script.

Valid for `ground_state` only; temperature-dependent concurrency is not currently implemented.

**renyi2** type: boolean.

Optional. Default: false.

Calculate the Renyi-2 entropy of each subsystem. More accurately, the quantity output to the data table is  $S_2^n = \sum_{ij} (\rho_{ij}^n)^2$ , (which differs from the Renyi-2 entropy by a minus sign and a logarithm) where  $\rho^n$  is the reduced density matrix of the  $n$ -th subsystem. The temperature-dependent estimate of the Renyi-2 entropy can then be obtained using the `finite_temp_analysis.py` script.

Valid for `instantaneous` only; ground-state Renyi-2 averaged over a single beta loop is not currently implemented. Requires `replica_tricks` to be enabled in order to obtain unbiased estimates.

**von\_neumann** type: boolean.

Optional. Default: false.

Calculate the unnormalised von Neumann entropy and the trace of the reduced density matrix at the end of each beta loop. The normalised von Neumann entropy can be calculated from this using the `average_entropy.py` script.

Valid for `ground_state` only; temperature-dependent von Neumann entropy is not currently implemented.

**write** type: boolean.

Optional. Default: false.

Print out the ground-state RDM to a file at the end of each beta loop. The file contains the trace of the RDM in the first line followed by elements of the upper triangle of the RDM labelled by their index.

Valid for `ground_state` only.

**ref\_projected\_energy** type: boolean.

Optional. Default: false.

Calculate the numerator and denominator for the projected energy as well as the total walker population for the reference row (or column) of the density matrix. Currently only available for read in systems.

## Full Configuration Interaction Quantum Monte Carlo (simple)

Find the ground state of a system via FCIQMC [Booth09].

```
simple_fciqmc {  
  sys = system,  
  sparse = true/false,  
  qmc = { ... },  
  restart = { ... },  
  reference = { ... },  
  qmc_state = qmc_state,  
}
```

**Returns:** a qmc\_state object.

`simple_fciqmc` performs a full configuration interaction quantum Monte Carlo (FCIQMC) calculation on a system using an explicitly calculated and stored Hamiltonian matrix.

**Warning:** This is an **extremely** simple implementation of FCIQMC. In particular it makes no effort to be efficient (in time or memory), is not parallelised, and does not include any advanced features. It is, however, useful for educational purposes and (occasionally) hacking experimental ideas quickly. Do **not** use for production calculations.

## Options

**sys** type: system object.

Required.

The system on which to perform the calculation. Must be created via a system function.

**sparse** type: boolean.

Optional. Default: true.

Store the Hamiltonian matrix in a sparse matrix format.

**qmc** type: lua table.

Required.

Further options that are common to all implemented QMC algorithms. Note that options relating to memory usage, excitation generation and real amplitudes are not implemented for `simple_fciqmc`. See [qmc options](#).

**restart** type: lua table.

Optional.

Further options to control restarting the calculation from a previous calculation. See [restart options](#).

**reference** type: lua table.

Optional.

Further options to select the reference state used. See [reference options](#).



**qmc\_state** type: qmc\_state object.

Optional.

Output of a previous calculation to resume.

**Warning:** The qmc\_state object must have been returned by a previous simple FCIQMC calculation. The validity of this is not checked. The system must also be unchanged.

**Warning:** This destroys the qmc\_state object and so it cannot be re-used in subsequent QMC calculations.

## MP1 wavefunction

```
psip_list = mpl_mc {
  sys = system,
  mp1 = {...},
  qmc = {...},
  ccmc = {...},
}
```

**Returns:** a particle\_t object.

mpl\_mc creates a deterministic MP1 wavefunction and stochastically coarse-grains (rounds down small amplitudes) it into a particle\_t object that can be used to initialise a subsequent CCMC calculation. The MP1 wavefunction will be ignored if restarting from a restart file.

## Options

**sys** type: system object.

Required.

The system on which to perform the calculation. Must be created via a system function.

**mp1** type: lua table.

Required.

Further options controlling the calculation.

**qmc** type: lua table.

Optional.

If provided, will override the mp1 input options where relevant.

**ccmc** type: lua table.

Optional.

If provided, will override the mp1 input options where relevant.

---

**Note:** If you wish to chain together a MP1 calculation and a CCMC calculation, one way to do it would be:

```
sys = {...}
qmc_opt = {...}
ccmc_opt = {...}

psip_list = mpl_mc{
    sys = sys,
    qmc = qmc_opts,
    ccmc = ccmc_opts,
}

ccmc {
    sys = sys,
    qmc = qmc_opts,
    ccmc = ccmc_opts,
    psip_list = psip_list,
    reference = {...},
}
```

Note the lack of commas after the main tables. This makes sure the MPI wavefunction (the `psip_list` object) is compatible with the subsequent CCMC calculation.

---

## MP1 options

**D0\_population** type: integer.

Required.

Set the initial population on the reference determinant.

---

**Note:** This will overwrite the value given in the `qmc` table.

---

**state\_size** type: integer.

Maximum number of excitors to store in the “main” list, which holds the number of particles on the state and related information such as the diagonal Hamiltonian matrix element. The number of elements that can be stored usually should be of the same order as the target population.

If negative, then the absolute value is used as the maximum amount of memory in MB to use for this information.

---

**Note:** This will overwrite the value given in the `qmc` table.

---

**real\_amplitudes** type: boolean.

Optional. Default: false.

Allow amplitudes to take non-integer weights. This will often significantly reduce the stochastic noise in the Monte Carlo estimates.

---

**Note:** This should be the same as the subsequent calculation.

---

**spawn\_cutoff** type: float.

Optional. Default: 0.01.

The threshold for stochastic rounding.

**rng\_seed** type: integer.

Optional. Default: generate a seed from a hash of the time and calculation UUID.

The seed used to initialise the random number generator.

**even\_selection** type: boolean.

Optional. Default: false.

---

**Note:** Must be true if true in the subsequent CCMC calculation.

---

## Common options

The following settings are common to multiple QMC algorithms. See the individual calculation documentation for *Full Configuration Interaction Quantum Monte Carlo*, *Coupled Cluster Monte Carlo* and *Density Matrix Quantum Monte Carlo* for details on how to perform the calculations as well as the documentation for each set of common options.

### qmc options

The following options in the `qmc` table are common to the FCIQMC, CCMC and DMQMC algorithms and control the core settings in the algorithms.

**tau** type: float.

Required.

The timestep to use.

A small timestep causes the particles sampling the wavefunction/matrix to evolve very slowly. Too large a timestep, on the other hand, leads to a rapid particle growth which takes a long time to stabilise, even once the shift begins to vary, and coarse population dynamics.

**init\_pop** type: float.

Required unless the calculations is initialised from a restart file or `qmc_state`.

Set the initial population on the reference determinant. For DMQMC calculations this option sets the number of psips which will be randomly distributed along the diagonal at the start of each beta loop.

**mc\_cycles** type: integer.

Required.

Number of Monte Carlo cycles to perform per “report loop”.

**nreports** type: integer.

Required.

Number of “report loops” to perform. Each report loop consists of `mc_cycles` cycles of the QMC algorithm followed by updating the shift (if appropriate) and output of information on the current state of the particle populations, including terms in the energy estimators.

**state\_size** type: integer.

Required unless `qmc_state` is given.

Maximum number of states (i.e. determinants, excitors or density matrix elements) to store in the “main” list, which holds the number of particles on the state and related information such as the diagonal Hamiltonian matrix element. The number of elements that can be stored usually should be of the same order as the target population.

If negative, then the absolute value is used as the maximum amount of memory in MB to use for this information.

Ignored if `qmc_state` is given.

---

**Note:** This is a **per processor** quantity. It is usually safe to assume that each processor has approximately the same number of states.

---

**spawned\_state\_size** type: integer.

Required unless `qmc_state` is given.

Maximum number of states (i.e. determinants, excitors or density matrix elements) to store in the “spawned” list, i.e. the maximum number of states which can be spawned onto at a given timestep. The amount of memory required for this is usually a small fraction of that required for `state_size`, unless `real_amplitudes` is in use, in which case this should be a sizeable fraction (or potentially even greater than the memory for `state_size`, if load balancing of states across processors is poor). The amount of memory required is also dependent on the value of `tau`.

If negative, then the absolute value is used as the maximum amount of memory in MB to use for this information.

Ignored if `qmc_state` is given.

---

**Note:** This is a **per processor** quantity. It is recommended that a short trial calculation is run and the spawning rate for the desired timestep examined in order to estimate a reasonable value for `spawned_state_size`.

---

**rng\_seed** type: integer.

Optional. Default: generate a seed from a hash of the time and calculation UUID.

The seed used to initialise the random number generator.

**target\_population** type: float.

Optional. Default: none.

Set the target number of particles to be reached before the shift is allowed to vary. This is only checked at the end of each report loop. Once the `target_population` is reached, the shift is varied according to

$$S(\tau) = S(\tau - A\delta\tau) - \frac{\zeta}{A\delta\tau} \ln \left( \frac{N_w(\tau)}{N_w(\tau - A\delta\tau)} \right)$$

where  $S$  is the shift,  $\tau$  the current imaginary time,  $\delta\tau$  the timestep,  $A$  `mc_cycles`,  $\zeta$  `shift_damping`, and  $N_w$  the number of particles (walkers).

**reference\_target** type: float.

Optional. Default: none.

Set a target reference population to be reached before the shift is allowed to vary. Cannot be used in conjunction with `target_population`.

**real\_amplitudes** type: boolean.

Optional. Default: false.

Allow amplitudes to take non-integer weights. This will often significantly reduce the stochastic noise in the Monte Carlo estimates.

Automatically enabled if semi-stochastic is used.

---

**Note:** Real amplitudes are handled using fixed precision and so numbers which can not be exactly represented are stochastically rounded to values that can be stored.

The preprocessor option POP\_SIZE=32 (default) uses 32-bit integers to store the amplitudes and stores amplitudes to within a precision/resolution of  $2^{-11}$  and to a maximum absolute population of  $2^{20}$ .

Consider using the preprocessor option POP\_SIZE=64 to allow a greater range of amplitudes to be encoded (precision of  $2^{-31}$  and maximum absolute population of  $2^{32}$  at the cost of doubling the memory required to store the amplitudes.

By default uses integer weights, i.e. with the minimum resolution of 1.

---

**real\_amplitude\_force\_32** type: boolean.

Optional. Default: false.

Force the precision of the real amplitudes to that used for POP\_SIZE=32 irrespective of the actual POP\_SIZE compile-time parameter.

---

**Note:** The main use-case for this is reproducing results produced by binaries compiled using POP\_SIZE=32 with binaries compiled using POP\_SIZE=64; it is not intended for use in production calculations.

---

**spawn\_cutoff** type: float.

Optional. Default: 0.01 if `real_amplitudes` is used, 0 otherwise.

The minimum absolute value for the amplitude of a spawning event. If a spawning event with a smaller amplitude occurs then its amplitude will probabilistically be rounded up to the cutoff or down to zero in an unbiased manner. A spawning event with an amplitude above the cutoff is stochastically rounded such that it can be stored in a fixed precision value. If `real_amplitudes` is not in use, the fixed precision corresponds to unit values.

Only relevant when using `real_amplitudes`.

**excit\_gen** type: string

Optional. Default: system dependent.

Possible values are system dependent (alternative, deprecated names in bracket):

System	Implemented	Default
chung	renorm, no_renorm	renorm
heisenberg	renorm, no_renorm	renorm
hubbard_k	renorm, no_renorm	renorm
hubbard_real	renorm, no_renorm	renorm
read	irenorm, no_renorm, renorm_spin, no_renorm_spin, heat_bath, heat_bath_uniform_singles (heat_bath_uniform), heat_bath_exact_singles (heat_bath_single), uniform_power_pitzer (power_pitzer_orderM), heat_bath_power_pitzer (power_pitzer_orderM_ij), heat_bath_power_pitzer_ref (power_pitzer_orderN), uniform_cauchy_schwarz (cauchy_schwarz_orderM), heat_bath_cauchy_schwarz (cauchy_schwarz_orderM_ij)	renorm
ringium	no_renorm	no_renorm
ueg	no_renorm, power_pitzer	no_renorm

The type of excitation generator to use. Note that not all types are implemented for all systems, usually because a specific type is not suitable for (large) production calculations or not feasible or useful.

The ‘renorm’ generator requires orbitals to be selected such that a valid excitation is possible, e.g. for a double excitation  $(i, j) \rightarrow (a, b)$ , the combination  $i, j, a$  is only selected if there exists at least one unoccupied orbital for  $b$  which conserves any symmetry and spin quantum numbers. This is efficient in terms of generating allowed excitations but involves an expensive renormalisation step. The ‘no\_renorm’ generator lifts this restriction at the cost of generating (and subsequently rejecting) such excitations; the excitation generation is consequently much faster. In general, ‘renorm’ is a good choice for small basis sets and ‘no\_renorm’ is a good choice for large basis sets, especially with a small number of electrons (such that forbidden excitations are rarely generated). ‘renorm\_spin’ and ‘no\_renorm\_spin’ are very similar to ‘renorm’ and ‘no\_renorm’ respectively but when selecting  $i$  and  $j$ , they first decide with probability `pattempt_parallel` whether  $i$  and  $j$  should have parallel spins or not. The idea is by Alavi and co-workers, see [Booth09] and [Booth14] for example for more details on these excitation generators.

Note that the implementations of the weighted excitation generators here are all described in [Neufeld19].

The ‘heat\_bath’ excitation generator is very similar to the “original” heat bath excitation generator described by Holmes et al. [Holmes16].  $i, j, a, b$  are chosen with weighted, precalculated probabilities that aim to make  $|H_{ij}|/p_{\text{gen}}$  as constant as possible. The difference to Holmes et al. is that we never do a single and a double excitation at the same time. When Holmes et al. decide to do both, we do a single excitation with probability of 0.5 and a double with 0.5. The ‘heat\_bath’ excitation generator can have a bias if for a valid excitation  $i$  going to  $a$ , there might be no occupied  $j$  that lets us select  $ija$ . See Holmes et al. for details. We check for the bias in the beginning of a calculation and stop it if necessary. The Cauchy-Schwarz ([Smartunpub], described in [Blunt17]) and Power-Pitzer excitation generators use approximate upper bounds for these weights. A version of Cauchy-Schwarz excitation generators is described in [Schwarz] but the weights used here and the implementation differ. Here, Cauchy-Schwarz uses Coulomb integrals and Power-Pitzer uses exchange integrals to approximate weights. ‘heat\_bath\_uniform\_singles’ is very similar to ‘heat\_bath’ but samples single excitations uniformly (mentioned by Holmes et al.) and ‘heat\_bath\_exact\_singles’ is also very similar but samples single excitations with the correct weighting (following a recommendation by Pablo Lopez Rios). ‘heat\_bath\_uniform\_singles’ and ‘heat\_bath\_exact\_singles’ do not have this potential bias that ‘heat\_bath’ can have.

Some of the Power-Pitzer excitation generators use elements of the heat-bath excitation generators ([Holmes16]) and their approximations for selecting  $a$  and  $b$  are inspired by the Cauchy-Schwarz excitation generators by Alavi and co-workers [Smartunpub]. See more details on all these weighted excitations generator in Ref. [Neufeld19].

The ‘power\_pitzer’ excitation generator generates double excitations using a Power-Pitzer [Power74] upper bound for the value of the Hamiltonian matrix element,  $|\langle ij|ab\rangle|^2 \Rightarrow \langle ia|ai\rangle\langle jb|bj\rangle (|\langle ij|ab\rangle|^2 \Rightarrow \langle ia|ia\rangle\langle jb|jb\rangle$  for Cauchy-Schwarz excitation generators). This involves some precalculated weights and alias tables, but should reduce both noise and shoulder heights. The weights to select a certain excitation are calculated for the reference in the beginning of the QMC calculation. Each time the excitation generator is called, the weights are mapped from the reference to the actual determinant we attempt a spawn from. Only available for the UEG and read\_in systems. The time spent in this excitation generator scales as  $\mathcal{O}(N)$ , where  $N$  is the number of electrons and the memory requirements are  $\mathcal{O}(NM)$ , where  $M$  is the number of basis functions. Single excitations are done uniformly.

‘uniform\_power\_pitzer’ uses a more refined upper bound for the Hamiltonian matrix elements, where the weights for selecting an excitation are calculated each time the excitation is called for the actual determinant we are spawning from. This requires  $\mathcal{O}(M)$  time cost for each particle being spawned from. The memory requirements are of  $\mathcal{O}(M)$ . ‘heat\_bath\_power\_pitzer’ is similar to ‘uniform\_power\_pitzer’ but samples selects  $i$  and  $j$  similarly to the heat bath excitation generators. The memory cost is  $\mathcal{O}(M^2)$ . ‘uniform\_cauchy\_schwarz’ is similar to ‘uniform\_power\_pitzer’ and ‘heat\_bath\_cauchy\_schwarz’ is similar to ‘heat\_bath\_power\_pitzer’, the distinction being the types of weights used to select  $ab$ .

The ‘heat\_bath\_power\_pitzer\_ref’ excitation generator [Neufeld19] uses precalculated weights and unlike ‘uniform\_power\_pitzer’, it also samples  $i$  and  $j$  with weighted probabilities. It also samples single excitations in a weighted manner. Its memory cost is  $\mathcal{O}(M^2)$ . This excitation generator can be use-

ful in single-referenced systems when doing CCMC especially where the basis set size gets too big for ‘heat\_bath\_power\_pitzer’ and ‘heat\_bath\_uniform\_singles’. The computational scaling is also more favourable than with ‘heat\_bath\_power\_pitzer’.

In the case of the UEG, the ‘power\_pitzer’ excitation generator pre-calculates Power-Pitzer like weights for the selecting of orbital  $a$ .  $i$  and  $j$  are selected like the ‘no\_renorm’ UEG excitation generator. If  $a$  is occupied, the excitation is forbidden.

---

**Note:** Our current advice for selecting an excitation generator to use with read\_in systems [Neufeld19]: First consider the ‘heat\_bath’ excitation generator. A bias test will be run at the beginning of the calculation then. If the bias test fails, try ‘heat\_bath\_uniform\_singles’. If ‘heat\_bath’ and/or ‘heat\_bath\_uniform\_singles’ fail due to memory constraints, try ‘heat\_bath\_power\_pitzer\_ref’. Note that only ‘heat\_bath’ requires a bias test.

---



---

**Note:** The Cauchy-Schwarz excitation generators are not implemented for complex read\_in systems.

---



---

**Note:** Currently only the no\_renorm and renorm excitation generators are available in DMQMC.

---

**power\_pitzer\_min\_weight** type: float.

Optional. Default: 0.01.

Only used in ‘power\_pitzer\_orderN’ excitation generator or in ‘read\_in’ systems if the ‘power\_pitzer’ excitation generator is used. This number (approximately) sets the minimum value of  $\text{weight}(\text{orbital to excite to})/(\text{total weights times number of orbitals to excite to})$ . The aim of this is to reduce the number of spawns with larger  $|H_{ij}|/p_{\text{gen}}$  which can happen if orbital connections with small values of  $p_{\text{gen}}$  are mapped to orbital connections with large values of  $|H_{ij}|$ .

**pattempt\_single** type: float.

Optional. Default: use the fraction of symmetry-allowed excitations from the reference determinant that correspond to single excitations.

The probability of generating a single excitation.

**pattempt\_double** type: float.

Optional. Default: use the fraction of symmetry-allowed excitations from the reference determinant that correspond to double excitations.

The probability of generating a double excitation.

---

**Note:** If `pattempt_single` and `pattempt_double` do not sum to 1, we renormalize them.

---

**pattempt\_update** type: boolean.

Optional. Default: False.

If true, then `pattempt_single` is varied during the run to attempt to align the means of  $|H_{ij}|/p_{\text{gen}}$  for single and double excitations. Mentioned in [Holmes16]. Update of `pattempt_single` only happens if shift has not started varying yet. Not applicable to “original” heat bath algorithm excitation generator (`excit_gen=“heat_bath”`). When restarting a calculation, if `pattempt_update` is set to true and both `pattempt_single` and `pattempt_double` are specified by the user, previous update information is lost and the update (provided shift has not started varying yet) starts from scratch (the information to update `pattempt_single` from previous runs is lost). If `pattempt_single` or `pattempt_double` are in

danger of getting too small, they will be set to 1/the number of allowed spawn attempts needed before they are updated again which is 10000 currently. A warning will be printed “WARNING: min. pattempt\_single/double!” if that is the case. Do make sure that before accepting a final pattempt\_single or pattempt\_double, this warning will have not been printed for a while.

---

**Note:** Currently not available in DMQMC.

---



---

**Note:** By the way we set the minimum values for pattempt\_single and pattempt\_double, the minimum value for these is 0.0001. If that is too high, consider setting them manually by specifying both (only one is not sufficient) in the input file.

---

**pattempt\_zero\_accum\_data** type: boolean.

Optional. Default: false.

If true and restarting a calculation, accumulated data needed to update pattempt\_single and pattempt\_double is reset (set to zero, overflow boolean is set to false). Only to be used together with pattempt\_update. Only to be used by experienced users.

**pattempt\_parallel** type: float.

Optional. Default: Estimate it using  $\frac{\sum_{i \parallel j \parallel ab} |H_{ijab}|}{\sum_{ijab} |H_{ijab}|}$ , where  $i \parallel j \parallel$  indicates  $i, j$  are restricted to having parallel spins.

Probability that  $i, j$  have parallel spins. Only to be used with excit\_gen == ‘no\_renorm\_spin’ and ‘renorm\_spin’.

Cannot be bigger than 1 and if negative, the default estimate is applied. It is recalculated in the beginning of each (restarted) calculation.

**initial\_shift** type: float.

Optional. Default: 0.0.

The initial value of the shift.

**shift\_damping** type: float.

Optional. Default: 0.05.

The shift damping factor,  $\zeta$ . This can be optimised using the auto\_shift\_damping keyword (see [blocking options](#)). On restarting the final value in the previous calculation will replace the usual default value if shift\_damping is not specified.

**shift\_harmonic\_forcing** type: float.

Optional. Default: 0.0.

The restoring force factor  $\xi$  in the improved shift update procedure from [Yang20]:

$$S(\tau) = S(\tau - A\delta\tau) - \frac{\zeta}{A\delta\tau} \ln \left( \frac{N_w(\tau)}{N_w(\tau - A\delta\tau)} \right) - \frac{\xi}{A\delta\tau} \ln \left( \frac{N_w(\tau)}{N_t} \right)$$

where  $N_t$  is the target population.

**shift\_harmonic\_crit\_damp** type: boolean.

Optional. Default: false.

If true, the shift\_harmonic\_forcing term will be set equal to the square of the shift\_damping term divided by 4 to obtain critical damping. If true, shift\_harmonic\_forcing will be ignored.



**shift\_harmonic\_forcing\_two\_stage** type: boolean.

Optional. Default: false.

A non-zero `shift_harmonic_forcing` factor allows the shift to be varied from the start of the calculation. However this would mean the target population is reached more slowly as more death events occur. If false, shift is varied from the start of the calculation, otherwise shift is only varied (with harmonic forcing turned on) when target population is reached.

**vary\_shift\_from**

type: float or string.

Optional. Default: `initial_shift`.

Specify a value to set the shift to when `target_population` is reached. If the string 'proje' is specified then the instantaneous projected energy is used. By instantly setting the shift to a value closer to the correlation energy, the total population can be stabilised substantially faster.

There is no guarantee that the instantaneous projected energy is a good estimate of the ground state (particularly in the real-space formulation of the Hubbard model), but it is likely to be closer to it than the default shift value of 0.

**initiator** type: boolean.

Optional. Default: false.

Enable the initiator approximation (FCIQMC: [Cleland10]; CCMC: [Spencer15]; DMQMC: [Malone16]) in which spawned particles are only kept if they are created onto states which already have a non-zero population, or were produced by states which are already highly occupied (see `initiator_threshold`), or multiple spawning events onto a previously unoccupied state occurred in the same timestep.

---

**Note:** The initiator approximation should be considered experimental for CCMC and DMQMC (see `initiator_level` option for DMQMC).

---

<p><b>Warning:</b> The initiator approximation is non-variational (due to the non-variational energy estimator used) and the error should be carefully converged by performing repeated calculations with increasing <code>target_population</code> values.</p>
---

**initiator\_threshold** type: float.

Optional. Default: 3.0.

Set the (absolute) population above which a state is considered to be an initiator state. A value of 0 is equivalent to disabling the initiator approximation.

**quadrature\_initiator** type: logical.

Optional. Default: true.

The initiator approximation in a complex spaces could be applied in (at least) two different ways. If this parameter is true, the magnitude of the instantaneous complex coefficient at each site is used to determine initiator properties for both real and imaginary parents.

If this parameter is false, the magnitude of the real and imaginary populations are compared separately and initiator flags for real and imaginary set individually.

---

**Note:** The comparative efficacy of these two approaches is currently under investigation.

---

**quasi\_newton** type: boolean.

Optional. Default: False.

Turn on quasi-Newton steps. Conventional FCIQMC and related methods take steps which are the equivalent of a scaled steepest-descent approach, which results in very long equilibration times, and requires smaller values of tau for stability. The quasi-Newton approach (partially) scales the steps according to the inverse difference in Fock energy to the reference determinant, reducing the contributions from very high-energy determinants.

For more details see V. A. Neufeld, A. J. W. Thom, JCTC (2020), 16, 3, 1503-1510.

---

**Note:** Not currently available for DMQMC. Due to Fock value calculations, only supported for read\_in systems and the 3D uniform electron gas. For semistochastic FCIQMC, determinants in the deterministic space are given weighting 1.

---

**quasi\_newton\_threshold** type: float.

Optional. Default: Energy difference between LUMO and HOMO.

Used when `quasi_newton` is true. The quasi-Newton approach (partially) scales the steps according to the inverse difference in Fock energy to the reference determinant (with Fock energy  $F_0$ ) for each determinant. Any determinant with energy less than  $F_0 + \Delta_{\text{QN}}$ , where  $\Delta_{\text{QN}}$  is the value given to `quasi_newton_threshold`, will have weighting  $v_{\text{QN}}^{-1}$ , where  $v_{\text{QN}}$  is the value given by `quasi_newton_value`. The shift containing term in the death step are scaled by `quasi_newton_pop_control` instead. This makes sure that that term is scaled by a constant, independent of the determinant/excitor involved, so that the energy does not diverge with fluctuations around the true energy.

For more details see V. A. Neufeld, A. J. W. Thom, JCTC (2020), 16, 3, 1503-1510.

**quasi\_newton\_value** type: float.

Optional. Default: `quasi_newton_threshold`.

See `quasi_newton_threshold`.

**quasi\_newton\_pop\_control** type: float

Set to 1 for original/non quasi-Newton propagation and otherwise for quasi-Newton, the default is  $1/\text{quasi\_newton\_threshold}$ .

See `quasi_newton_threshold`.

**tau\_search** type: boolean.

Optional. Default: false. Not currently implemented in DMQMC.

Update the timestep, `tau`, automatically if by scaling it by 0.95 if a bloom event is detected. A bloom event is defined as one which spawns more than three particles in a single spawning event in FCIQMC and one which spawns more than 5% of the total current population in a single spawning event in CCMC.

---

**Note:** Experimental option. Feedback on required flexibility or alternative approaches is most welcome.

---

**use\_mpi\_barriers** type: boolean.

Optional. Default: false.

Perform MPI\_Barrier calls before the main MPI communication calls (both for communication of the spawned list, and any semi-stochastic communication). These are timed, and the total time spent in these calls is reported at the end of a simulation. This is useful for assessing issues in load balancing, as it will allow you to see when

certain processors take longer to perform their work than others. This is turned off by default because such calls may have an initialisation time which scales badly to many processors.

**vary\_shift** type: boolean.

Optional.

If present, overrides any value of `vary_shift` set by a previous calculation contained either in a restart file or a `qmc_state` object. If set to true, the shift is set to `initial_shift`.

---

**Note:** The shift will still be varied when `target_population`, if set, is reached.

---

**Warning:** If reading in from a restart file and `vary_shift = false`, the shift will be set to `initial_shift` for the first iteration, which defaults to zero. Leave it unset if this is not intended.

**shift\_harmonic\_forcing** type: float.

Optional. Default: 0.00

If present, this sets the restoring force factor value in the harmonic population control algorithm. This differs from the canonical two-step population control by an additional term based on the target population, as follows

$$S(t) = S(t - A\tau) - \frac{\xi}{A\tau} \log \left( \frac{N_p(t)}{N_p(t - A\tau)} \right) - \frac{\zeta}{A\tau} \log \left( \frac{N_p(t)}{N_t} \right)$$

where  $S$  is the shift,  $t$  the current imaginary time,  $\tau$  the timestep,  $A$  `mc_cycles`,  $\xi$  `shift_damping`,  $\zeta$  is the restoring force factor described here,  $N_p$  the number of particles and  $N_t$  is the target population.

For more details see M. Yang, E. Pahl and J. Brand, J. Chem. Phys. 153, 174103 (2020) (DOI:10.1063/5.0023088).

---

**Note:** The original population control algorithm is obtained if set equal to zero.

---



---

**Note:** When used, the shift will vary throughout the entire simulation, even if the target population has not been reached.

---



---

**Note:** The harmonic population control algorithm will not work with target populations less than or equal to zero.

---

**shift\_harmonic\_crit\_damp** type: boolean.

Optional. Default: false.

If set to true, the value of `shift_harmonic_forcing` will be set to the square of `shift_damping` divided by four to obtain critical damping.

**chebyshev** type: lua table or boolean.

Optional. Default: false.

Input options (or switch) relating to the wall-Chebyshev projector ([Zhang16]). If set to true, then the default options of `chebyshev_order = 5`, `chebyshev_shift = 0.0`, `chebyshev_scale = 1.1`, `skip_gershgorin = false` are used.

**chebyshev\_order** type: integer.

Optional. Default: 5.

The order of the Chebyshev expansion of the wall function. The theoretical speed up compared to the linear projector with the largest allowable  $\delta\tau$  is  $(m + 1)/3$ .

**chebyshev\_shift, chebyshev\_scale** type: float.

Optional. Default: 0.0 and 1.1.

For the estimated highest eigenvalue of the Hamiltonian,  $E_{N-1}$ ,  $E_{N-1} = (E_{N-1} + a) * b$ , where  $a$  is the shift and  $b$  is the scale.

**skip\_gershgorin** type: boolean.

Optional. Default: false.

As the estimation of the highest eigenvalue by the Gershgorin circle theorem requires summing entries in the highest row of the Hamiltonian, this could be time consuming. If `true`, then only the highest diagonal element is used as the estimate, which can then be modified with the shift and scale parameters above.

## reference options

The `reference` table contains options used to control the Hilbert space used in the calculation and trial function for the projected estimator.

**det** type: vector of integers.

Optional. Default: a simple (but potentially not optimal) guess which satisfies the spin and, if provided, symmetry options using the Aufbau principle. In most cases the default (which for molecules typically corresponds to the Hartree–Fock determinant) is sufficient.

Specify the determinant (as a list of indices corresponding to occupied single-particle orbitals) to be used as the reference determinant, which is used in the trial function for calculating the projected energy estimator. Typically this should be the determinant expected to have the greatest overlap with the desired wavefunction.

**hilbert\_space\_det** type: vector of integers.

Optional. Default: set to `det`.

Specify the determinant (as a list of indices corresponding to occupied single-particle orbitals) used to generate the Hilbert space. Using different determinants to control the Hilbert space and the trial function allows, for example, spin-flip calculations to be performed.

---

**Note:** Only relevant if the Hilbert space is not equivalent to the FCI space, i.e. `ex_level` is smaller than the number of electrons in the system.

---

**ex\_level** type: integer.

Optional. Default: set to the number of electrons in the system (i.e. consider all determinants in the FCI space).

Maximum excitation level to consider relative to the determinant given by `hilbert_space_det`.

## restart options

The `restart` table contains options relating to checkpointing within QMC calculations.

HANDE currently uses one restart file per MPI rank with a filename of the form `HANDE.RS.X.pY.H5`, where `X` is the restart index and `Y` is the MPI rank.

**read** type: boolean or integer.

Optional. Default: false.

Start a QMC calculation from a previous calculation if `true` or an integer. If `true`, then the highest value of `X` is used for which a set of restart files exists, otherwise specifies the value of `X` to use.

---

**Note:** The calculation should be the same as the one that produced the output file, but it is possible to restart a calculation using an enlarged basis. The orbitals of the old (small) basis must correspond to the first orbitals of the new (larger) basis.

---

**write** type: boolean or integer.

Optional. Default: false.

Write out checkpointing files at the end of the calculation if `true` or an integer. If `true`, then the highest value of `X` is used for which a set of restart files doesn't exist, otherwise specifies the value of `X` to use.

**write\_shift** type: boolean or integer.

Optional. Default: false.

Write out checkpointing files when the shift is allowed to vary (i.e. once `target_population` is reached) if `true` or an integer. If `true`, then the highest value of `X` is used for which a set of restart files doesn't exist, otherwise specifies the value of `X` to use.

**write\_frequency** type: integer.

Optional. Default:  $2^{31} - 1$ .

Write out checkpointing files every  $N$  report loops, where  $N$  is the specified value.

---

**Note:** The index used for the restart files created with this option is the next unused index. Depending upon the frequency used, a large number of restart files may be created. As such, this option is typically only relevant for debugging or explicitly examining the evolution of the stochastic representation of the wavefunction.

---

**rng** type: boolean

Optional. Default: true.

Restart the state of the DSFMT random number generator from the previous calculation, allowing restarted calculations to follow the same Markov chain as if the entire series of calculations had been performed as a single calculation.

---

**Note:**

1. Calculations using OpenMP threads will not follow the same Markov chain due to the non-deterministic load balancing behaviour of the OpenMP implementation.
2. Restart files from older restart files do not contain the necessary information to recreate the RNG state. This option is ignored automatically in such cases.
3. Due to each processor using its own RNG stream, this functionality can only be used when restarting calculations on the same number of processors. Restart files created by the `redistribute` function will not contain RNG information as a result. This option is automatically ignored in such cases.
4. The presence of the RNG information in a restart file can be detected by running the command

```
$ h5dump -A -d rng/state <restart file>
```

where `<restart file>` is the appropriate filename, which will return some metadata information on the `rng/state` dataset if the RNG state is present and an error otherwise.

---

## semi\_stoch options

The semi-stochastic approach [Petruziolo12], [Blunt15] divides the Hilbert space into two regions: a small region in which the action of the Hamiltonian is applied exactly, and the remainder of the Hilbert space, in which the action is applied stochastically. This can substantially reduce the stochastic error in many cases.

**space** type: string.

Required.

Possible values: 'read', 'high', 'ci'.

The type of deterministic space to use. Using 'read' uses a deterministic space produced from a previous calculation and saved to file using the `semi_stoch write` option (the `write_determ_space` can be used but is now deprecated). Using 'high' sets the deterministic space to consist of the states with the highest population when the semi-stochastic projection is enabled. Using 'ci' sets the deterministic space to consist of a (small!) truncated configuration interaction space relative to a reference determinant.

**size** type: integer.

Required if `space` is 'high', otherwise ignored.

The number of states to include in the deterministic space.

**ci\_space** type: reference table. See [reference options](#) for options.

Required if `space` is 'ci', otherwise ignored. Must contain at least `ex_level`. The reference determinant, if not supplied, is identical to that given in the calculation's `reference` option.

Defines the deterministic space to contain all determinants in a small (truncated) configuration interaction space.

**start\_iteration** type: integer.

Optional. Default: 1.

The number of iterations to perform, during which the action of the Hamiltonian is applied entirely stochastically, before semi-stochastic projection is enabled. This allows for a period for the population to grow and the ground-state wavefunction to emerge before the deterministic space is selected if `space` is set to 'high'.

---

**Note:** If the calculation is restarted from a previous one, this value refers to the iteration index of the entire set of calculations. If it is less than the iteration from which the calculation is started, semi-stochastic projection is enabled immediately.

---

**shift\_start\_iteration** type: integer.

Optional. Default: None. Overrides `start_iteration`.

The number of iterations to perform after the shift is varied (i.e. after the `target_population` is reached) before the semi-stochastic projection is enabled.

---

**Note:** If the calculation is restarted from a previous one and the shift is already varying, then semi-stochastic projection is enabled immediately.

---

**separate\_annihilation** type: boolean.

Optional. Default: true.

If true, the deterministic amplitudes are communicated separately at the cost of an additional MPI call. If false, the annihilation of particles created from deterministic and stochastic projections are performed together, which removes the need for an additional MPI call at the cost of communicating an additional  $\mathcal{O}(N_p N_D)$  more amplitudes, where  $N_p$  is the number of processors and  $N_D$  the size of the deterministic space. If the deterministic space is small and communication latency high, setting `separate_annihilation` to false might improve performance. For most systems and computer architectures, the default value is faster.

**write** type: boolean or integer.

Optional. Default: false.

Write out the deterministic space to file of form `SEMI.STOCH.X.H5`, where `X` is the file id. If set to true, `X` will be the smallest non-negative id such that `SEMI.STOCH.X.H5` does not already exist, otherwise the value provided is used as the file id.

**read** type: integer.

Optional. Default: largest value of `X` such that the file `SEMI.STOCH.X.H5` exists.

Index of the file containing the deterministic space produced from a previous calculation.

## logging options

The `logging` table contains options relating to outputting additional logs from QMC calculations.

Use of this functionality requires compiling HANDE with debug flags (using the `-g` option with `mkconfig`). This enables implementation of logging without having an appreciable impact upon timings of an optimised build.

This functionality is recommended for developers only. It should allow easy identification of the causes of any changes in Markov chain between two calculations.

Additional logging functionality can be added upon request. Current coverage is by no means complete.

---

**Note:** This functionality cannot be used with OpenMP parallelisation.

---

**calc** type: integer

Optional. Default: 0.

Determines level of logging output related to high-level behaviour within a calculation. Currently implemented levels are:

- 0 returns no extra information.
- 1 returns summary of events within a calculation (currently only for FCIQMC and CCMC).

Any information is produced in files `CALC.Y.pX.log` within the working directory, where `Y` is the same for all files produced in the same calculation and is set to the lowest value not present, and `X` is the process number.

**spawn** type: integer

Optional. Default: 0.

Determines level of logging output related to spawning within a calculation. Current levels are:

- 0 returns no extra information.
- **1 returns information on each spawning event creating at least one particle within a calculation** (currently only for FCIQMC and generic systems).
- **2 returns information on each spawning event within a calculation, regardless of result** (currently only for FCIQMC on generic systems and CCMC).

Any information is produced in files SPAWN.Y.pX.log within the working directory, where Y is the same for all files produced in the same calculation and is set to the lowest value not present, and X is the process number.

**death** type: integer

Optional. Default: 0.

Determines level of logging output related to death within a calculation. Current levels are:

- 0 returns no extra information.
- **1 returns information on each death or cloning event resulting in a change in particle number** within a calculation (currently only for FCIQMC and generic systems).
- **2 returns information on each death or cloning event within a calculation, regardless of result** (currently only for FCIQMC on generic systems and CCMC).

Any information is produced in files DEATH.Y.pX.log within the working directory, where Y is the same for all files produced in the same calculation and is set to the lowest value not present, and X is the process number.

**stoch\_selection** type: integer

Optional. Default: 0.

Determines level of logging output related to stochastic cluster selection within a ccmc calculation. Current levels are:

- 0 returns no extra information.
- **1 returns information on each stochastic selection attempt within a calculation resulting in a valid cluster** (only for CCMC).
- **2 returns information on each stochastic selection attempt within a calculation, regardless of validity of resulting cluster** (only for CCMC).

Any information is produced in files STOCH\_SELECTION.Y.pX.log within the working directory, where Y is the same for all files produced in the same calculation and is set to the lowest value not present, and X is the process number.

**start** type: integer

Optional. Default: 0.

Defines the iteration from which logging information should be produced.

**finish** type: integer

Optional. Default:  $2^{31} - 1$ .

Defines the iteration after which logging information should cease to be produced.



## output options

The `output` table contains options relating to directing calculation output. This is currently only compatible with *Full Configuration Interaction Quantum Monte Carlo*, *Coupled Cluster Monte Carlo* and *Monte Carlo estimate of size of the Hilbert space*, though extension to other calculations would be relatively simple.

**filename** type: string.

Optional. Default: 'stdout'.

Filename to write any calculation output to. If set to default value, all calculation information is printed to stdout.

**reprint\_sys** type: boolean.

Optional. Default: true.

If true all information on system single particle basis and symmetry that would usually be printed during initialisation is also reprinted at the head of any output file. This is useful when identifying what system a calculation was performed on a while later.

## blocking options

The `blocking` table contains options used to control the options for performing blocking analysis on the fly.

**blocking\_on\_the\_fly** type: boolean.

Optional. Default: false

If true, the data for blocking analysis is collected every report loop and blocking analysis is performed on the fly while the calculation is running. At the end of the calculation, Estimated correlation energy and its error together with reference energy is printed to the HANDE output file. Zero is printed if insufficient data are collected for the blocking analysis.

**start\_save\_frequency** type: integer.

Optional. Default: -1

Log2 of the frequency at which the potential start points of the blocking analysis is saved. When negative, the frequency is the nearest integer to the  $\log_2(\text{nreports}) - 8$ .

**start\_point\_number** type: integer.

Optional. Default: -1

Number of potential start points of the blocking analysis that is to be saved. If negative, the integer part of  $\text{nreports}/2^{(\text{start\_save\_frequency})}$ .

**filename** type: string.

Optional. Default: 'BLOCKING'

Filename to which the blocking analysis report is written.

**start\_point** type: integer.

Optional. Default: -1

The iteration number from which the data for blocking analysis is collected. When negative the data is collected when `target_population` is reached.

**error\_limit** type: real.

Optional. Default: 0

One of two conditions for termination of the calculation together with `blocks_used`. This specifies the upper limit of the sum of standard error and the error in error of projected energy.

**min\_blocks\_used** type: integer.

Optional. Default: 10

The minimum number of optimal reblock lengths required for a calculation to terminate. The calculation will not terminate due to the standard error falling below `error_limit` until at least this number of optimal reblock lengths are included within the calculation. This ensures that our error estimate is reliable at termination. Larger `min_blocks_used` ensures a more reliable blocking analysis but increases the minimum length of calculations.

**blocks\_used** type: integer.

Optional. Default:  $2^{*31}-1$

Independent of the `error_limit`, if the number of blocks used to estimate the standard error of projected energy is more than the `blocks_used`, the calculation is terminated. Larger `blocks_used` ensures a more reliable blocking analysis.

**auto\_shift\_damping** type: boolean.

Optional. Default: false

Whether to automatically optimise the shift damping using information from blocking on the fly. This optimises the shift damping to ensure that the standard deviations of the instantaneous projected energy and shift are approximately equal. The allowable range of values is currently set to allow the shift standard deviation to be between 50% and 200% of that of the instantaneous projected energy, though this could easily be exposed to the user if required.

---

**Note:** This approach will modify the shift damping to ensure a reasonable variation in the shift during a calculation. Updates to the shift damping will be printed within the output file, and the final shift damping written into restart files to be used in any restarted calculations. If no `shift_damping` is provided to a restarted calculation in the qmc table the final value from the restarted calculation will be used. If we read in from a legacy restart file and no `shift_damping` is provided in the qmc table, the `shift_damping` defaults to the original default, 0.05.

---



---

**Note:** Once an optimisation has been completed the calculation will not modify the shift damping unless `force_shift_damping_opt` is true. This is to avoid the user having to know if an optimisation has been completed when configuring a calculation restart.

---

**shift\_damping\_precision** type: real.

Optional. Default: 2.0\_p

How precisely the standard deviations of the projected energy and shift should match. This defines the maximum allowed ratio between the two in any combination. For values above this a further optimisation will be attempted. A lower value will lead to a longer optimisation period before statistics can be collected but a more reliably optimised value. The minimum allowed ratio is 1.5\_p, as convergence to below this accuracy is not guaranteed.

**force\_shift\_damping\_opt** type: boolean.

Optional. Default: false

Forces shift damping optimisation when we have previously performed an optimisation. Useful when restarting from previous calculation with a higher target population.

## state\_histogram options

The `state_histogram` table contains options used to control the options for calculating the state histograms during a *Full Configuration Interaction Quantum Monte Carlo* or *Density Matrix Quantum Monte Carlo* simulation.

This is a generalization of the state histograms original proposed by Cleland and coworkers for FCIQMC: [Cleland12]. The generalization is to treat DMQMC in addition to FCIQMC. In the case of FCIQMC the behavior is nearly identical to that of the original algorithm.

In FCIQMC, the histograms are calculate based on the excitation levels relative to the reference determinant. In DMQMC, we add an additional excitation index based on the excitation level between the two determinants used to label the density matrix site.

**report\_frequency** type: integer.

Optional. Default: `nreports`

The frequency in report cycles to calculate and report the state histograms. A histogram is always reported at the beginning and end of a calculation regardless of whether it falls within the frequency provided.

**nbins** type: integer.

Optional. Default: 5

The number of histogram bins to use per decade of walker population. As an example, if we have a walker population 10 to 100, there are bins from: [10, ~ 15.85), [15.85, ~ 25.12), [25.12, ~ 39.81), [39.81, ~ 63.10), and [63.10, ~ 100).

**decades** type: integer.

Optional. Default: 3

The number of decades of particle populations to include in the histogram bins past the decades of  $\lfloor \log_{10}(N_w) \rfloor$ . Where  $N_w$  is the simulations `target_population` set in the *qmc options*.

---

**Note:** If this value is too small, and the simulations population grows well pass the target population, the histogram population bins may not cover the number of particle on a single site. In this case the simulation will terminate with an error message to prevent an out of bounds index.

---

**skip\_memory\_check** type: boolean.

Optional. Default: false.

Controls the memory check performed when collecting state histograms. Normally an estimate is made for the memory cost to store all the state histogram files, if the estimate exceeds 1 gigabyte the calculation will halt. Setting this flag to true will ignore the memory check.

## 1.7.3 Utilities

### Utilities

#### Redistribution of restart files

```
redistribute {
    -- options
}
```

For speed in reading in restart files and for simplicity, HANDE produces restart files specific to the number of MPI ranks used in the calculation and hence by default calculations can only be restarted on the same number of MPI ranks the original calculation ran on. The `redistribute` function reads in a set of restart files and produces a new set to be used on a different number of processors.

---

**Note:**

- It is convenient to place this before the QMC calculation call in the input file. However, the process of redistributing particles is a somewhat serial task and hence `redistribute` may not scale well to large numbers of processors. Hence it may be more computationally efficient to do the redistribution targeting a large (ie 100s or 1000s) of processors using a much smaller number of processors in a separate run of HANDE.
  - Load balancing settings are reset to their default values.
- 

HANDE uses one restart file per MPI rank with a filename of the form `HANDE.RS.X.pY.H5`, where X is the restart index and Y is the MPI rank.

Options:

**nprocs** type: integer.

Optional. Default: number of processors the calculation is running on.

Set the number of processors that the new set of restart files are to be used on.

**read** type: integer.

Optional. Default: highest non-negative integer for which a set of restart files exists.

Set the index, X of the set of restart files to be read in.

**write** type: integer.

Optional. Default: highest non-negative integer for which a set of restart files does not yet exist.

Set the index, X of the set of restart files to be written out.

**move\_frequency** type: integer.

Optional. Default: use the value from the original calculation.

Relevant only for CCMC calculations. See corresponding option in *ccmc options* for details.

**sys** type: system object.

Optional.

Only used to determine the number of basis functions, if changing the value of `DET_SIZE` for the restart files.

**Warning:** Each processor must be able to access the entire set of existing restart files, which are assumed to be in the working directory.

## MPI information

```
mpi_root()
```

**Returns:** true if the processor is the MPI root processor and false otherwise.

The input file is processed and run by each processor. It is occasionally useful to perform (for example) additional I/O from lua but only on one processor. Testing if the processor is the MPI root processor is a safe way to do this, e.g.

```

if mpi_root() then
    print('root says hello from lua!')
end

```

## Memory management

Objects returned from functions (e.g. `system` and `qmc_state` objects) are deallocated by Lua's garbage collector when they are no longer required. This can either be because the variable goes out of scope or is set to `nil`. This level of memory management is sufficient in most calculations. However, there may be a substantial memory overhead when running multiple separate calculations in the same input file as the garbage collection need not take place immediately. As such, objects which are no longer required can be explicitly freed using `free` methods on all objects returned by HANDE's functions. For example, for `qmc_state` objects:

```

system = hubbard_k {
    lattice = { { 10 } },
    electrons = 6,
    ms = 0,
    sym = 1,
    U = 1,
}

qs1 = fciqmc {
    sys = system,
    qmc = {
        tau = 0.01,
        init_pop = 10,
        mc_cycles = 20,
        nreports = 100,
        target_population = 50000,
        state_size = 5000,
        spawned_state_size = 500,
    },
}

-- Deallocate all memory associated with qs1 produced by the first FCIQMC calculation.
qs1:free()

qs2 = fciqmc {
    sys = system,
    qmc = {
        tau = 0.02,
        init_pop = 10,
        mc_cycles = 10,
        nreports = 100,
        target_population = 50000,
        state_size = 5000,
        spawned_state_size = 500,
    },
}

```

and similarly for `system` objects.

## Write HDF5 system file

```
hdf5_name = write_read_in_system {  
    sys = system,  
    filename = filename,  
}
```

Options:

**sys** type: system object.

Required.

The system on which to perform the calculation. Must be created via the `read_in` function.

**filename** type: string. Optional.

Filename to dump system hdf5 file to. If unset will generate a filename to dump to based on the template: `int_file + CAS_information + .H5`, where `int_file` and the CAS information are set in the call to `read_in` which create the `system` object.

Returns:

type: string.

name of HDF5 file created. This is currently only available on the root processor and can be passed into subsequent calls to `read_in` safely as only the root processor reads from integral and system files.

When running a calculation using a system generated from a FCIDUMP, the `system` object created by `read_in` can be dumped in HDF5 format for reuse in subsequent calculations; this speeds initialisation by a factor of ~100x and reduces the required file size by ~16x for large FCIDUMPs. When running in parallel on a large number of cores this is particularly important to utilise as it overcomes an inherent serialisation point in the calculation initialisation.

For example:

```
sys = read_in {  
    int_file = "FCIDUMP",  
    nel = 24,  
    ms = 0,  
    sym = 0,  
}  
  
hdf5_name = write_read_in_system {  
    sys = sys,  
}
```

produces an HDF5 file entitled "FCIDUMP.H5" and return this value to the variable `hdf5_name`. Passing this as the argument to `int_file` within `read_in` will use it in future calculations – the HDF5 format of the file is automatically detected.

If a CAS is used to produce the system object used to produce such a file it will be labelled as such and only information for basis functions within the CAS will be stored; conversion between different CAS within this functionality is not currently supported.

The FCIDUMP.H5 file does not specify the symmetry sector on which to perform a calculation. This is instead set as in *Generic systems*.

---

**Important:** When using a HDF5 file to initialise a system either both of `nel` and `ms` must be specified or neither; if neither are specified the values stored within the system HDF5 file will be used and otherwise the given values override

those stored.

## 1.7.4 Appendix

### A short introduction to lua

Lua is a lightweight programming language which is easy to embed and is well-suited to the task of controlling a simulation. For a quick introduction to lua, please read [Learn Lua in 15 Minutes](#). However, for most cases the input file format can be treated as follows:

Assignment is performed by setting a variable name equal to an object, e.g.

```
pi = 3.141592654
```

Strings are created by enclosing characters in quotation marks:

```
msg = 'hello world'
```

and boolean variables can be set using the `true` and `false` keywords:

```
yes = true
yes = false
```

A key data structure in lua is the *table*, which serves both as an array and an associative array or map, and is denoted using braces. First, the following creates a table to hold a 1D vector:

```
v = { 1, 2, 3 }
```

whilst using key=value pairs creates a table as an associative array:

```
v = { x = 3, y = 4, type = 'dual' }
```

Tables can be nested.

Functions are called using:

```
x = fname(arg1, arg2, ...)
```

where *fname* is the name of the function, which returns a single value (which is stored in *x* in the above example). Keywords can be passed in by using a table. If the function takes a single table, then the parentheses need not be included, such that the following calls are identical:

```
x = fname1({ x = 3, y = 4, type = 'dual' })
x = fname1{ x = 3, y = 4, type = 'dual' }
```

All options are passed into HANDE by using a table as an associative array. Each function exposed by HANDE to the lua script takes a single (nested) table.

Lua handles multiple return values from functions in a convenient manner. If a function call returns values that are then not set to a variable, the additional values are discarded. If a function call returns fewer values than are the variables set to hold the results of the function call, the additional variables are set to `nil`. See (e.g.) <http://www.lua.org/pil/5.1.html> for more details.

**Warning:** lua, and by extension the HANDE input file, is case sensitive.

## Cookbook

Having lua control a HANDE simulation allows for some pretty clean ways to run complicated simulations. Here we will list some examples.

### Twist Averaging

To aid in the removal of single-particle finite size effects it is often helpful to perform twist averaging. Here we want to average results over multiple twist vectors  $\mathbf{k}_s$  where each component of  $\mathbf{k}_s$  can be chosen to lie within the simulation cell Brillouin zone. Normally we would need to run multiple independent simulations yielding many output files, which can be problematic for file systems. Lua allows us to run the calculations from a single input file.

In the example below we show this for a twist averaged canonical total energy calculation, which can be useful for correcting incomplete twist averaged QMC calculations which are typically much more expensive.

```
-- Function to generate a random twist.
function get_twist()
    ks = {}
    -- 3D UEG.
    for i = 0, 2 do
        -- For the UEG, we only need to generate a twist vectors whose components lie
        -- the range  $[-\pi/L, \pi/L]$ . In HANDE we interpret the input ks as being in
        -- of  $2\pi/L$ , so we need to randomly pick components in the range  $[-0.5, 0.5]$ .
        sign = math.pow(-1, math.random(0, 1))
        ks[i] = 0.5*sign*math.random()
    end
    return ks
end

-- The number of simulations to average over.
ntwists = 3000
math.randomseed( os.time() )

for i = 1, ntwists do
    ks = get_twist()
    sys = ueg {
        nel = 19,
        ms = 19,
        dim = 3,
        cutoff = 20,
        rs = 0.5,
        twist = ks,
        verbose = false,
    }
    mc_state = canonical_estimates {
        sys = sys,
        canonical_estimates = {
            beta = 16,
            nattempts = 10000,
            ncycles = 10,
            fermi_temperature = true,
        },
    }
    sys:free() -- Free up memory.
end
```



The output file can then be analysed to obtain the canonical total energy estimate for each twist angle using

```
$ analyse_canonical.py --sim canonical_twist.out
```

where `canonical_twist.out` is the output filename.

## 1.8 Interacting with running calculations

It is possible to interact with running calculations.

After each report loop, HANDE checks for the existence of the file `HANDE.COMM` in the current working directory for all processors. If `HANDE.COMM` exists, then the file is read and any modified parameters are then used for the rest of the calculation. `HANDE.COMM` is deleted after it is read in to prevent it from being detected on subsequent report loops and to enable multiple interactions with a running calculation.

`HANDE.COMM` is a lua script, in a similar fashion to the input file, but has a much more restricted range of options. Options which can be set or modified are:

**softexit** type: boolean.

End the calculation immediately but still perform any post-processing (e.g. dumping out a restart file). This is useful for cleanly terminating a converged calculation or cleanly stopping a calculation before the walltime is reached to allow it to be restarted.

The `send_softexit.py` script in the `tools` subdirectory is useful for running HANDE on a queueing system as it writes **softexit = true** to `HANDE.COMM` a certain amount of time before the walltime is reached.

**write\_restart** type: boolean or integer.

If true or set to an integer, restart files will be written out at the end of the calculation, with the index given by the integer if supplied. See [restart options](#) for more information. This overwrites the value (if any) given to `write` in the `restart` table set in the input file. Note that warnings relating to restart files (e.g. blocking on the fly information not stored) will not be printed.

**tau** type: float.

Change the timestep to be used.

**target\_population** type: integer.

Change the number of particles to be reached before the calculation starts varying the shift. Meaningless if the calculation has already started varying the shift. If smaller than the current population (or negative) then the shift is immediately allowed to vary.

**shift** type: float or 1D vector of floats.

Adjust the current value of the shift. If the calculation has already entered variable shift mode then the shift will still be updated every report cycle, otherwise this is equivalent to changing the **initial\_shift** value.

Passing a single value such as:

```
shift = -1
```

sets the shift in **all** spaces to the specified value. Different spaces can be modified separately by passing in a vector. For example:

```
shift = { -1, -2 }
```

sets the shift in the first space to -1, in the second space to -2 and leaves it unmodified in all other spaces.

## 1.9 Analysis

The following provides a brief overview for the most common analysis required for each type of Monte Carlo calculation. The guides in [Tutorials](#) provide a step-by-step guide to analysing HANDE calculations and explain the reasoning behind the required analysis parameters.

HANDE includes a variety of scripts and utilities in the `tools` subdirectory. However, these only provide a simple, command-line interface. A comprehensive python module, *pyhande*, drives all the analysis. *pyhande* is extremely powerful for dealing with complex analysis, data-driven investigation or bulk data analysis.

### 1.9.1 FCIQMC and CCMC

#### Fundamental Usage

QMC calculations print out data from a block of iterations (a ‘report loop’), the length of which is controlled by the `mc_cycles` input option. Care should be taken analysing this data and, in particular, producing accurate estimates of the errors in the means of the energy estimators. Almost all data is averaged over the report loop (see output for further details).

Note that no data is lost when quantities are summed over report loops, as the correlation length in the data is substantially longer than the length of the report loop (typically 10-20 iterations).

As the particle distribution at one iteration is not independent from the distribution at the previous iteration, estimators at each iteration are not independent. This correlation in the data needs to be taken into account when estimating standard errors. A simple and effective way of doing this is to use a blocking analysis [\[Flyvbjerg89\]](#).

The `reblock_hande.py` script (in the `tools` subdirectory) does this. Run

```
$ reblock_hande.py --help
```

to see the available options. Estimates for the shift and projected energy are typically obtained using

```
$ reblock_hande.py --start N out
```

respectively, where `N` is the starting iteration from which data should be blocked (i.e. after the calculation has equilibrated) and `out` is the file to which the calculation output was saved. Without `--start` option, this script automatically estimates the appropriate `N`, so you usually don’t have to give `N` by yourself.

Note that `reblock_hande.py` can accept multiple output files for the case when a calculation is restarted as follows:

```
$ reblock_hande.py -m out1 out2 out3
```

More complicated analysis can be performed in python by using the `pyhande` library — `reblock_hande.py` simply provides a convenient interface for the most common analysis tasks.

#### Hybrid method

Hybrid method is different choice to estimate errors from blocking analysis, which is available as

```
$ reblock_hande.py -a hybrid out
```

Our experiment has shown that hybrid method makes more reliable estimation of errors than blocking analysis: We prepared 1000 different CCMC-SD energy time-series for Nitrogen atom, with the same calculation setting but just different random seeds. Then, the energy means and the standard errors were obtained by hybrid method and blocking analysis, and it was examined how many means coincide with the CCSD energy within the range of the errors,

respectively. The expected coincidence rate for 1 sigma accuracy is 68.27%. Thus, when the actual coincidence rate is closer to this percent, the post-analysis is more reliable.

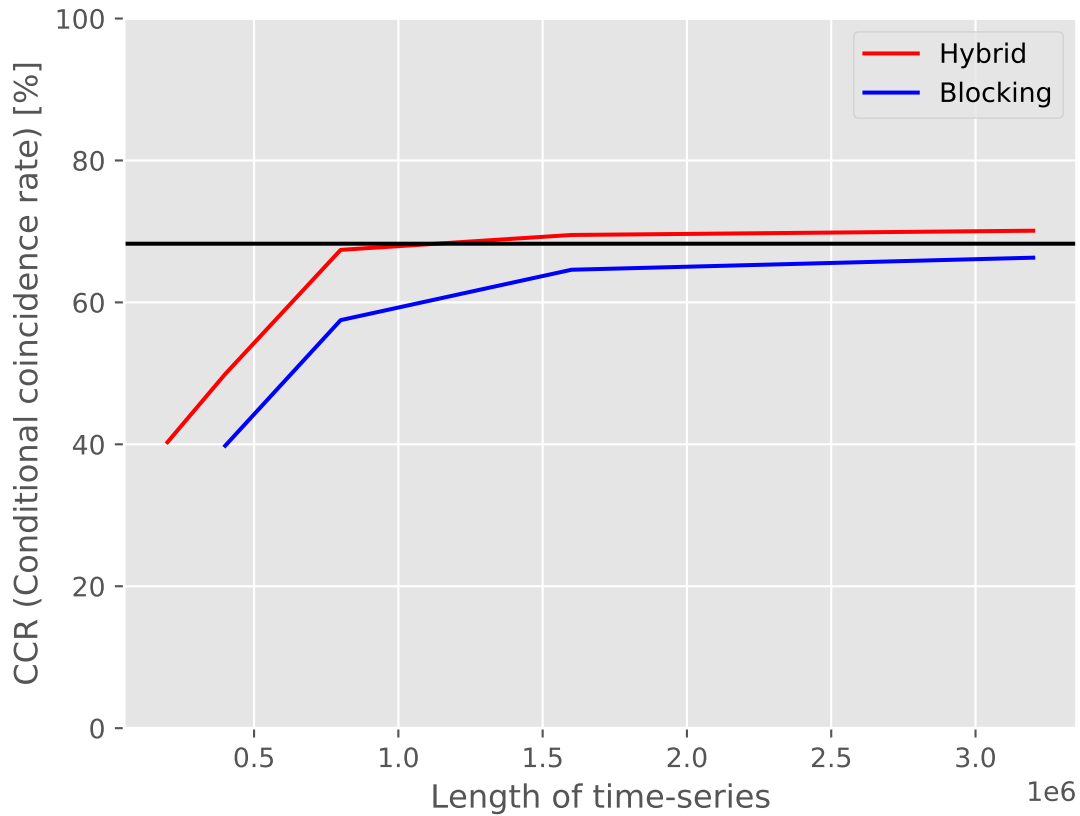
We employed two types of coincidence rate to compare reliabilities, conditional coincidence rate (CCR) and unconditional coincidence rate (UCR), which are defined by

$$\text{CCR} = \text{Hit} / (\text{Total} - \text{Failed}) * 100,$$

$$\text{UCR} = \text{Hit} / \text{Total} * 100.$$

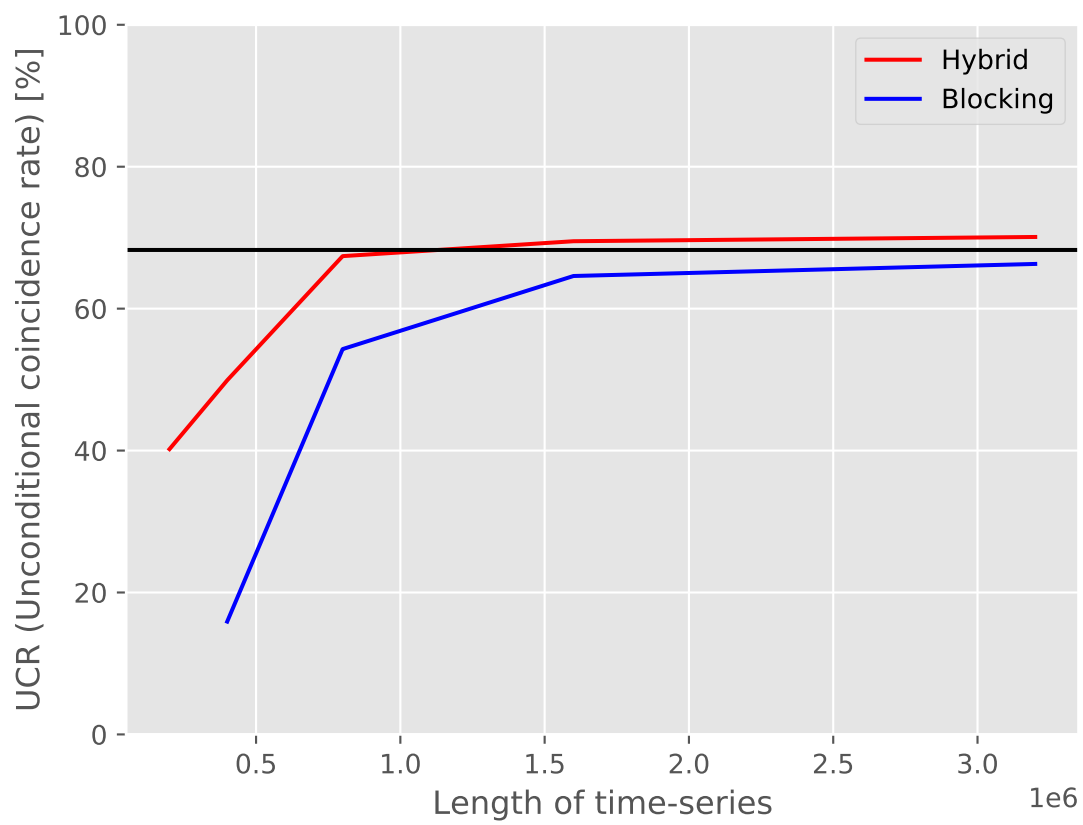
Here, ‘Total’ is the total number of post-analyses (=1000), ‘Failed’ is the number of post-analyses which fails to make an estimation of the error(\*), and ‘Hit’ is the number of post-analyses which makes an estimation of the error and the energy mean coincides with the CCSD energy within the standard error. (\*: e.g. ‘Shift is not started yet’ in the case of blocking method)

In the following figures, the former (latter) compares the CCRs (UCRs) obtained using hybrid method and blocking analysis for different lengths of time-series. Both figure shows that the CR of hybrid method is closer to 68.27% for short lengths of time-series.



## MSER minimization

There are two choices of method to estimate starting iterations, one is originally implemented in reblock\_hande.py (here call it ‘WREE minimization’) and the other is the newly implemented, named ‘MSER minimization’. The new



method is available as

```
$ reblock_hande.py -b mser_min out
```

These two methods are compared in a unpublished work, where it is established that WREE minimization discards extra much iterations, when length of time-series is large. On the other hand, MSER minimization always gives constant estimation of starting iterations, independent of length of time-series.

## 1.9.2 Canonical Total Energy MC

The configurations and resulting estimates in a canonical total energy calculation are statistically independent and therefore no blocking analysis is required. The `analyse_canonical.py` script is available in `tools/canonical_energy/` which performs the appropriate averaging and standard error analysis on the output file using the pyhande suite.

## 1.9.3 DMQMC

No blocking analysis is required for the error analysis of DMQMC calculations as estimates are averaged over statistically independent runs. The `finite_temp_analysis.py` script in `tools/dmqmc` can be used to perform a standard error analysis of the Monte Carlo data for a number of different observables.

## 1.10 Generating integrals

HANDE can treat *systems* other than model Hamiltonians by reading in the necessary integrals in the FCIDUMP format [Knowles89]. Many quantum chemistry packages can generate them following Hartree-Fock calculations, including:

**HORTON** <https://theochem.github.io/horton/>

**MOLPRO** <https://www.molpro.net>

**PSI4** <http://psicode.org>

A short tutorial can be found *below*.

**Q-Chem** <http://www.q-chem.com> FCIDUMP code contributed by Alex Thom.

We most frequently use PSI4 and Q-Chem and so these tend to be better tested. Note that the computational cost of the calculations in HANDE vastly outweighs the cost of the underlying SCF calculations and so the efficiency of the code used to generate the integrals is usually not a key factor. Please consult the documentation of the code of interest regarding how to run SCF calculations and generate the integrals in the FCIDUMP format.

Please note that not all programs use exactly identical FCIDUMP formats and some may not be compatible with HANDE. The differences are typically in the namelist header. It may be possible to resolve these differences by hand or a script.

### 1.10.1 A short tutorial for generating FCIDUMPs by Psi4

#### Installation

The Psi4 package can be simply installed in an Anaconda environment via

```
$ conda install psi4 python=3.8 -c psi4
```

Psi4 provides two APIs to access it, the Psithon interface (`$ psi4 H2.in > H2.out`), or by using it like a Python module. The latter is covered by this tutorial as it is more intuitive to use and renders post-calculation analysis easier.

## Typical usage

The following examples runs a RHF calculation on carbon dimer at cc-pVDZ at a clamped orbital occupancy, producing a FCIDUMP file at the end.

```
import psi4

psi4.core.clean() # Clean local scratch files
psi4.set_memory('2000 MB')

dump = 'c2_1.200.FCIDUMP'
outfile = 'c2_1.200.psi4out'
psi4.core.set_output_file(outfile, False)
# There are many ways to specify geometry, see documentation
mol = psi4.geometry("""
C
C 1 r
r = 1.200
""")
# Default SCF_TYPE is density fitting, which produces slightly different results than
# other packages like PySCF.
# Provide 'SCF_TYPE':'DIRECT' in the option dictionary if it's concerning
psi4.set_options({'basis':'cc-pvdz', 'docc':[2,0,0,0,0,2,1,1]})
E, wfn = psi4.energy('scf', return_wfn=True)
# oe_ints has to be specified exactly like this
psi4.fcidump(wfn, fname=dump, oe_ints=['EIGENVALUES'])
```

## Custom basis set

Sometimes a custom basis set is needed (for example many chromium dimer benchmarks are done with an 'Ahlich's SV' basis, which requires deleting a diffuse p basis from the def2-SV(P) basis set for Cr). This can be done either in the input file (<https://psicode.org/psi4manual/master/basissets.html#user-defined-basis-sets>) or by writing a basis set definition in the python module folder (which should be `/home/{user}/anaconda3/envs/{env-name}/share/psi4/basis/`, see the link above for basis set file naming convention).

## Post-calculation analysis

The returned wavefunction object `wfn` can be inspected and analysed. For methods summary see [here](#). But most basically you can call

```
wfn.epsilon_a().nph
```

which returns all the HF eigenvalues grouped by symmetry.

## Symmetry

Psi4 uses ‘Cotton ordering’ for the irreps of  $D_{2h}$ , albeit inconsistently (e.g. the DOCC option takes in a list of irrep occupation with normal ordering, i.e.,  $A_g, B_{1g}, B_{2g}, \dots$ ). But in the &FCI namelist, the symmetry labels are Cotton-ordered, i.e. [1, 2, 3, 4, 5, 6, 7, 8] means  $[A_{1g}, B_{3u}, B_{2u}, B_{1g}, B_{1u}, B_{2g}, B_{3g}, A_u]$ .

## Freezing orbitals

For large systems, if you’re already planning on freezing electrons in the HANDE calculation, it might be sensible to freeze them in the FCIDUMP. Psi4 can do this for you by just adding 'freeze\_core':True in the options dictionary above (more precise control is available, see [here](#)), and export FCIDUMP in exactly the same way.

### 1.10.2 FCIDUMP format

The format of FCIDUMP files used by HANDE is partially defined in [Knowles89]. It consists of a namelist header, containing various pieces of information about the system, and a body containing all integral values.

**&FCI** Starts FCI namelist.

/ Terminates a namelist. Most compilers also implement the extension where &END is used to terminate the namelist instead.

**x i a j b** Format for integral values within body of the FCIDUMP. x is a float or complex value as appropriate for the system. i, j, a and b are integers.

#### &FCI namelist

**NORB** Number of orbitals in the basis. See note on basis indices below. Must be provided in FCIDUMP namelist.

**NELEC** Number of electrons in system. Must be provided either in FCIDUMP namelist or input file.

**MS2** Spin polarisation. Must be provided either in FCIDUMP namelist or input file.

**ORBSYM** Array containing symmetry label of each orbital. See symmetry notes below. If not provided in FCIDUMP namelist we assume the system has no symmetry.

**UHF** True if FCIDUMP file was produced from an unrestricted Hartree-Fock calculation. See note on basis indices below. If not provided in FCIDUMP namelist RHF calculation is assumed.

---

**Note:** We assume that in UHF calculations the number of spin-up basis functions is equal to the number of spin-down basis functions.

---

**ISYM** Currently unused. Defined solely for compatibility with NECI FCIDUMP files. Gives the symmetry of the wavefunction formed by occupied the NELEC lowest energy spin-orbitals.

**SYML** Currently unused. Defined solely for compatibility with NECI FCIDUMP files. Array containing L (angular momentum) for each orbital. Set to -1 if L is not a good quantum number.

**SYMLZ** Array containing  $L_z$  (angular momentum along the z-axis) for each orbital. For example  $d_{xz}$  would have  $L = 2$  and  $L_z = 1$ , and  $d_{yz}$   $L = 2$ ,  $L_z = -1$ . If not provided in FCIDUMP assume no  $L_z$  symmetry in system. See [Generic systems](#) for more details, and also on how to generate  $L_z$ -transformed FCIDUMPs.

**NPROP** Dimensions of the supercell used in translationally symmetric systems.

**PROPBITLEN** Length in bits of each kpoint index dimension in translationally symmetric systems.

## Integrals

if  $i = j = a = b = 0$ ,  $E_{\text{core}} = x$ , where  $E_{\text{core}}$  contains the nuclear-nuclear and other non-electron contributions to the Hamiltonian.

if  $a = j = b = 0$ ,  $\epsilon_i = x$ , the single-particle eigenvalue of the  $i$ -th orbital.

if  $j = b = 0$ ,  $\langle i|h|a \rangle = x$ , the one-body Hamiltonian matrix element between the  $i$ -th and  $a$ -th orbitals, where  $h = T + V_{\text{ext}}$ .

otherwise  $\langle ij|1/r_{12}|ab \rangle = x$ , the Coulomb integral between the  $i$ -a co-density and the  $j$ -b codensity. Note the Coulomb integrals are given in Chemists' notation.

### 1.10.3 Basis indices

**RHF** All indices are in terms of spatial orbitals. NORB is the number of spatial orbitals.

**UHF** All indices are in terms of spin orbitals. NORB is the number of spin orbitals.

---

**Note:** Basis functions (as stored by `basis_fns`) are always stored as spin orbitals (the memory saving involved in storing only spatial orbitals is not worth the additional overhead/headache, as FCIQMC involves working in spin orbitals). Integrals are expensive to store, so we store them in as compressed format as possible.

---

**Warning:** The single-particle basis is assumed to be orthonormal.

### 1.10.4 Symmetry

Molecular orbitals are defined by the D2h point group (or a subgroup thereof) by the quantum chemistry packages (QChem, MOLPRO) used to produce FCIDUMP files, so we need only concern ourselves with Abelian symmetries.

ORBSYM( $i$ ) = S+1, where S is the symmetry label defining the irreducible representation spanned by the  $i$ -th orbital. See notes in `pg_symmetry` about the symmetry label for Abelian point groups.

If ORBSYM( $i$ ) = 0, then the symmetry of the  $i$ -th orbital is not well-defined. In this case, we can only resort to turning off all symmetry (i.e. set all orbitals to be totally symmetric).

**Warning:** Note that this has memory implications for the integral storage.

For periodic systems symmetries are defined by their kpoint vector. ORBSYM( $i$ ) contains this vector in a format defined by `PROPBITLEN`, which is decoded within HANDE.

## 1.11 Tips

Some suggestions from the HANDE developers for using HANDE... heed our words!



### 1.11.1 Compilation

For optimised versions of HANDE, explore using:

- compiler-specific optimisation flags

In general adding ‘high-level’ optimisation flags (`-O3`, `-Ofast`, etc.) makes a substantial impact on the calculation speed.

- interprocedural optimisation

Many compilers can perform interprocedural optimisation, whereby optimisations are performed at link-time instead of compile-time. This allows optimisations to be performed (including inlining) on procedures specified in different source files. On some compilers (e.g. GCC, Intel) this can have a substantial benefit; on other compilers the difference is less marked.

- popcnt instruction

If the processor being used includes it, uses the `popcnt` instruction rather than a software implementation to count bits set in an integer. This can have a impact of the order of a few percent for the entire calculation.

- `DET_SIZE=64`

Use 64-bit integers rather than 32-bit integers to store the representation of the determinant/excitor/tensor labels. This can make certain calculations quicker (i.e. those involving more than 32 single-particle basis functions) by reducing the amount of bit operations that need to be performed.

### 1.11.2 Plotting calculation output using gnuplot

The first section of the output file contains information about the basis functions used in the calculations. This gives spurious data points when the contents of the file is plotted using gnuplot. They can be removed by creating an executable file called `gphande` in the user’s `$PATH`, containing:

```
#!/bin/sed -nf
1,/iterations/d
/^ *[0-9]/p
```

When plotting in gnuplot, using the command

```
plot '<gphande file'
```

instead of

```
plot 'file'
```

will then remove the extra points.

## 1.12 Old (removed) functionality

Unused and **not useful** functionality is occasionally removed from HANDE, in order to remove the maintenance burden for code that really has no benefit. In general, keeping failed experiments in the codebase is not helpful to developers (more work) and users (not obvious if an option should or should not be used). When it transpires that something falls into the category, we may hence remove it and detail it below. If you are interested in resurrecting this functionality, please dig through the git history and/or speak to a developer.

**folded-spectrum FCIQMC** The folded-spectrum approach allows, in principle, access to excited states in FCIQMC via using the Hamiltonian  $(H - \epsilon)^2$ , where  $\epsilon$  is an energy offset. It emerged in practice to be very painful/impossible to converge to excited states for systems beyond the reach of conventional FCI.

**defining an initiator determinant via a complete active space** Originally the initiator space was defined by a population threshold and a complete active space (CAS). It turns out that it is simpler to allow the initiator space to emerge naturally just through the population threshold (as used in later studies), whereas defining a CAS that is small but effective is not easy in large systems. Furthermore, using just a population threshold makes the initiator approximation easier to extend to other algorithms (i.e. CCMC and DMQMC).

## 1.13 Tutorials

The tutorials below demonstrate how to set up and run Monte Carlo calculations in HANDE. The input files in the test suite also demonstrate how calculations can be performed. The aim here is to provide an introduction to setting up, running and analysing calculations and only basic input options are considered; for advanced options please consult the appropriate section of the manual.

The tutorials assume that HANDE has been successfully compiled and the test suite has been successfully run. Any reference to `hande.x` should be replaced with the full path to the HANDE executable and similarly for the `reblock_hande.py`, `finite_temperature_analysis.py` and `analyse_canonical.py` scripts.

---

**Note:** The exact command to launch HANDE with MPI depends upon the exact configuration of MPI. The command may be different (e.g. `mpirun` instead of `mpiexec`) and might require the number of processors to be passed as an argument. The tutorials show the exact command we used, which varies depending upon the machine used to run the tutorials. We regularly use the OpenMPI implementation (`mpiexec -np <# processors>` or `mpirun -np <# processors>`), Intel MPI (`mpiexec`) and Cray-MPICH (`aprun`).

---

The input and output files from the calculations performed in the tutorials can be found under the `documentation/manual/tutorials/calcs/` directory. The example calculations are deliberately not trivial and may require up to a few hundred core hours to run as shown. Smaller calculations can be performed by reducing the system size (e.g. using fewer electrons or orbitals) or running for fewer iterations.

---

**Note:** None of the tutorials fix a random number seed (as this is the best approach for running multiple production calculations on the same system) so results will not be exactly identical (but should agree statistically) from those in the above dataset unless the same seeds (which can be found in the output files) are used.

---

We recommend working through the FCIQMC tutorial before the iFCIQMC, CCMC or DMQMC tutorials.

### 1.13.1 Full Configuration Interaction Quantum Monte Carlo

In this tutorial we will run FCIQMC on the 18-site 2D Hubbard model at half filling with  $U/t = 1.3$ . The input and output files can be found under the `documentation/manual/tutorials/calcs/fciqmc` subdirectory of the source distribution. Knowledge of the terminology and theory given in [Booth09] and [Spencer12] is assumed.

First, we will set up the system and estimate the number of determinants in Hilbert space with the desired symmetry using a Monte Carlo approach.

We are interested in the state with zero crystal momentum, as there is theoretical work showing this will be the symmetry of the overall ground state. HANDE uses an indexing scheme for the symmetry label. The easiest way to find this out is to run an input file which only contains the system definition:

```

hubbard = hubbard_k {
  lattice = {
    { 3, 3 },
    { 3, -3 },
  },
  electrons = 18,
  ms = 0,
  U = 1.3,
  t = 1,
}

```

This file can be run using:

```
$ hande.x hubbard_sym.lua > hubbard_sym.out
```

The output file, `hubbard_sym.out`, contains a symmetry table which informs us that the wavevector  $(0,0)$  corresponds to the index 1; this value should be specified in subsequent calculations to ensure that the calculation is performed in the desired symmetry subspace.

It is useful to know the size of the FCI Hilbert space, i.e. the number of Slater determinants that can be formed from the single-particle basis given the number of electrons and total spin. Whilst the full space can be determined from simple combinatorics, the size of the subspace containing only determinants of the desired symmetry is less straightforward and it is the latter number that is of interest as it only includes determinants that are connected via non-zero Hamiltonian matrix elements and hence can be accessed in a Monte Carlo calculation. A fast way to determine the size of the accessible subspace is to use Monte Carlo sampling [Booth10] with an input file containing:

```

hubbard = hubbard_k {
  lattice = {
    { 3, 3 },
    { 3, -3 },
  },
  electrons = 18,
  ms = 0,
  U = 1.3,
  t = 1,
  sym = 1,
}

hilbert_space {
  sys = hubbard,
  hilbert = {
    nattempts = 100000,
    ncycles = 30,
  }
}

```

The Monte Carlo algorithm produces `nattempts` random determinants per cycle, from which it estimates the size of the Hilbert space. The independent cycles are used to provide an estimate of the mean and standard error of the data; the running estimates of these are printed every cycle and the final estimate at the end.

This calculation can be run in a similar fashion to before:

```
$ hande.x hubbard_hilbert.lua > hubbard_hilbert.out
```

Inspecting the output, we find that the Hilbert space contains  $1.3 \times 10^8$  determinants with the desired symmetry.

FCIQMC requires a critical population to be exceeded in order to converge to the correct answer. This system-specific population is determined by the plateau. A calculation initially uses a constant energy offset ('shift') and a small

starting population and hence the population grows exponentially. A plateau in the population growth spontaneously appears, during which the correct sign structure of the ground state wavefunction emerges. The plateau is equally spontaneously exited and the population grows at an exponential rate (albeit slower than the initial growth).

The simplest way to find the plateau is to run an FCIQMC calculation with a small initial population and allow the population to grow until a large size; this can be accomplished by setting `target_population`, which is the population at which the shift is allowed to vary, to a large value (i.e. effectively infinite) such that the plateau should occur before it. This is done using an input file like<sup>1</sup>:

```
hubbard = hubbard_k {
  lattice = {
    { 3, 3 },
    { 3, -3 },
  },
  electrons = 18,
  ms = 0,
  U = 1.3,
  t = 1,
  sym = 1,
}

fcirqmc {
  sys = hubbard,
  qmc = {
    tau = 0.002,
    mc_cycles = 20,
    nreports = 500,
    init_pop = 100,
    target_population = 10^10,
    state_size = -1000,
    spawned_state_size = -100,
  },
}
```

As the input file is a lua script, we can use lua expressions (e.g. `10^10` for  $1 \times 10^{10}$ ) at any point.

The choice of timestep is beyond the scope of a simple tutorial; broadly it is chosen such that the population is stable and there are no ‘blooms’ (spawning events which create a large number of particles). HANDE will print out a warning and a summary at the end of the calculation if blooms occur. The other key values are how many iterations to run for and the amount of memory to use for the main and spawned particle data objects. These were chosen such that enough states could be stored and the plateau occurs within the iterations used. Choosing these for a new system typically requires some trial and error. Given the large population, we will run this calculation in parallel using MPI:

```
$ mpiexec hande.x hubbard_plateau.lua > hubbard_plateau.out
```

The parallel scaling of HANDE depends upon the system being studied and quality of the hardware being used. Typically using a minimum population per core of  $\sim 10^5$  (assuming perfect load balancing, which can rarely be achieved) results in an acceptable performance.

The output file is (hopefully!) fairly intuitive. The QMC output table contains one entry per ‘report loop’ (a set of Monte Carlo cycles). `pyhande` can be used to extract this information so that the population growth can be easily plotted:

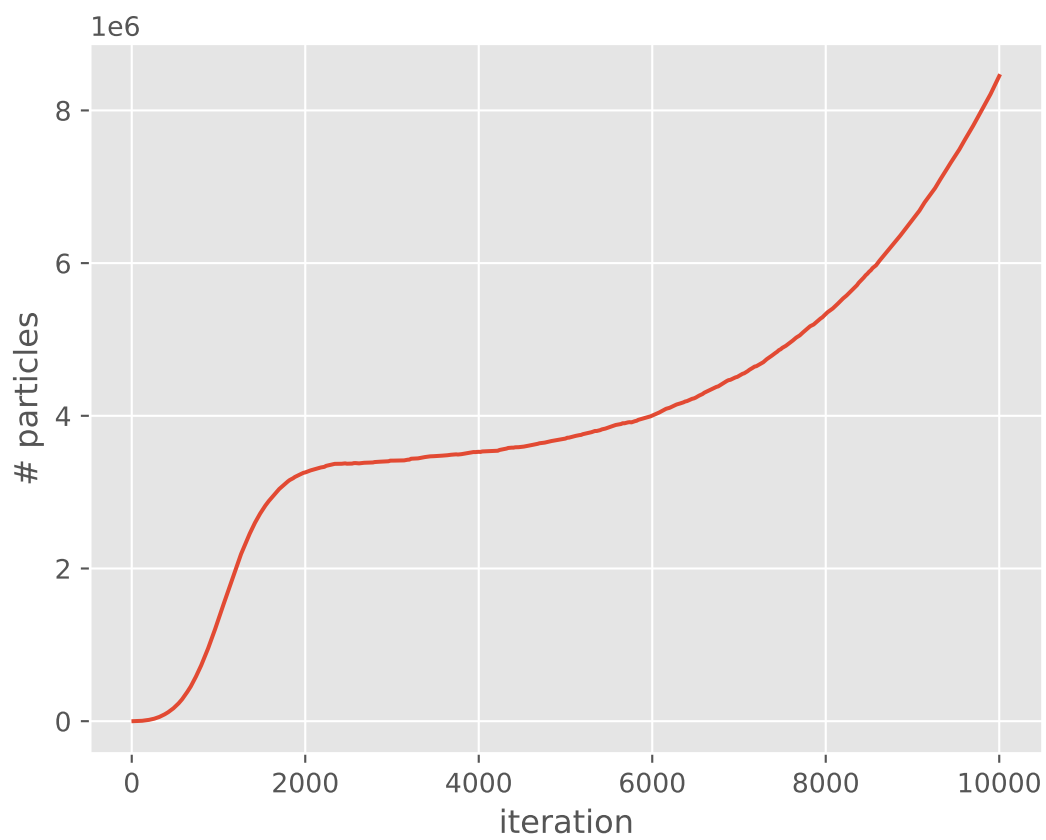
We hence see that the plateau occurs at around  $3.5 \times 10^6$  ( $\sim 2.8\%$  of the entire Hilbert space) and hence FCIQMC is very successful for this system.

---

**Note:** In some cases the plateau may not be present (e.g. in sign-problem free systems) or not easily visible (e.g. in

---

<sup>1</sup> With some scripting it is possible to automatically detect the plateau and interact with the calculation at this point.



systems with a small Hilbert space) or appear as a shoulder (common in CCMC calculations). *pyhande* contains two algorithms for determining the plateau, which are helpful in such cases or for automatically analysing large numbers of calculations.

We can now run a production calculation to find the ground state energy of this system. To do so, we make two changes to the input used to find the plateau: `target_population` is set to a value above the plateau (but not so large that the computational cost is overwhelming) and the simulation is run for more iterations, i.e.:

```
hubbard = hubbard_k {
  lattice = {
    { 3, 3 },
    { 3, -3 },
  },
  electrons = 18,
  ms = 0,
  U = 1.3,
  t = 1,
  sym = 1,
}

fciqmc {
  sys = hubbard,
  qmc = {
    tau = 0.002,
    mc_cycles = 20,
    nreports = 10000,
    init_pop = 100,
    target_population = 4*10^6,
    state_size = -1000,
    spawned_state_size = -100,
  },
}
```

and can again be run using:

```
$ mpiexec hande.x hubbard_fciqmc_real.lua > hubbard_fciqmc.out
```

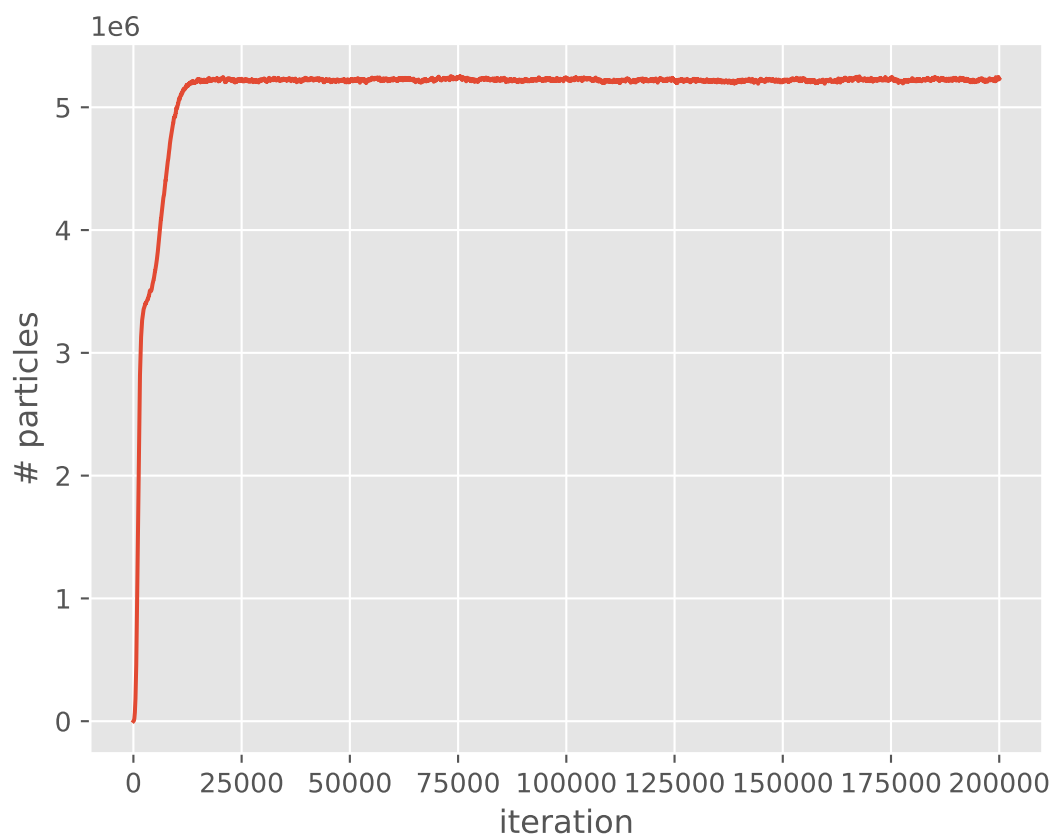
This time, the population starts to be controlled after it reaches the desired `target_population`:

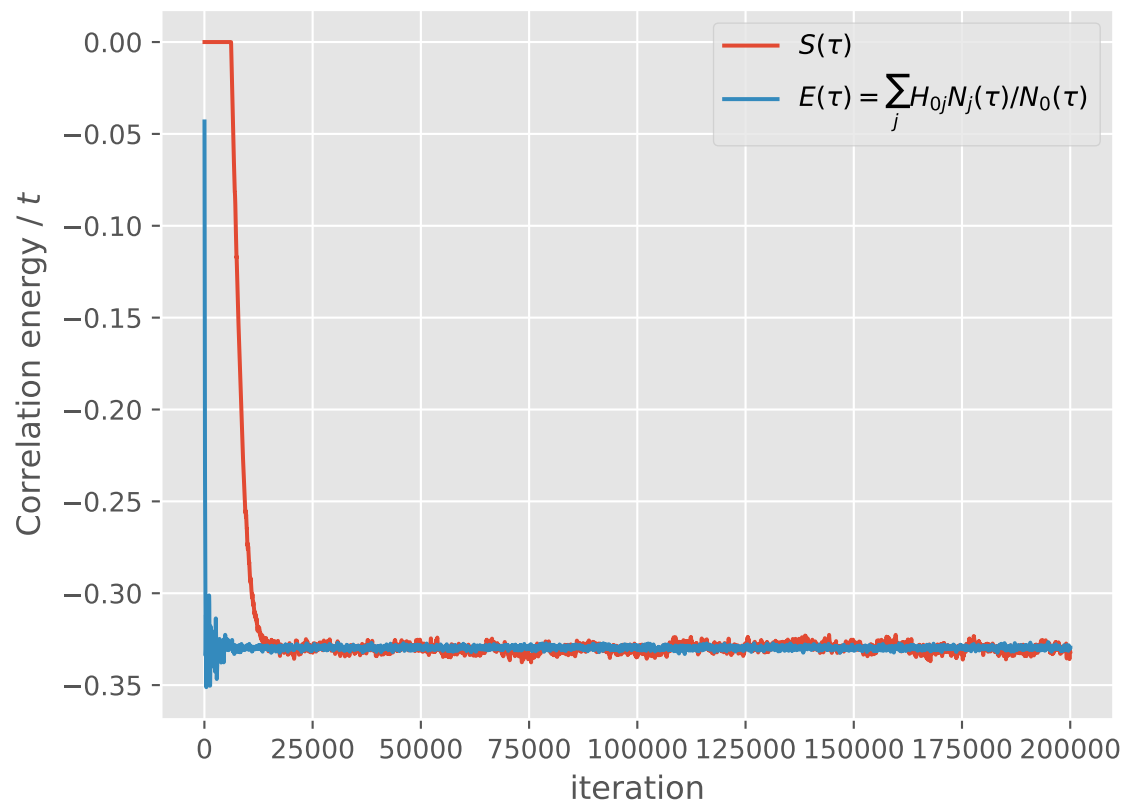
Note that it takes some time for the population to stabilise as the shift gradually decays towards the ground state correlation energy. Once the population is stable, both the shift and the **instantaneous** projected energy vary about a fixed value, namely the ground state energy:

Care must be taken in evaluating the mean and standard error of these quantities, however. The state of a simulation at one iteration depends heavily upon the state at the previous iteration and hence each data point is not independent. Further, in the case of the projected energy estimator, the correlation between the numerator and denominator must be taken into account. The former issue is dealt with using a blocking analysis [Flyvbjerg89]; the latter by taking the covariance into account. Both of these are implemented in *pyhande* and the `reblock_hande.py` script provides a convenient command line interface to this functionality. See *Analysis* for more information. The above graphs show that the population, shift and instantaneous projected energy estimator have all stabilised by iteration 30000, so we will accumulate statistics from that point onwards. `reblock_hande.py` can produce a lot of useful output but for now we'll only concern ourselves with the best guess of the standard error [Lee11], hence the use of the `--quiet` flag:

```
$ reblock_hande.py --quiet --start 30000 hubbard_fciqmc.out
```

which gives







Recommended statistics **from optimal** block size:

	# H	psips	\sum H_0j	N_j	N_0	Shift	Proj.	
↪Energy								
fciqmc/hubbard_fciqmc.out	5222000	(1000)	-7791	(7)	23630	(20)	-0.3299	(3)
↪32969	(2)						-0.	

The stochastic error can be reduced by running with more particles and/or running for longer. Another very effective method is to allow determinants to have fractional numbers of particles on determinants rather than just using a strictly integer representation of the wavefunction. This is done using the `real_amplitudes` keyword:

```
hubbard = hubbard_k {
  lattice = {
    { 3, 3 },
    { 3, -3 },
  },
  electrons = 18,
  ms = 0,
  U = 1.3,
  t = 1,
  sym = 1,
}

fciqmc {
  sys = hubbard,
  qmc = {
    tau = 0.002,
    mc_cycles = 20,
    nreports = 10000,
    init_pop = 100,
    target_population = 4*10^6,
    state_size = -1000,
    spawned_state_size = -100,
    real_amplitudes = true,
  },
}
```

The calculation can be run and analysed in the same manner:

```
$ mpiexec hande.x hubbard_fciqmc_real.lua > hubbard_fciqmc_real.out
$ reblock_hande.py --quiet --start 30000 hubbard_fciqmc_real.out
```

which results in:

Recommended statistics **from optimal** block size:

	# H	psips	\sum H_0j	N_j	N_0	Shift	Proj.	
↪Proj. Energy								
fciqmc/hubbard_fciqmc_real.out	5230600	(100)	-15460	(2)	46890	(6)	-0.32976	(3)
↪329694	(4)						-0.	

Whilst using real amplitudes is substantially slower, the reduction in stochastic error more than compensates; it is much more efficient than simply running for longer. Real amplitudes also reduce the plateau height in some cases (as is the case here) though this has not been investigated carefully in a wide variety of systems.

One reason that the calculation with real amplitudes took so much longer than that with integer amplitudes is due to the nature of the Hubbard model: all non-zero off-diagonal Hamiltonian matrix elements are identical in magnitude. Carefully inspecting the output in `hubbard_fciqmc_real.out` reveals that there is almost one spawning event

for every particle<sup>2</sup>. This results in a costly communication overhead every timestep. We can improve this by changing the `spawn_cutoff` parameter, which is the minimum absolute value of a spawning event [Overy2014]. A spawning event with a smaller cutoff is probabilistically rounded to zero or the cutoff value<sup>3</sup>. The default cutoff value, 0.01, need only be changed in cases such as this and is set using the `spawn_cutoff` parameter in the `qmc` table:

```
hubbard = hubbard_k {
  lattice = {
    { 3, 3 },
    { 3, -3 },
  },
  electrons = 18,
  ms = 0,
  U = 1.3,
  t = 1,
  sym = 1,
}

fciqmc {
  sys = hubbard,
  qmc = {
    tau = 0.002,
    mc_cycles = 20,
    nreports = 10000,
    init_pop = 100,
    target_population = 4*10^6,
    state_size = -1000,
    spawned_state_size = -100,
    real_amplitudes = true,
    spawn_cutoff = 0.1,
  },
}
```

Note that a value of 1 is comparable to using integer amplitudes except for the death step, which acts without stochastic rounding if `real_amplitudes` is enabled.

We can run calculations with different values of `spawn_cutoff` as before; here we set use values of 0.1, 0.25 and 0.5. `reblock_hande.py` can analyse multiple calculations at once and so we can easily see the impact of changing `spawn_cutoff` compared to the default value and the original FCIQMC calculation using integer amplitudes:

```
$ reblock_hande.py --quiet --start 30000 hubbard_fciqmc*out
```

Recommended statistics from optimal block size:

	# H psips	\sum H_0j	N_j	N_0	
↪ Shift Proj. Energy					
fciqmc/hubbard_fciqmc.out	5222000 (1000)	-7791 (7)	23630 (20)	-0.	
↪ 3299 (3) -0.32969 (2)					
fciqmc/hubbard_fciqmc_real.out	5230600 (100)	-15460 (2)	46890 (6)	-0.	
↪ 32976 (3) -0.329694 (4)					
fciqmc/hubbard_fciqmc_real_sc0.1.out	5225400 (200)	-13172 (1)	39952 (4)	-0.	
↪ 32968 (5) -0.329704 (6)					
fciqmc/hubbard_fciqmc_real_sc0.25.out	5219300 (400)	-10627 (4)	32230 (10)	-0.	
↪ 3298 (1) -0.329696 (9)					

(continues on next page)

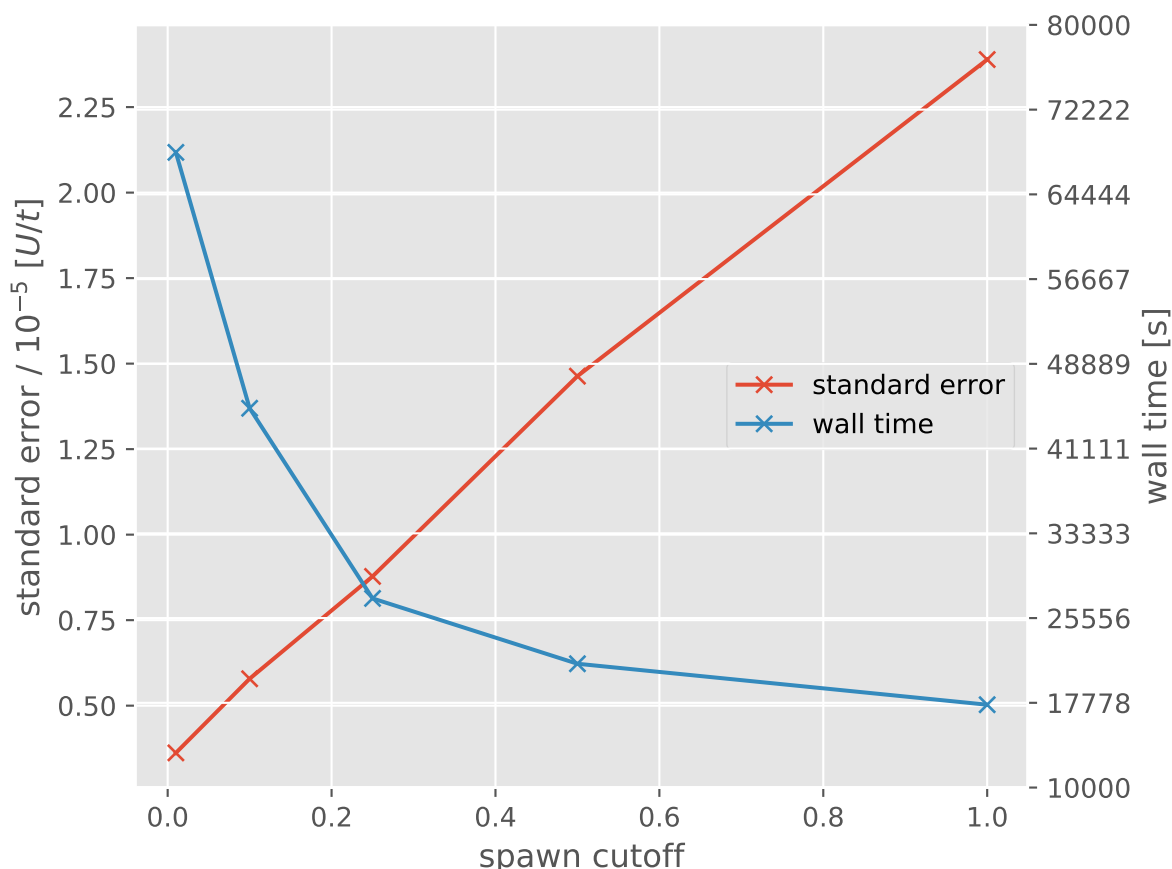
<sup>2</sup> This can be confirmed analytically using knowledge of the internal excitation generators and the associated probabilities, the value of  $U/t$  and the calculation timestep.

<sup>3</sup> One can hence view the integer amplitudes algorithm, ignoring death and spawning events which produce multiple particles, as having a `spawn_cutoff` of 1.

(continued from previous page)

```
fciqmc/hubbard_fciqmc_real_sc0.5.out    5220500 (600)    -9595 (4)    29100 (10)    -0.
↪ 3296 (2)    -0.32970 (1)
```

As expected, increasing the `spawn_cutoff` results in an increase in the stochastic error (linear, in this case, due to the identical magnitude of non-zero off-diagonal Hamiltonian matrix elements). Finally, we can compare the change in stochastic error to the wall time of the calculation:



For convenience, the integer amplitude calculation is shown as having a `spawn_cutoff` of 1. Clearly there is a payoff between the computational cost and the desired stochastic error; choosing a value of 0.25 for `spawn_cutoff` in this case seems sensible as it is around the point where the rate of change in the wall time begins to slow<sup>4</sup>.

### 1.13.2 Initiator Approximation to FCIQMC

We shall again calculate the ground state energy of the 18-site 2D Hubbard model at half-filling and with  $U/t = 1.3$ , as in the *FCIQMC tutorial*. The initiator approximation [Cleland10] greatly reduces the number of particles required to sample the wavefunction. The drawback, however, is that the approximation must be carefully controlled to obtain an accurate estimate of the FCI energy by running multiple calculations with increasing populations.

It is efficient (both computationally and in terms of elapsed time) to treat each calculation separately. For compactness, we shall simply run multiple calculations with different `target_population` values one after the other in the same HANDE calculation. This is trivial to do by using a lua loop as `fciqmc` is simply a function call:

<sup>4</sup> A more comprehensive approach to assessing the efficiency of the calculations can be found in [Vigor16].

```

hubbard = hubbard_k {
    lattice = {
        { 3, 3 },
        { 3, -3 },
    },
    electrons = 18,
    ms = 0,
    U = 1.3,
    t = 1,
    sym = 1,
}

targets = {2.5*10^3, 5*10^3, 7.5*10^3, 10^4, 2.5*10^4, 5*10^4, 1*10^5, 2.5*10^5, 5*10^
↪5, 1*10^6}
for i,target in ipairs(targets) do
    qmc_state = fciqmc {
        sys = hubbard,
        qmc = {
            tau = 0.002,
            mc_cycles = 20,
            nreports = 10000,
            init_pop = 100,
            target_population = target,
            state_size = -1000,
            spawned_state_size = -100,
            initiator = true,
        },
    }
    -- For memory efficiency, explicitly free qmc_state after each calculation.
    qmc_state:free()
end

```

The only difference between the above input and an FCIQMC calculation is the setting `initiator = true`. As in the examples in the [FCIQMC tutorial](#), this can be run using:

```
$ mpiexec hande.x hubbard_ifciqmc.lua > hubbard_ifciqmc.out
```

Again, the exact command to launch MPI will vary with MPI implementation and local configurations.

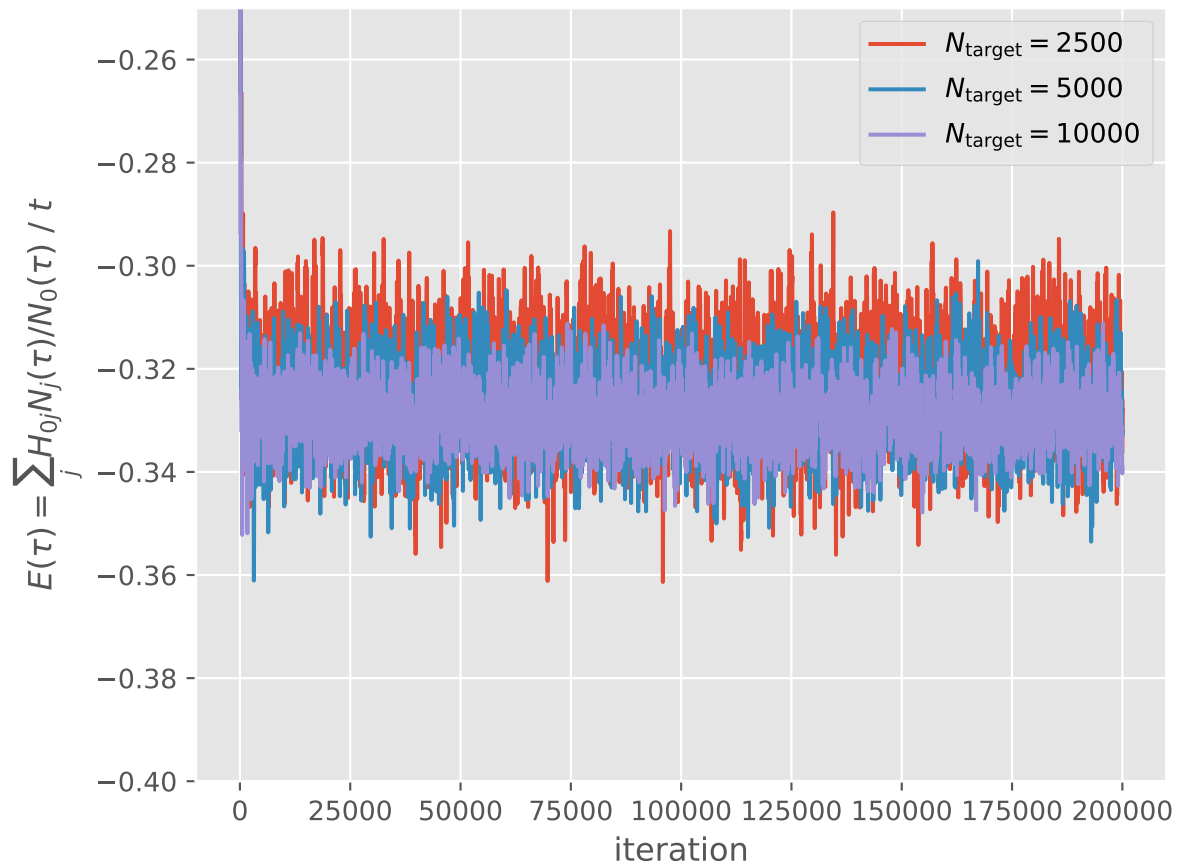
Inspecting the output, we see one iFCIQMC calculation was run for each call to the `fciqmc` function. `pyhande` (and, by extension, `reblock_hande.py`) can handle such cases, so we easily extract and inspect the data for each calculation.

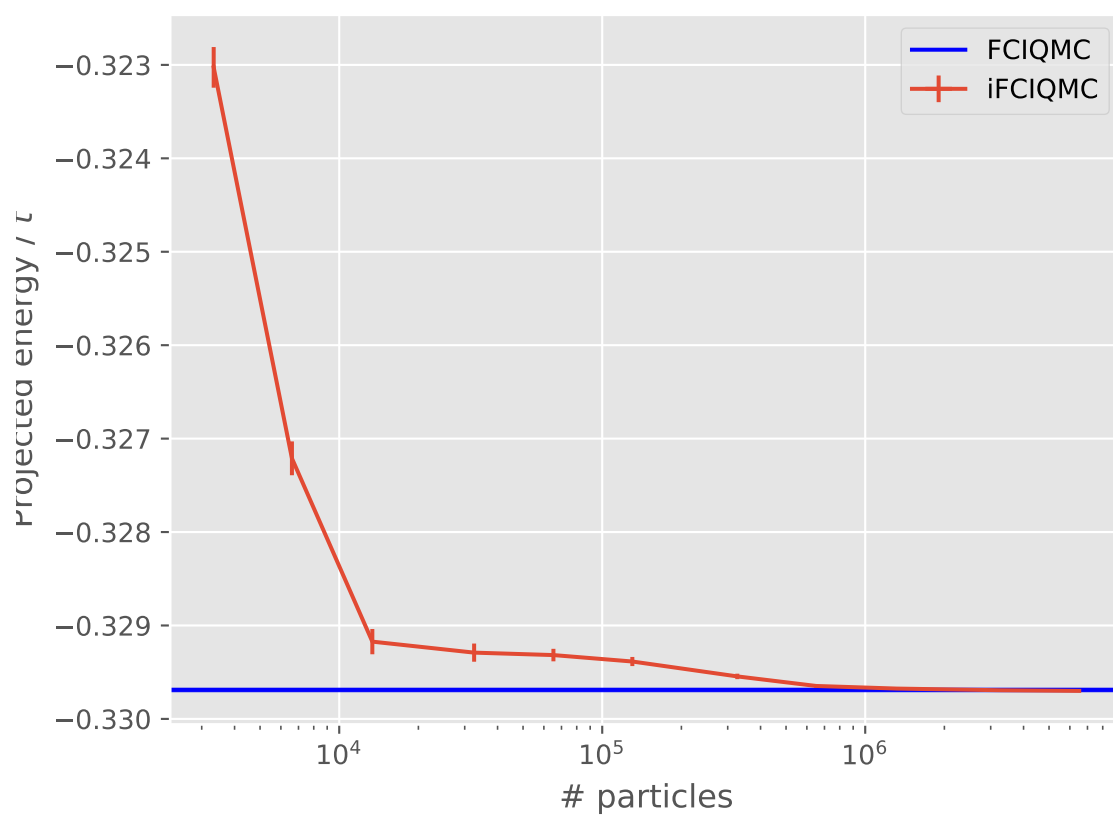
Let's start by inspecting instantaneous projected energy estimator for the three smallest populations:

Whilst the difference is small on this scale, it is evident that the calculation with the smallest population has a slightly higher mean than calculations with larger populations. To confirm this, we will plot the energy as a function of population. As `target_population` is the population at which the population **starts** to be controlled, we should consider the average population (which is somewhat higher). We can also compare directly to the FCIQMC energy in this case, as the population required for the FCIQMC calculation is sufficiently small:

The light blue region indicates the extent of the FCIQMC stochastic error, as calculated in the [FCIQMC tutorial](#). In this case, the initiator approximation reduces the population required by a factor of  $\sim 2$ . However, many studies (including on the electron gas and molecular systems) have demonstrated the initiator approximation can reduce the population required by many orders of magnitude.

The estimates for each calculation can be found directly by using `reblock_hande.py`:





```
$ reblock_hande.py --quiet --start 30000 hubbard_ifciqmc.out
```

where again we chose the start point from inspecting the population growth. This gives:

Recommended statistics **from optimal** block size:

	#	$H$	$psips$	$\backslash sum$	$H_{-0j}$	$N_{-j}$	$N_{-0}$	$Shift$	
↪ Proj. Energy									
ifciqmc/hubbard_ifciqmc.out	0	3332	(6)	-91.6	(1)	283.6	(4)	-0.325	(2)
↪ -0.3230									
	1	6609	(9)	-153.6	(2)	469.4	(8)	-0.328	(2)
↪ -0.3272									
	2	13360	(10)	-293.3	(3)	890.9	(7)	-0.329	(1)
↪ -0.3292									
	3	32580	(20)	-718.7	(4)	2182	(2)	-0.3293	(6)
↪ -0.3293									
	4	65230	(30)	-1403.2	(6)	4261	(2)	-0.3291	(5)
↪ -0.32932									
	5	130170	(30)	-2586.4	(5)	7853	(2)	-0.3289	(3)
↪ -0.32939									
	6	326320	(60)	-5520.8	(8)	16753	(3)	-0.3298	(2)
↪ -0.32955									
	7	651010	(80)	-9937	(1)	30146	(4)	-0.3296	(1)
↪ -0.32965									
	8	1318400	(100)	-19354	(2)	58707	(6)	-0.32969	(9)
↪ -0.32968									
	9	3279800	(200)	-48971	(4)	148530	(20)	-0.32962	(7)
↪ 0.329693									
	10	6512700	(200)	-97670	(4)	296240	(10)	-0.32971	(5)
↪ 0.329700									

reblock\_hande.py can also handle the case where each calculation is run separately and each separate file is passed in as a separate argument on the command line.

**Note:** We highly recommend a visual inspection of the plot of the initiator error as a function of population as the convergence can be non-monotonic and, as a result, at least two calculations at different populations with statistically equivalent results are required in order to confirm the error due to the initiator approximation is smaller than the stochastic error.

Finally, using real populations can, as with the *FCIQMC tutorial*, have a significant impact on the stochastic error. Again, this is done by setting `real_amplitudes = true` in the input file (see `hubbard_ifciqmc_real.lua`). We also choose to set `spawn_cutoff` to 0.25 following the investigation in *FCIQMC tutorial*; this results in a small increase in the stochastic error but results in the calculation taking roughly half the time. Again, note this is somewhat unique to the Hubbard model. Running:

```
$ mpiexec hande.x hubbard_ifciqmc_real.lua > hubbard_ifciqmc_real.out
```

followed by the blocking analysis on the output:

```
$ reblock_hande.py --quiet --start 30000 hubbard_ifciqmc_real.out
```

results in

Recommended statistics **from optimal** block size:

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		# H	psips	\sum H_0j	N_j	N_0	
↪Shift	Proj. Energy						
ifciqmc/hubbard_ifciqmc_real.out	0	3271	(2)	-91.03	(5)	280.7	(2) -0.
↪3234	(9) -0.3243	(1)					
	1	6643	(4)	-148.28	(8)	451.5	(3) -0.
↪3298	(7) -0.32844	(7)					
	2	13100	(7)	-288.8	(2)	877.4	(7) -0.
↪3285	(7) -0.32917	(7)					
	3	32762	(7)	-744.6	(2)	2261.7	(7) -0.
↪3290	(3) -0.32925	(5)					
	4	65570	(20)	-1510.1	(4)	4586	(1) -0.
↪3300	(3) -0.32930	(3)					
	5	130830	(20)	-2855.0	(3)	8669	(1) -0.
↪3295	(1) -0.32934	(2)					
	6	326640	(30)	-5821.8	(6)	17665	(2) -0.
↪3296	(1) -0.32957	(1)					
	7	660180	(40)	-10118.3	(5)	30694	(2) -0.
↪32981	(7) -0.32965	(1)					
	8	1303850	(60)	-19413	(1)	58882	(4) -0.
↪32958	(5) -0.329689	(8)					
	9	3287160	(90)	-51020	(2)	154749	(5) -0.
↪32969	(3) -0.329699	(5)					
	10	6548200	(100)	-103229	(2)	313100	(10) -0.
↪32967	(2) -0.329698	(3)					

Again, there is a general trend (though not entirely smooth) for the energy estimators to converge to the same energy as a function of total population. It is interesting to take a close look at the convergence of the projected energy estimator:

The cluster of results around populations of  $5 \times 10^5$  shows that it is vital to reduce the stochastic error before deciding the remaining initiator error is negligible. Further, it is interesting to note that the initiator approximation results in a much more efficient sampling of the Hilbert space: for a similar population ( $\sim 10^6$ ), the iFCIQMC calculations have a **much** smaller stochastic error for a similar computational cost.

### 1.13.3 Semi-Stochastic FCIQMC

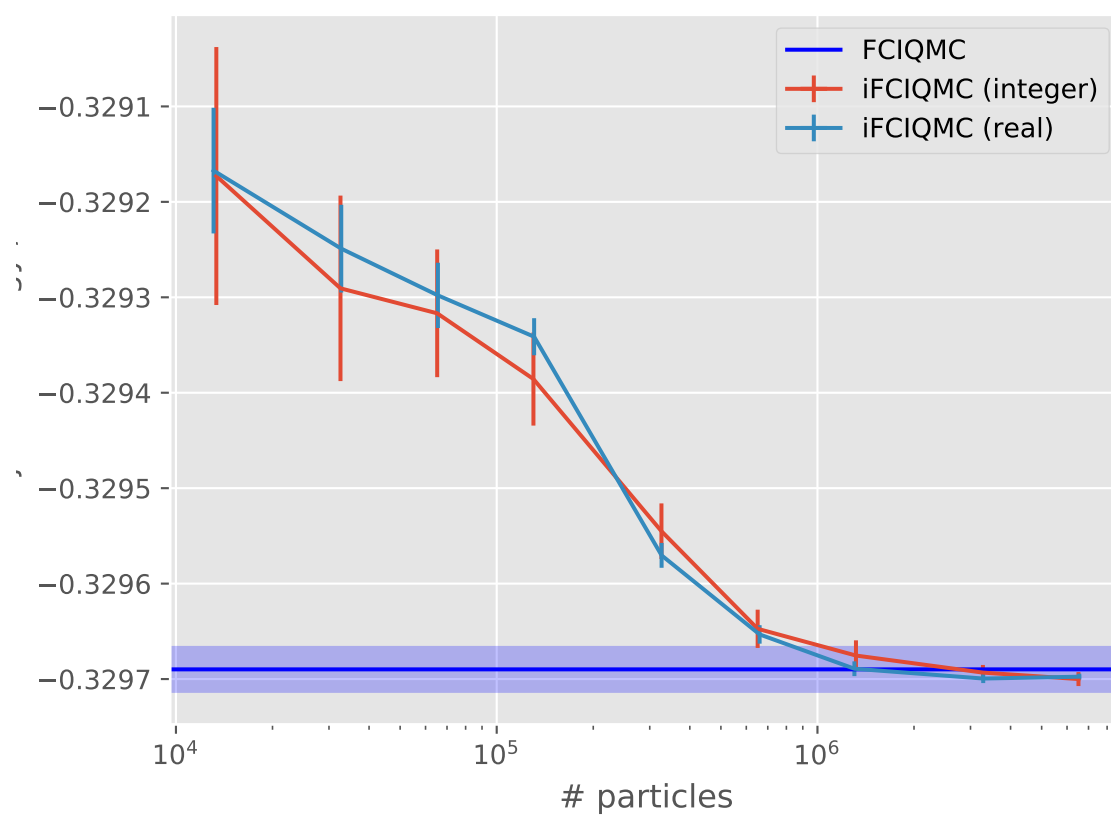
In this tutorial we will explain how to run FCIQMC calculations using the semi-stochastic adaptation to reduce stochastic errors [Petruziello12]. We will consider the half-filled 18-site 2D Hubbard model at  $U/t = 1.3$ , as previously considered in the basic *Full Configuration Interaction Quantum Monte Carlo* tutorial. In particular, we shall begin from the input file presented at the end of the FCIQMC tutorial, which introduces the use of non-integer psip amplitudes through the `real_amplitudes` keyword:

```
hubbard = hubbard_k {
  lattice = {
    { 3, 3 },
    { 3, -3 },
  },
  electrons = 18,
  ms = 0,
  U = 1.3,
  t = 1,
  sym = 1,
}

fcIQMC {
  sys = hubbard,
```

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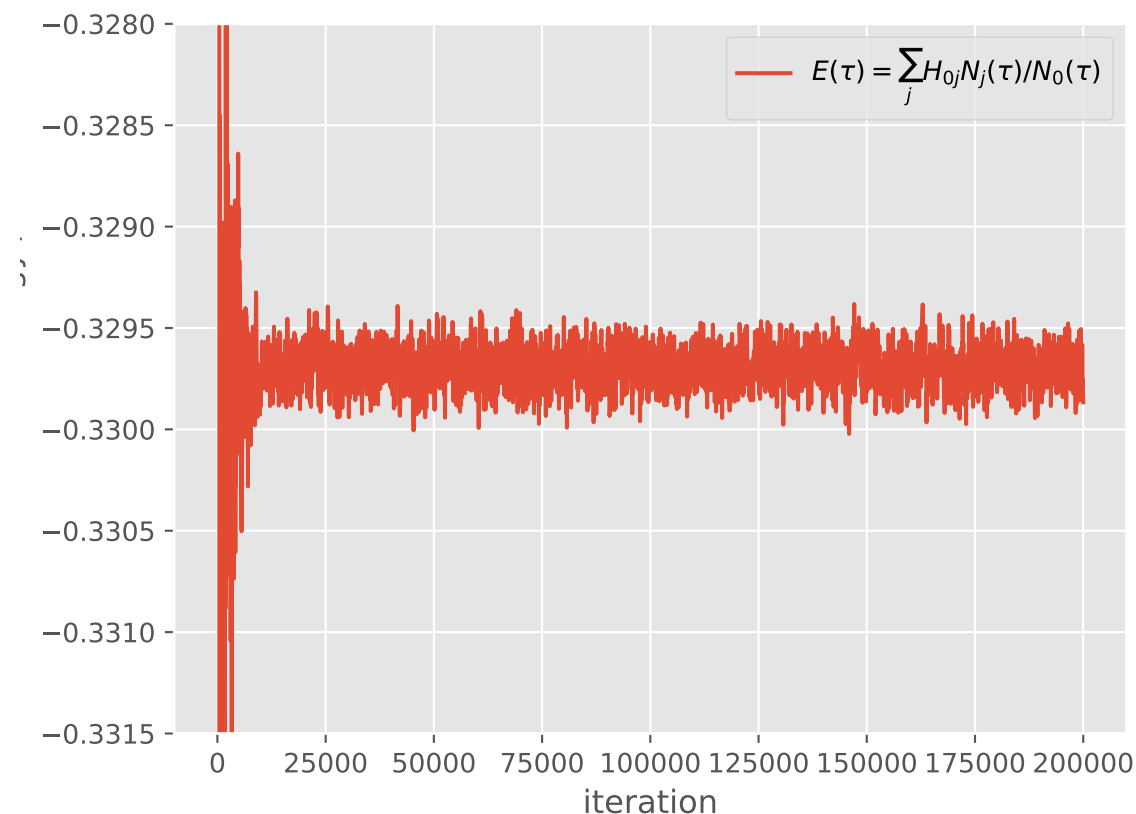
(continued from previous page)

```

qmc = {
    tau = 0.002,
    mc_cycles = 20,
    nreports = 10000,
    init_pop = 100,
    target_population = 4*10^6,
    state_size = -1000,
    spawned_state_size = -100,
    real_amplitudes = true,
},
}

```

and which results in the following simulation:



The semi-stochastic adaptation provides a way to reduce the stochastic noise in such simulations. It does so by choosing a certain subspace (called the deterministic subspace), which is deemed to be most important (in that most of the wave function amplitude resides in this subspace), and performing projection exactly within it. Projection outside the subspace is performed by the usual FCIQMC stochastic spawning.

Thus, we simply need to specify what subspace to use for the exact projection. One way of doing this is by using the scheme of [Blunt15], where the subspace is formed from the determinants on which the largest number of psips reside. We therefore simply need to tell HANDE what iteration to start using the semi-stochastic adaptation, and how many determinants to form the deterministic subspace from.

There are a couple of things to consider when choosing the size of the deterministic space. Firstly, within the deter-

ministic subspace, the Hamiltonian is stored exactly in a sparse form. Therefore, using semi-stochastic does increase memory requirements. The deterministic Hamiltonian storage (and multiplication) is distributed across processing cores, which allows larger subspaces to be used. The other consideration is that, for very large deterministic spaces, and for certain systems (particularly strongly correlated systems), semi-stochastic can slow simulations down slightly. Through investigation (for example, see [Blunt15]), it has been found that a deterministic space of size  $10^4$  allows a very large reduction in stochastic error for most simulations, while not increasing simulation time. We therefore suggest this as a black box subspace size. This is also small enough that the deterministic Hamiltonian can always be stored, even if using only a typical desktop computer.

Note that because semi-stochastic does not usually reduce iteration time much (and sometimes increases it), one should not worry that we do not use semi-stochastic from the first iteration. We are only concerned with reduction in stochastic error from the point where data will be averaged later.

Looking at the above simulation, it appears that the energy has converged by iteration  $2 \times 10^4$ . This is not a guarantee that the wave function is also fully converged, but full convergence is not critical – so long as the most important determinants are in the deterministic subspace, then a large reduction in stochastic error will occur. As discussed above, a reasonable deterministic space size is  $10^4$ . So, to start using a deterministic space of size  $10^4$  at iteration  $2 \times 10^4$ , we modify the above input to the following:

```
hubbard = hubbard_k {
    lattice = {
        { 3, 3 },
        { 3, -3 },
    },
    electrons = 18,
    ms = 0,
    U = 1.3,
    t = 1,
    sym = 1,
}

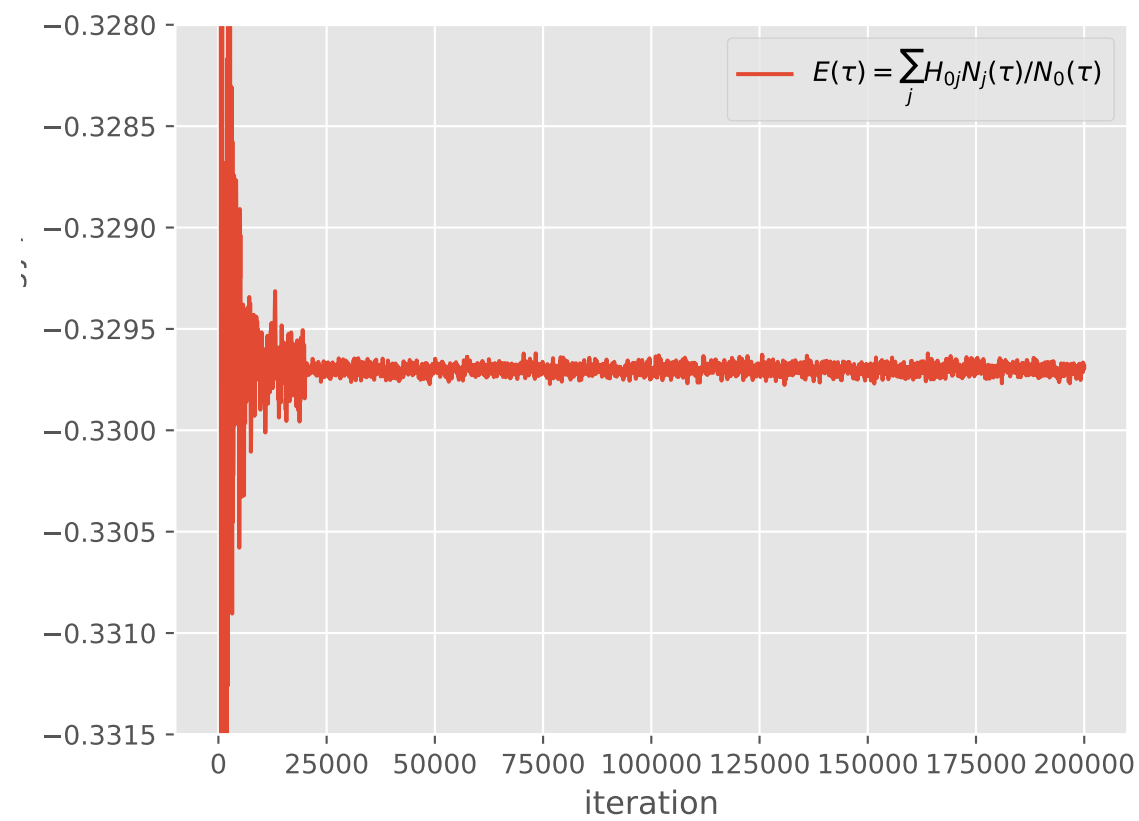
fcqmcc {
    sys = hubbard,
    qmc = {
        tau = 0.002,
        mc_cycles = 20,
        nreports = 10000,
        init_pop = 100,
        target_population = 4*10^6,
        state_size = -1000,
        spawned_state_size = -100,
        real_amplitudes = true,
    },
    semi_stoch = {
        size = 10000,
        start_iteration = 20000,
        space = "high",
    },
}
```

Here, the semi-stoch table contains three keywords. The use of size and start\_iteration keywords is hopefully clear. The space keyword determines which method is used to generate the deterministic space - in this case by choosing the determinants with the highest weights.

This results in the following simulation:

As can be seen, at iteration  $2 \times 10^4$  there is a large reduction in stochastic error.

When performing a blocking analysis, the user should not begin averaging data until after the semi-stochastic adapta-



tion has been turned on, since there is a significant change in the probability distributions of data beyond this point. This is particularly true in initiator FCIQMC simulations, where the use of semi-stochastic can alter the initiator error (although we typically find that semi-stochastic does not alter the magnitude of initiator error significantly, it can in some cases, see [Petruszielo12]). We can therefore analyse the above simulation using

```
$ reblock_hande.py --quiet --start 30000 hubbard_semi_stoch_high.out
```

which results in:

Recommended statistics **from optimal** block size:

	# H	psips	\sum H_0j	N_j	N_0	Shift	Proj.
↪Energy							
hubbard_semi_stoch_high.out	5216460	(80)	-15356	(2)	46576	(5)	-0.32970
↪3296994	(8)						-0.

Compared to the equivalent non-semi-stochastic simulation performed in the *FCIQMC tutorial* tutorial, the error bars on the shift and projected energy estimators have reduced from  $4 \times 10^{-5}$  and  $3 \times 10^{-6}$  to  $2 \times 10^{-5}$  and  $8 \times 10^{-7}$ , respectively.

Note that if you do not specify a `start_iteration` value in the `semi_stoch` table of the input file, then the semi-stochastic adaptation will be turned on from the first iteration. This should not be done when starting a new simulation, because wave functions in HANDE are initialised as single determinants. However, if restarting a simulation from an HDF5 file then this is a sensible approach - the simulation will begin from the wave function stored in the HDF5 file, and the deterministic space will be chosen from the most populated determinants in this wave function. An input file for such a restarted simulation would contain the following `semi_stoch` and `restart` tables within the `fcimc` table:

```
fcimc {
  sys = hubbard_k{...},
  qmc = {...},
  semi_stoch = {
    size = 10000,
    space = "high",
  },
  restart = {
    read = 0,
  },
}
```

(see the *restart options* entry in the documentation for more options relating to restarting simulations).

Finally, when restarting simulations which were already using the semi-stochastic adaptation, it is important to use exactly the same deterministic space to ensure that estimators are statistically consistent before and after restarting. However, the approach in HANDE uses the instantaneous FCIQMC wave function to generate the deterministic space, which changes during the simulation. Using the above approach would therefore lead to a slightly different space being generated after restarting. One can get around this by outputting the deterministic space in use to a file, and reading it back in for the restarted calculation. For example, to generate a deterministic space from the  $10^4$  most populated determinants at iteration  $2 \times 10^4$ , and to then print this space to a file, one should use the `write` keyword in the `semi_stoch` table:

```
fcimc {
  sys = hubbard_k{...},
  qmc = {...},
  semi_stoch = {
    size = 10000,
    start_iteration = 20000,
    write = "deterministic_space.h5",
  },
}
```

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```

        space = "high",
        write = 0,
    },
}

```

Here, the value of the `write` keyword, 0, is an index used in the name of the resulting file. Note that `write` can also be a boolean, in which case HANDE will find and use the smallest unused id available in the directory.

When restarting the simulation, one can then specify the `space` option to read a semi-stochastic HDF5 file, using:

```

fcimc {
    sys = hubbard_k{...},
    qmc = {...},
    semi_stoch = {
        space = "read",
    },
}

```

The deterministic space file is an HDF5 file. As such, both writing and reading of such files requires *compilation* of HANDE with HDF5 enabled, which is the default compilation behaviour.

### 1.13.4 Coupled Cluster Monte Carlo

In this tutorial we will run CCMC on the carbon monoxide molecule in a cc-pVDZ basis. For details of the theory see [Thom10] and [Spencer15].

This tutorial only presents the basic options available in a CCMC calculation; for the full range of options see the main *documentation*.

To perform calculations on a molecular system in HANDE, we need the one- and two- electron *integrals* in some appropriate basis from an external source. For the calculations in this tutorial, the integrals were calculated using Psi4; input and output files can be found with the files from the calculations herein in the `documentation/manual/tutorials/calcs/ccmc` subdirectory.

The system definition is exactly the same as for FCIQMC:

```

sys = read_in {
    int_file = "CO.CCPVDZ.FCIDUMP",
    nel = 14,
    ms = 0,
}

```

Note that we have not specified an overall symmetry. In this case HANDE uses the Aufbau principle to select a reference determinant.

A CCMC calculation can be run in a very similar way to FCIQMC. As for FCIQMC we can substantially reduce stochastic error by using real amplitudes, which we do for all calculations presented here. The most significant difference from an FCIQMC input is that it is standard to use truncation with CCMC, specified by the `ex_level` option, (i.e. 2 for CCSD, 3 for CCSDT, etc.). The determination of a plateau and hence a suitable value for `target_population` is exactly analogous to *FCIQMC*, as the sign problem is similar between the two methods; we will not discuss it further here. The CCSDTMC calculation can be run using an input file such as:

```

sys = read_in {
    int_file = "CO.CCPVDZ.FCIDUMP",
    nel = 14,
    ms = 0,
}

```

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```

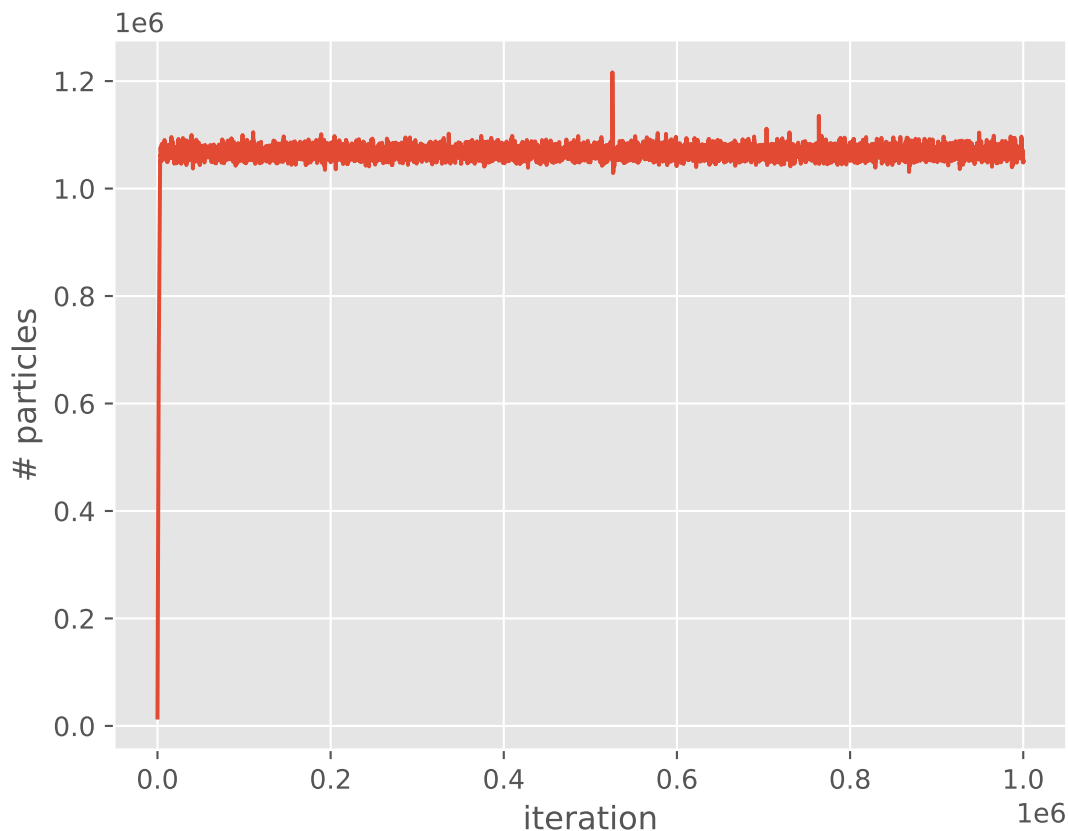
}

ccmc {
  sys = sys,
  qmc = {
    tau = 1e-3,
    mc_cycles = 10,
    nreports = 1e5,
    state_size = -500,
    spawned_state_size = -200,
    init_pop = 1e4,
    target_population = 1e6,
    real_amplitudes = true,
  },
  reference = {
    ex_level = 3,
  },
}

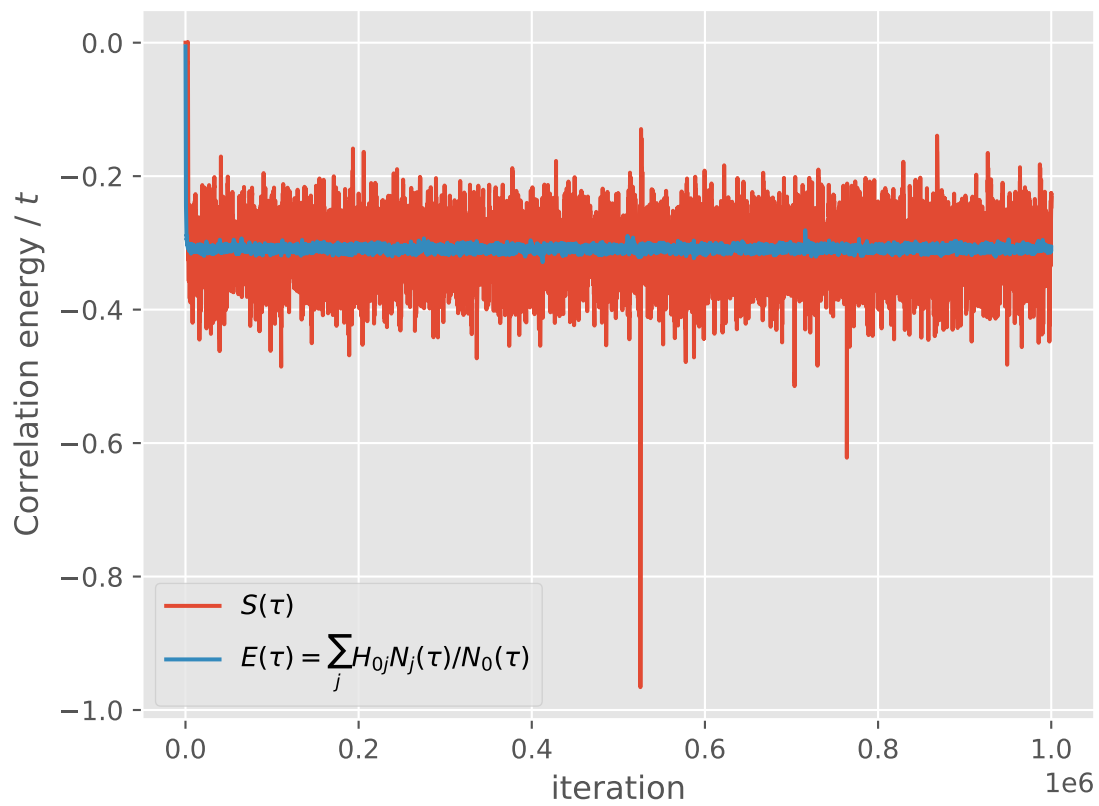
```

Note the much larger initial population compared to an FCIQMC calculation; if this is too low the correct wavefunction will not be obtained.

Looking at the output, we see the evolution of the population has a similar form to FCIQMC:



and the shift and projected energy vary about the correlation energy:





The output of the calculation can be analysed in exactly the same way as for FCIQMC:

```
$ reblock_hande.py --quiet --start 100000 co_ccmc.out
```

giving

Recommended statistics **from optimal** block size:

	# H psips	\sum H_0j N_j	N_0	Shift Proj. Energy
ccmc/co_ccmc.out	1066600(100)	-6510(10)	21040(40)	-0.3092(6) -0.30925(7)

Due to the sampling of the wavefunction in CCMC, it is more prone to “blooming” events where many particles are created in a single spawning event than is FCIQMC. Details of blooming during a calculation are reported at the end of the output. It can be seen that significant blooming occurred. This substantially increases the stochastic error, and in particularly severe cases can cause the calculation to not give a correct result due to the instability. These events can be avoided by reducing the timestep, but the timestep required to eliminate them entirely is often prohibitively small. Another way of reducing them is the use of the `cluster_multispawn_threshold` keyword, whereby large spawning attempts are divided into a number of smaller spawns:

```
sys = read_in {
    int_file = "CO.CCPVDZ.FCIDUMP",
    nel = 14,
    ms = 0,
}

ccmc {
    sys = sys,
    qmc = {
        tau = 1e-3,
        mc_cycles = 10,
        nreports = 1e5,
        state_size = -500,
        spawned_state_size = -200,
        init_pop = 1e4,
        target_population = 1e6,
        real_amplitudes = true,
    },
    ccmc = {
        cluster_multispawn_threshold = 10,
    },
    reference = {
        ex_level = 3,
    },
}
```

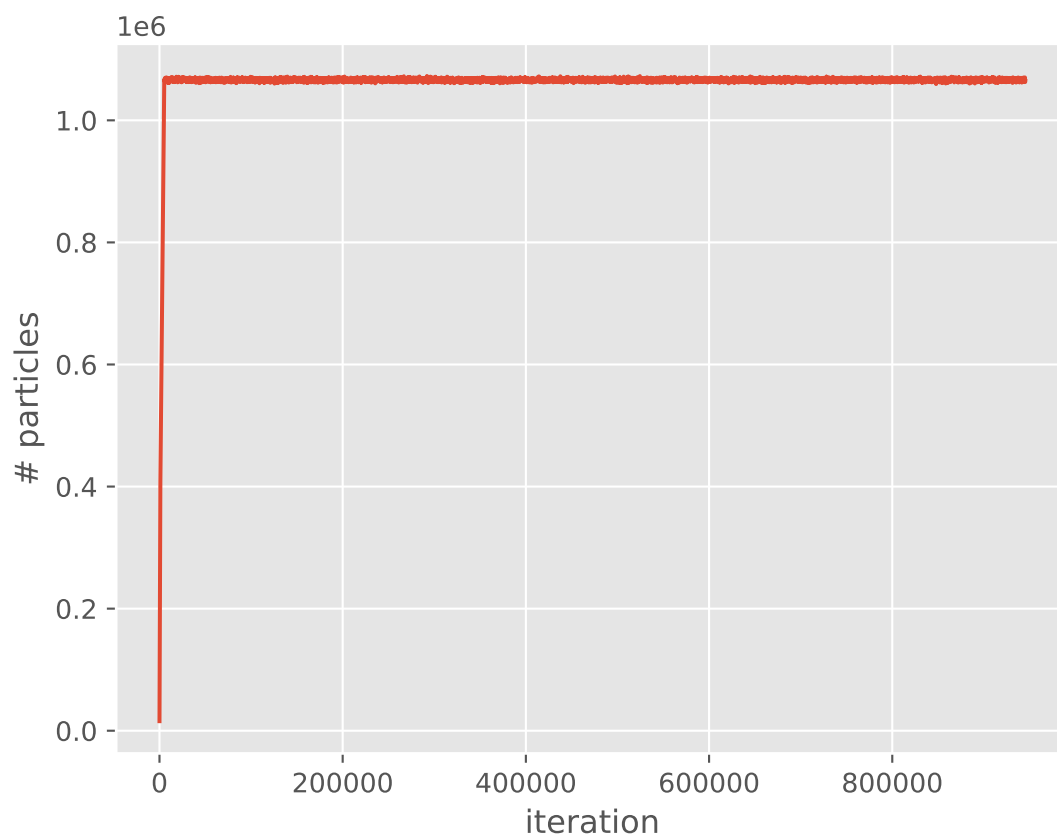
Running as before, and inspecting the output, it can be seen that there are now no blooms. Additionally, plotting the population growth and comparing to the previous plot we see that there are now no spikes in the population:

This substantially reduces the stochastic error:

Recommended statistics **from optimal** block size:

	# H psips	\sum H_0j N_j	N_0	Shift Proj. Energy
ccmc/co_ccmc_multispawn.out	1066160(30)	-11191(1)	36178(7)	-0.3091(1) -0.30933(3)

The extra spawning causes the calculation to run more slowly, but the reduction in error bars can often more than make



up for this.

### 1.13.5 Density Matrix Quantum Monte Carlo

In this tutorial we will run DMQMC on the 2D Heisenberg model and the uniform electron gas. The input and output files can be found under the `documentation/manual/tutorials/calcs/dmqmc` subdirectory of the source distribution. Knowledge of the terminology and theory given in [Booth09], [Blunt14] and [Malone15] is assumed.

To begin we will focus on the 6x6 antiferromagnetic Heisenberg model on a square lattice with periodic boundary conditions. The input file for this system is given as

```
sys = heisenberg {
    lattice = {
        {6, 0},
        {0, 6},
    },
    J = -1.0,
    ms = 0,
}

dmqmc {
    sys = sys,
    qmc = {
        tau = 0.001,
        init_pop = 5e6,
        rng_seed = 19838,
        mc_cycles = 10,
        nreports = 500,
        shift_damping = 0.5,
        target_population = 5e6,
        state_size = -400,
        spawned_state_size = -400,
    },
    dmqmc = {
        beta_loops = 1,
    },
    operators = {
        energy = true,
        excit_dist = true,
    },
}
```

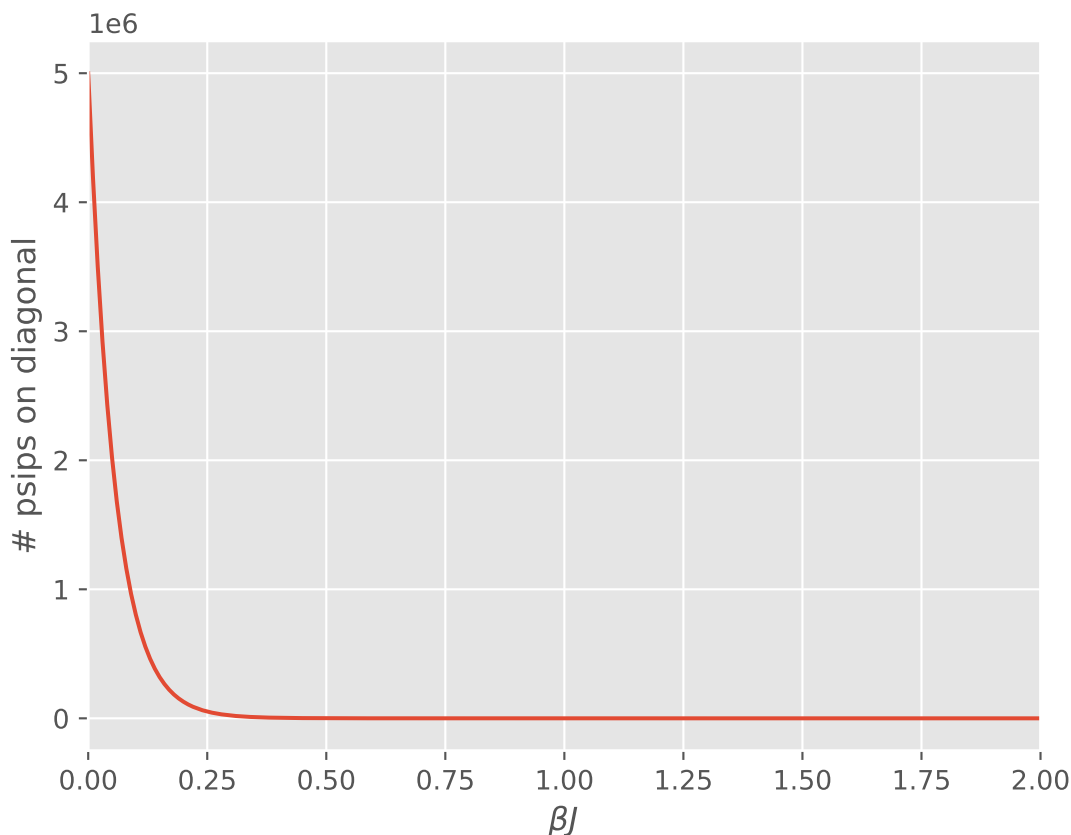
and is largely analogous to that found in the *FCIQMC tutorial*. We refer the reader to the discussion there and the manual for system specific input options. Note that `init_pop` here controls the population with which the density matrix at  $\beta = 0$  is sampled. Typically the shift is allowed to vary from the beginning of a simulation by setting `target_pop` equal to `init_pop`. Here we will attempt to run to a final temperature of  $\beta = 5/J$ . The `beta_loops` option determines the number of independent simulations over which observables are averaged, see *dmqmc options* for more options. The operators table specifies which observables are to be evaluated in a given simulation. Here only the total energy is considered, a full list is available in *operators options*.

An issue encountered when applying DMQMC to larger systems is that the population on the diagonal (denoted Trace in the output file) decays with increasing  $\beta$  which results in poor estimates for observables. The seriousness of this problem needs to be assessed on a system by system basis and should be tested for as a first step, which we'll do now.

To do this we set `beta_loops` to 1 in the input file and run the code as:

```
$ aprun -B hande.x heisenberg_dmcmc.lua > heisenberg_dmcmc.out
```

We find that for this system the population on the diagonal does indeed decay to zero rapidly:

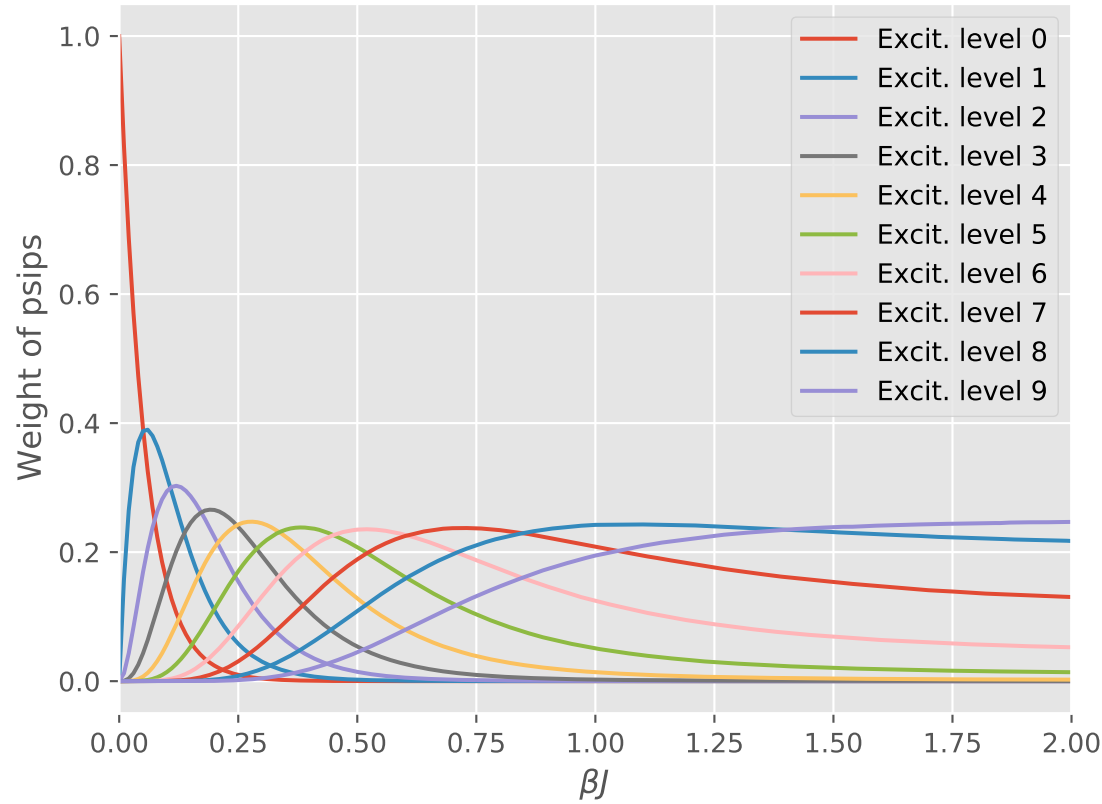


The source of this problem can be investigated by analysing the distribution of psips on different excitation levels of the density matrix, which was calculated in anticipation of this result using the `excit_dist` option in the operators table. Here the excitation level is defined as the difference between the bra and ket of a density matrix element i.e., number of spin flips or number of particle-hole pairs for electronic systems. We see the majority of the total weight is redistributed from the diagonal to highly excited determinants.

To overcome this [Blunt14] invented an unbiased importance sampling scheme to encourage psips to stay on or near the diagonal by penalising spawning moves away from excitation levels. This is sensible as typically the majority of the weight contributing to most physically significant observables originates from the determinants at lower excitation levels which we wish to sample more regularly.

Practically this amounts to first running a calculation with the `find_weights` option. This will output importance sampling weights which are appropriate as input for the production calculation. It is worthwhile to run the calculation for a few `beta_loops` to ensure the weights are not fluctuating too much, and also check they don't fluctuate too much with the `target_population`. The algorithm currently tries to ensure that the number of walkers on each excitation level is roughly constant once the ground state is thought to have been reached. The iteration number where this is deemed to have been reached is controlled by the `find_weights_start` option.

For this system we do



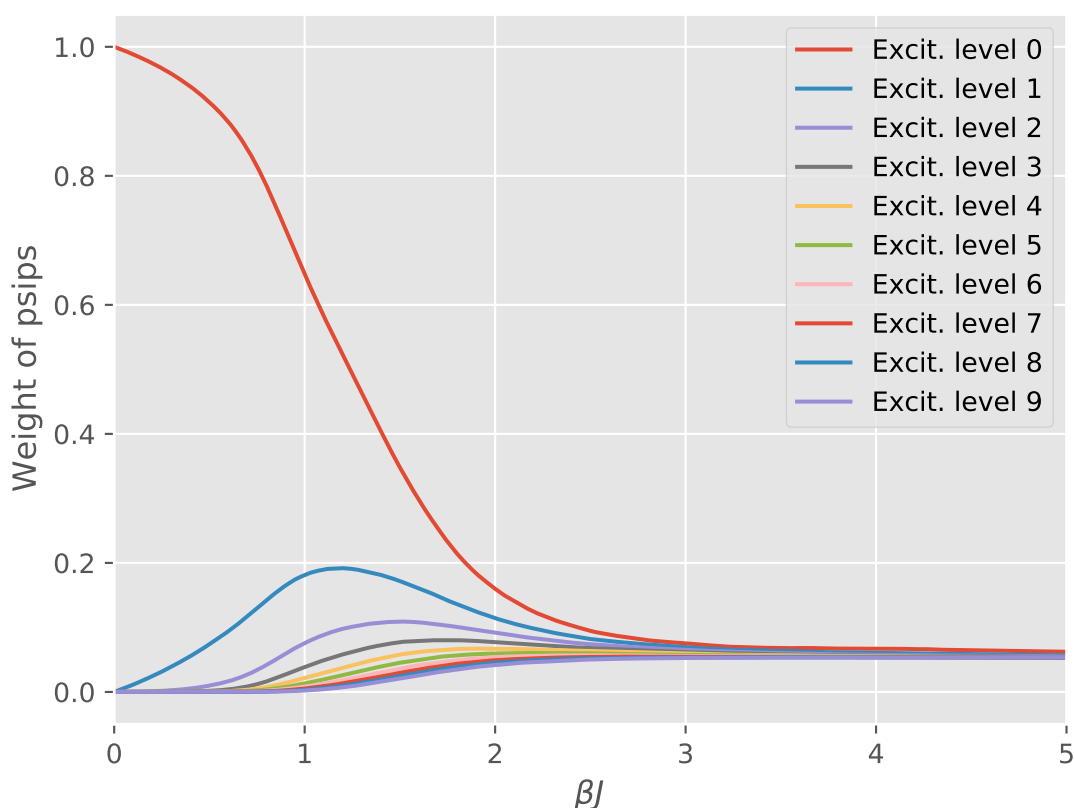
```
$ aprun -B hande.x heisenberg_find_weights.lua > heisenberg_reweighted.out
```

Here we first run a simulation for 10 beta loops to find the weights and then use the last iteration's weights as input to the production calculation. This procedure can be simplified using lua as seen in the input file.

To see what is going on we can copy the weights from the output file and run for a single iteration and again examine the excitation distribution

```
$ aprun -B hande.x heisenberg_reweight_single.lua > heisenberg_reweight_single.out
```

and we find that the psips are now more equally distributed among excitation levels:



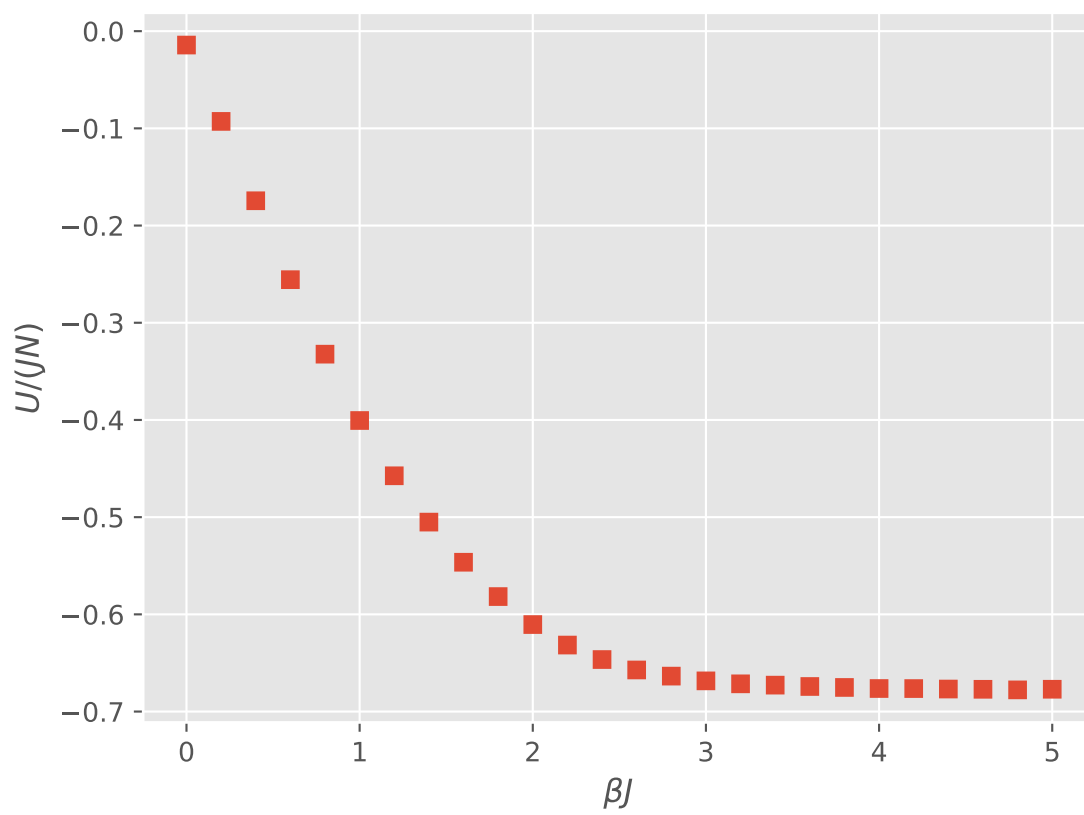
The results of the full reweighted calculation can be analysed using the `finite_temperature_analysis.py` script provided in the `tools/dmcmc` subdirectory:

```
$ finite_temp_analysis.py heisenberg_reweighted.out > heisenberg_reweighted_block.out
```

Finally, we can plot the results of the internal energy,  $U$ , as a function of temperature:

### 1.13.6 Interaction Picture Density Matrix Quantum Monte Carlo

It turns out that the original formulation of DMQMC can run into problems for moderately weakly interacting systems which are relatively well described by Hartree–Fock theory. An extreme example of this is the uniform electron gas (UEG) especially at higher densities (low  $r_s$ ). This issue is largely overcome by switching to the interaction



picture which enables us to start from a (temperature dependent) mean-field distribution at  $\tau = 0$  ensuring low energy determinants are initially sampled. See [Malone15] for details. For systems with a good mean-field ground state the user should consider using IP-DMQMC.

Most of the running details for IP-DMQMC are the same as for DMQMC, however there are some additional considerations. This is best demonstrated by running a simulation. We will focus on a 7-electron, spin polarised system in 319 plane waves at  $r_s = 1$ .

Looking at the input file

```
sys = ueg {
    nel = 7,
    ms = 7,
    sym = 1,
    dim = 3,
    cutoff = 10,
    rs = 1,
}

dmqmc {
    sys = sys,
    qmc = {
        tau = 0.001,
        rng_seed = 7,
        init_pop = 10000,
        mc_cycles = 10,
        nreports = 100,
        target_population = 10000,
        state_size = -200,
        spawned_state_size = -100,
    },
    dmqmc = {
        fermi_temperature = true,
        all_sym_sectors = true,
        beta_loops = 100,
    },
    ipdmqmc = {
        target_beta = 1.0,
        initial_matrix = 'free_electron',
        grand_canonical_initialisation = true,
        symmetric = false,
    },
    operators = {
        energy = true,
    },
}
```

we see most of the same options are present as for dmqmc. Note that unlike DMQMC where estimates for the whole temperature range are gathered in a single simulation, in IP-DMQMC only one temperature value is (directly) accessible, specified by the `target_beta` option. We've also set the energy scale to be determined by the Fermi energy of the corresponding (thermodynamic limit) free electron gas so that the temperatures are interpreted as fractions of the Fermi temperature (here  $\Theta = 0.5$ ). `all_sym_sectors` ensures all momentum symmetry sectors are averaged over. To average over spin polarisation the `all_spin_sectors` option must be specified.

Moving on through the `ipdmqmc` table we've set the `initial_matrix` to be the free electron density matrix, i.e., Fermi-Dirac like. Additionally we're using the `grand_canonical_initialisation` option to initialise this density matrix (see [Malone15]). This is the recommended method to initialise the density matrix; the Metropolis algorithm should only be used for testing.



Finally we will use the asymmetric form of the original IP-DMQMC algorithm by specifying `symmetric` to be false. The symmetric algorithm is somewhat experimental but can lead to better estimates for quantities other than the internal energy especially at lower temperatures. This is thought to be due to sampling issues at low temperatures where the initial mean field guess becomes significantly different (in terms of energy scales) to the fully interacting theory. Symmetrising the equations allows psips to move along rows and which improves sampling. See [Malone16].

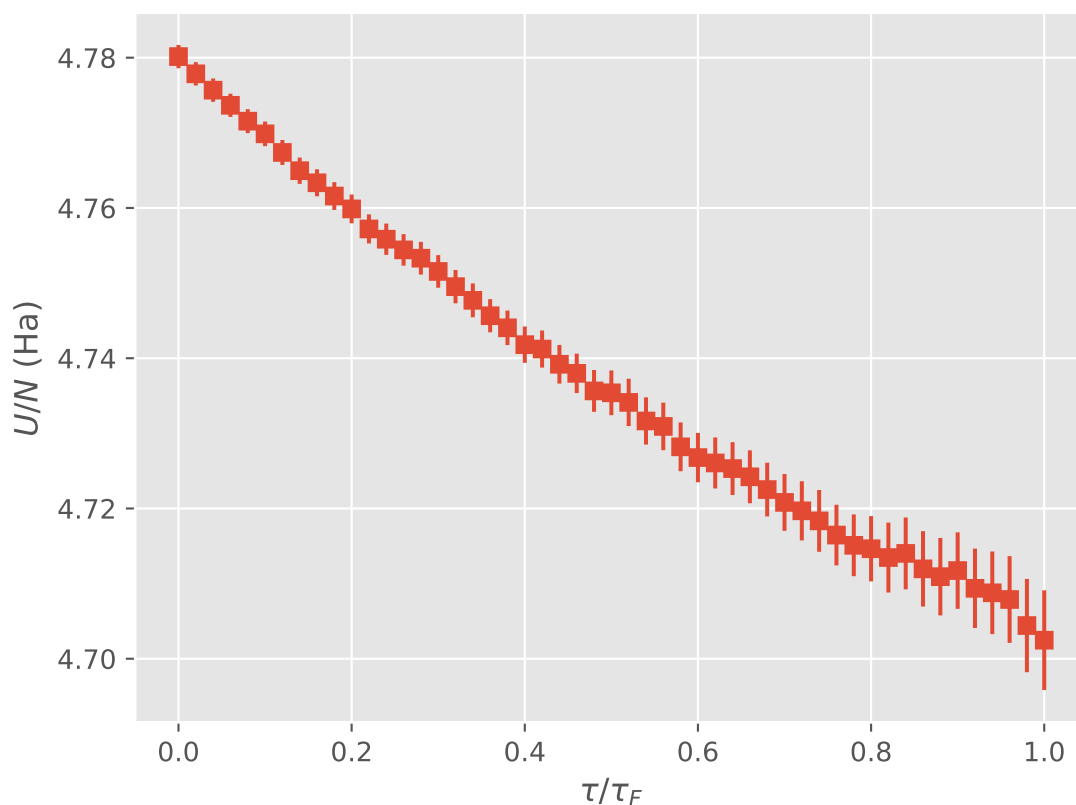
Running the code

```
$ hande.x ipdmqmc_ueg.lua > ipdmqmc_ueg.out
```

and analysing the output:

```
$ finite_temp_analysis.py ipdmqmc_ueg.out > ipdmqmc_ueg_block.out
```

we find



where again only estimates at the final iteration are physical, i.e., when  $\tau = \beta$ . Note that the estimates do not contain a Madelung constant.

The initiator approximation can significantly extend the range of applicability of DMQMC but is somewhat experimental. See the options, in particular `initiator_level` in the manual for more discussion. The user should ensure results are meaningful by comparing answers at various walker populations. See [Malone16] for further discussion.

### 1.13.7 Canonical Estimates

In this tutorial we will discuss how estimates for various mean-field properties of a system can be evaluated in the canonical ensemble at finite temperatures. These estimates are useful for basis set extrapolation as well as comparison to the fully interacting results and are non-trivial to evaluate analytically. See [Malone15] for details.

The input file is fairly simple:

```
sys = ueg {
    nel = 7,
    ms = 7,
    dim = 3,
    cutoff = 10,
    rs = 1,
}

canonical_estimates {
    sys = sys,
    canonical_estimates = {
        beta = 1,
        nattempts = 10000,
        ncycles = 1000,
        fermi_temperature = true,
    },
}
```

Here we attempt to generate  $N$  particle states making `nattempts` attempts and then run the simulation for `ncycles*nattempts` iterations in total. The only other options available are the inverse temperature desired, which can be scaled by the Fermi temperature (where appropriate). Here we restrict ourself to the fully spin polarised UEG in  $M=389$  plane waves, which can be compared to the IP-DMQMC simulation in the [DMQMC tutorial](#).

Running the input file we find

```
$ hande.x canonical_estimates.lua > canonical_estimates.out
```

Inspecting the output, we see a number of columns for various estimates including the kinetic, potential, internal, free energy and entropy - precise definitions of everything can be found in the output file. The data can be analysed to find the mean and standard error using the `analyse_canonical.py` script in the `tools/canonical_energy` subdirectory:

```
$ analyse_canonical.py canonical_estimates.out
```

which gives

	Beta	U_0	U_0_error	T_0	T_0_error	F_0	F_0_error	U_HF
→ V_0	V_0_error	N_ACC/N_ATT	N_ACC/N_ATT_error	T_HF	T_HF_error			
→ error	S_0	S_0_error						
→ U_HF_error		V_HF	V_HF_error					
1.00000000e+00	3.34489604e+01	7.12207413e-03	3.42505858e+01	7.00598613e-03	-8.			
→ 01625332e-01	1.43282029e-04	1.67618487e-01	1.16924926e-04	-1.83693842e+01	2.			
→ 03921704e-03	1.79999929e+01	2.45760105e-03	3.37906337e+01	6.93061658e-03	3.			
→ 29774580e+01	7.04945348e-03	-8.13175652e-01	1.46382195e-04					

In particular, we can compare the values of  $U_0$  and  $U_{HF}$  to the value of 32.91(4) Ha from the IP-DMQMC tutorial.

### 1.13.8 Shoulder Plots

This tutorial looks further into finding the optimal target particle population in more detail. It is advisable to have read the [FCIQMC](#) and [CCMC](#) tutorials before this one. More information and details on shoulder plots can be found in [\[Spencer15\]](#).

The example used here is a CCSDT Monte Carlo calculation on water in a cc-pVDZ basis [\[Dunning89\]](#). As in the [CCMC tutorial](#), the integrals were calculated with PSI4 (see [Generating integrals](#) for details). Input and output files are in `documentation/manual/tutorials/calcs/shoulder/`.

The first calculation was run using

```
sys = read_in {
    int_file = "H2O_INTDUMP",
    nel = 10,
    ms = 0,
}

ccmc {
    sys = sys,
    qmc = {
        tau = 1e-4,
        mc_cycles = 10,
        nreports = 2e4,
        state_size = -500,
        spawned_state_size = -200,
        init_pop = 200,
        real_amplitudes = true,
        target_population = 3e5,
    },
    reference = {
        ex_level = 3,
    },
}
```

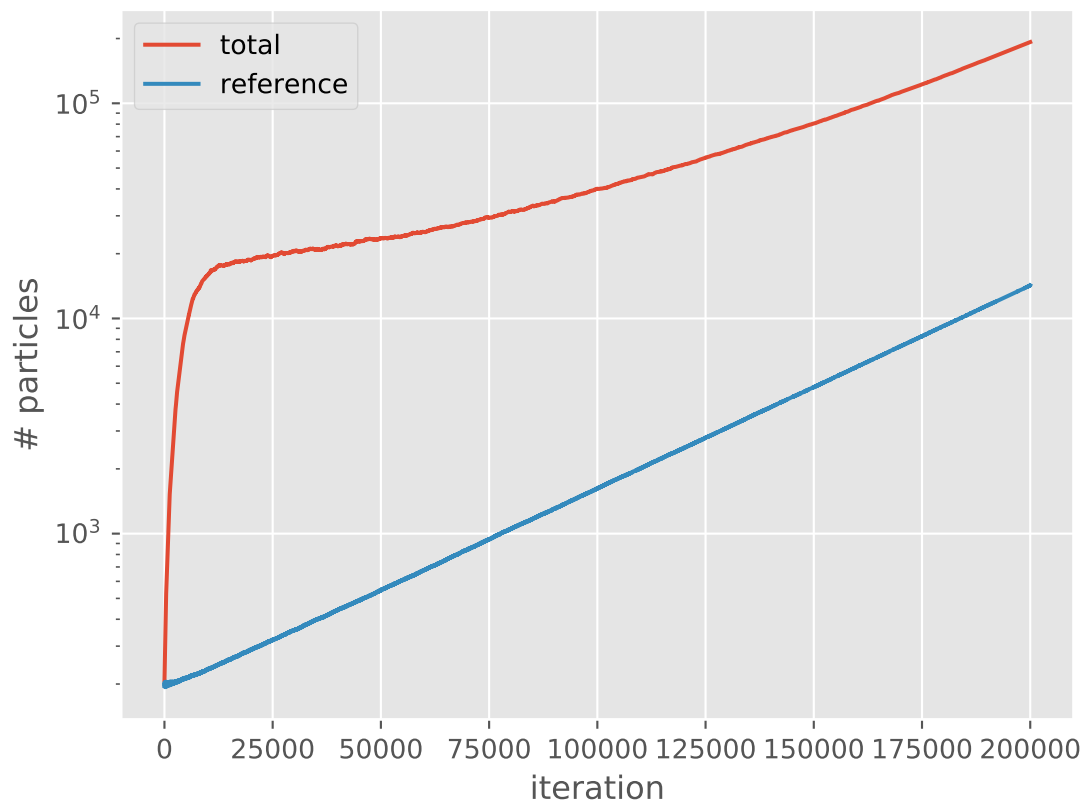
Just like [FCIQMC](#), a plateau can be seen in a total population vs iteration plot, which indicates roughly the minimum particle number to make the calculation stable:

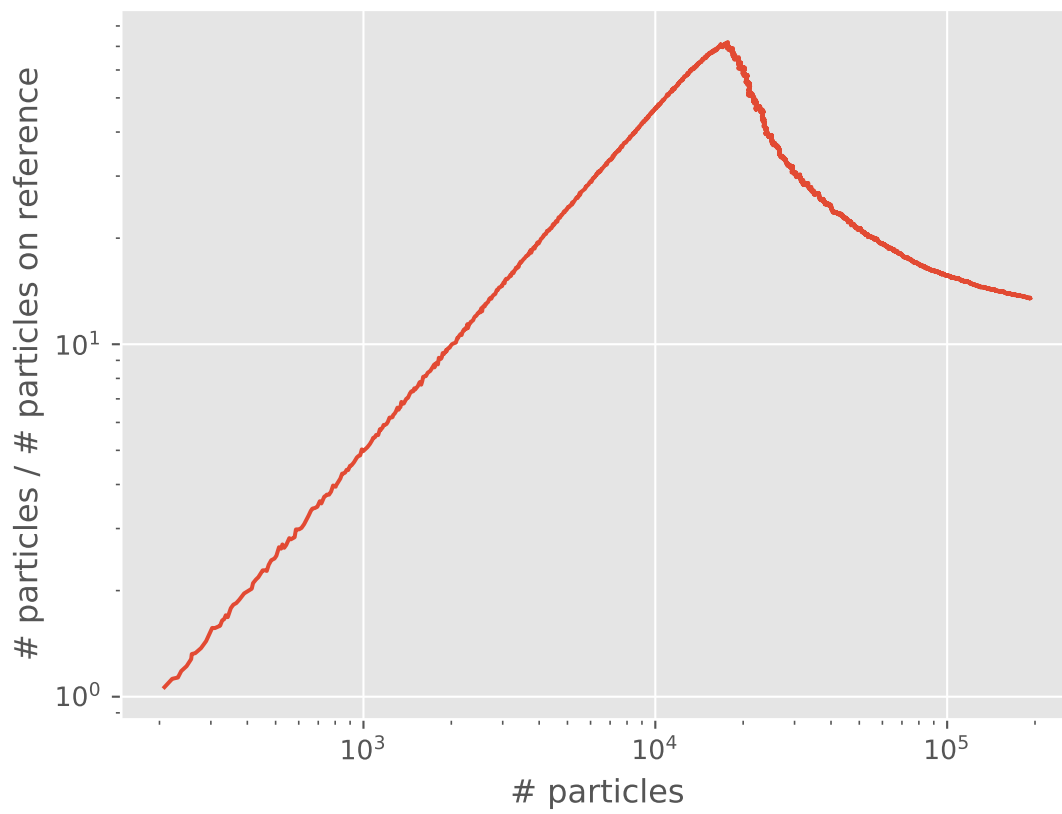
The plateau is clearly visible at around 20000 particles. This is one technique but the plateau is frequently not so easy to observe by visual inspection, especially for CCMC and being able to estimate it computationally is useful for analysing large numbers of calculations.

In the beginning of a typical simulation, only the reference is occupied. Its particles then spawn to occupy parts of the remaining Hilbert space, making the total population grow at a greater pace than the population on the reference does. At the plateau point, annihilation, spawning and death balance each other which temporarily leads to a constant total population while the reference population keeps growing. After a bit, the total population grows again and leaves the plateau. It then grows at a smaller or the same rate as the reference population because the system is now converged and the distribution of particles stochastically represents the ground state wavefunction of the system. See [\[Spencer12\]](#) and [\[Spencer15\]](#) for details.

The ratio of total population to population on the reference therefore peaks at roughly the plateau with respect to the total population. A good way to find the position of the plateau is therefore to look at the ratio of total population to population on the reference vs total population plots and find the position of the peak. We call this “shoulder” plot and the peak, or “shoulder height”, is an upper limit for the position of the plateau, see [\[Spencer15\]](#). The shoulder plot for our example from above is:

The position of the shoulder is at about 20000 which corresponds to the position of the plateau.





**Note:** `pyhande` contains two functions to estimate the position of the plateau/shoulder: `pyhande.analysis.plateau_estimator()`, which looks for the peak in the shoulder plot [Spencer15], and `pyhande.analysis.plateau_estimator_hist()`, which uses a histogram approach to identifying the plateau [Shepherd14]. As a result of the difference in approaches, the former tends to pick up the population at the start of the plateau whilst the latter favours the end of the plateau and is less well suited to cases without a clear plateau.

In this case, `plateau_estimator` gave 18481 with an estimated standard error of 38 for the shoulder height and `plateau_estimator_hist` gave 20155 (rounded to 0 d.p.). The difference is not important as the plateau is not exactly constant; its value to a few significant values is the important quantity.

---

The position of the plateau/shoulder is somewhat sensitive to input parameters and can be varied with changing the time step `tau` or the `cluster_multispawn_threshold` (if applicable) for example, more details below. A large initial population `init_pop` can also lead to overshooting of the shoulder.

## Effects of the Time Step

Now we will run another calculation with a higher time step, see input file below:

```
sys = read_in {
    int_file = "H2O_INTDUMP",
    nel = 10,
    ms = 0,
}

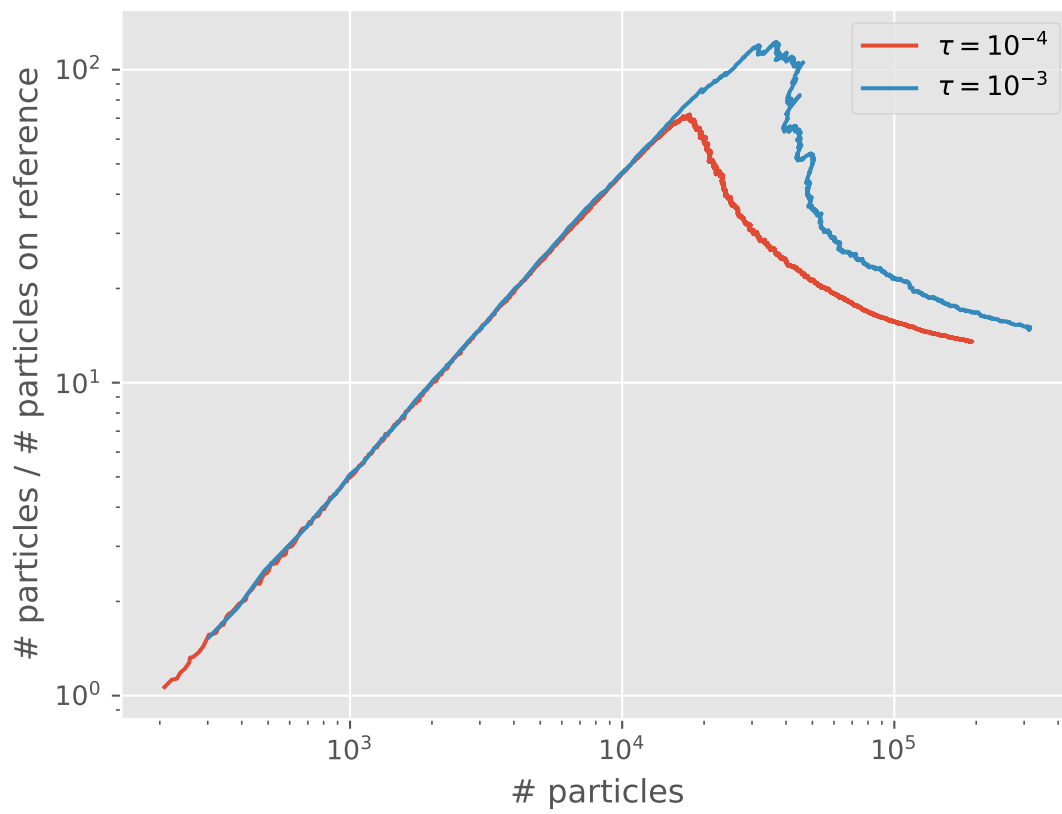
ccmc {
    sys = sys,
    qmc = {
        tau = 1e-3,
        mc_cycles = 10,
        nreports = 3.6e3,
        state_size = -500,
        spawned_state_size = -200,
        init_pop = 200,
        real_amplitudes = true,
        target_population = 3e5,
    },
    reference = {
        ex_level = 3,
    },
}
```

The two resulting shoulders are shown in the following graph:

A smaller time step can lead to fewer particles at the shoulder position, as described in [Booth09], [Vigor16].

## Effects of Cluster Multispawn Threshold

This part looks at changing the multispawn threshold. This is another feature which can change the number of particles at the shoulder. Positive effects of that have already been shown in *CCMC*. Note that while changing the time step changes the position of the plateau for FCIQMC for example as well, cluster multispawn threshold is specific to CCMC. The lower the multispawn threshold, the lower will be the number of “blooming” events which spawn multiple particles at the same spawning attempt. “Blooming” events can lead to greater uncertainty as the wavefunction is then sampled in a more coarse and less fine manner. It is therefore not surprising that less particles are needed to converge to the correct wavefunction for a lower multispawn threshold.



To demonstrate the effects of decreasing the multispawn threshold, we will run the following calculation with a low multispawn threshold:

```
sys = read_in {
  int_file = "H2O_INTDUMP",
  nel = 10,
  ms = 0,
}

ccmc {
  sys = sys,
  qmc = {
    tau = 1e-4,
    mc_cycles = 10,
    nreports = 2e4,
    state_size = -500,
    spawned_state_size = -200,
    init_pop = 200,
    real_amplitudes = true,
    target_population = 3e5,
  },

  ccmc = {
    cluster_multispawn_threshold = 0.1,
  },

  reference = {
    ex_level = 3,
  },
}
```

The plot below compares the shoulder plot of this and the first calculation on top of this tutorial:

Note that “multispawn threshold = none” means that there is no threshold within computer number representation limits.

Clearly, setting a low multispawn threshold lowers the total number of particles at the shoulder. This is, like with a smaller timestep, due to more efficient sampling: an exciton with a large amplitude is allowed to explore more of the space (via multiple spawning attempts) than an exciton with a smaller amplitude.

## Effects of Initial Population

In this part of the tutorial we will see that a large initial population can lead to overshooting the shoulder.

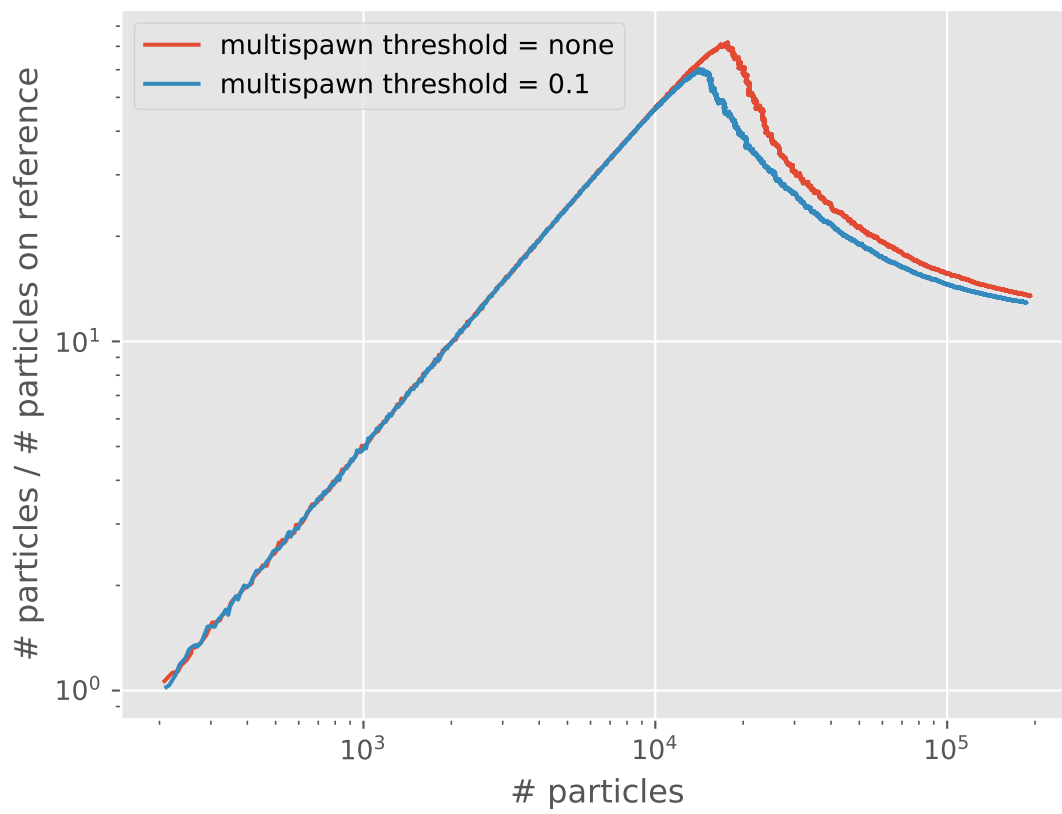
As a demonstration, we look at almost the same calculation as the first one but with a larger initial population.

```
sys = read_in {
  int_file = "H2O_INTDUMP",
  nel = 10,
  ms = 0,
}

ccmc {
  sys = sys,
  qmc = {
    tau = 1e-4,
    mc_cycles = 10,
    nreports = 2e4,
```

(continues on next page)





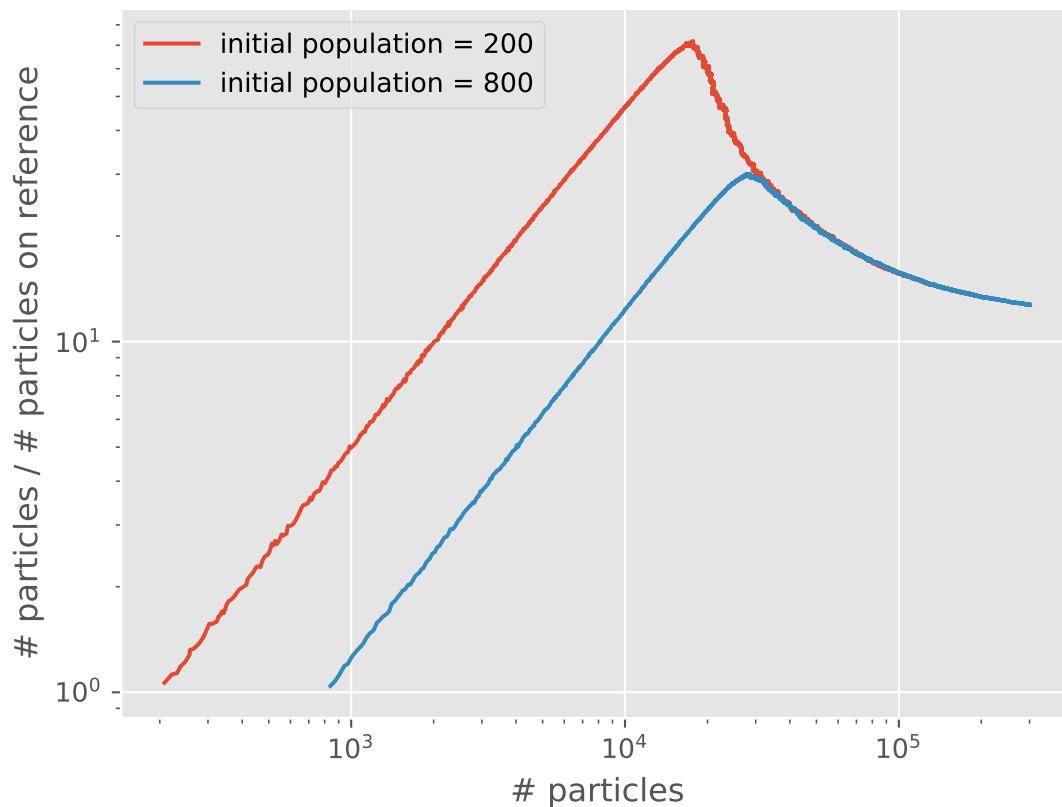
(continued from previous page)

```

state_size = -500,
spawned_state_size = -200,
init_pop = 800,
real_amplitudes = true,
target_population = 3e5,
},
reference = {
    ex_level = 3,
},
}

```

The following plot compares the original with the calculation starting with a large initial population:



We see that the calculation with a larger initial population has a shoulder at a larger number of particles, effectively overshooting the shoulder. At yet larger numbers of particles than this, we expect the calculation to be stable once population control is enabled (i.e. the shift is allowed to vary).

The overshooting can be explained by considering that the only significant difference between the two curves above is that they start with a different population at the reference. Before they reach a shoulder, each calculation has a very fast growth in total population without changing the reference population. This results in an initial linear growth on the shoulder plots, which lasts until the reference populations begin to grow.

The calculation with the greater initial population will require a greater total population to reach this point, and it occurs when this calculation's curve hits that which begins with a smaller population.

Once a calculation has passed its shoulder, the location on the shoulder plot can generally be used to describe its 'state'. Two calculations with different initial populations, but otherwise identical, will end up on the same curve once equilibrated, and will follow the curve if total particle numbers are allowed to grow. Modifying the algorithm (e.g. with `multispawn_threshold`) or changing the timestep will cause the equilibrium curve to shift position, and therefore affect the position of the shoulder.

### 1.13.9 Solid state calculations

In this tutorial we will run periodic boundary conditions CCMC calculation on a diamond crystal in STO-3G basis with 2x1x1 sampling of the Brillouin zone. Familiarity with *CCMC* and *FCIQMC* tutorials is assumed. The input and output files can be found under the `documentation/manual/tutorials/calcs/ccmc_solids` subdirectory of the source distribution.

First of all, we need the one- and two- electron integrals from an external source. We will use *PySCF* software package [Sun18] to perform preliminary Hartree-Fock calculation and generate the integrals. *PySCFDump* script can be used to save the integrals in the FCIDUMP format readable by HANDE<sup>1</sup>.

To correctly address exchange divergence, additional exchange integrals are needed. Those are written in a FCIDUMP\_X file by *PySCFDump*. Theoretical details of this procedure will be elaborated on as part of an upcoming paper.

Cell object can be conveniently prepared using `build_cell` function of the `pyscfdump.helpers` module and *ASE* library. Set of basis functions, kinetic energy cutoff and pseudopotential used are specified.

The `run_khf` function of the `pyscfdump.scf` module is used to run the HF calculation. Number of k-points in each dimension is specified. By default, the Monkhorst-Pack grid is used. If `gamma` is set to true, the grid will be shifted to include the Gamma point. Exchange divergence treatment scheme should also be chosen. The function returns the converged HF calculation object and a list of scaled k-points (i.e. (0.5,0.5,0.5) is at the very corner of the Brillouin zone).

Finally, `fcidump` function of the `pyscfdump.pbfcidump` module is used to dump the integrals to a file. Name of the resulting file, SCF calculation object, number of k points, list of scaled k points and boolean variable MP (true if the grid is Monkhorst-Pack - i.e. not shifted to include the gamma point for even grids) must be provided.

```
from ase.lattice import bulk
import pyscfdump.scf as scf
from pyscfdump.helpers import build_cell
from pyscfdump.pbfcidump import fcidump

A2B = 1.889725989          #angstrom to bohr conversion

a=3.567                    #lattice parameter
ke=1000                    #kinetic energy cutoff in units of rydberg
basis='sto-3g'             #basis set choice
nmp = [2,1,1]             #k point sampling

#prepare the cell object
ase_atom = bulk('C', 'diamond', a=a*A2B)
cell = build_cell(ase_atom, ke=ke, basis=basis, pseudo='gth-pade')

#run the HF calculation
kmf,scaled_kpts = scf.run_khf(cell, nmp=nmp, exxdiv='ewald', gamma=True)

#dump the integrals
fcidump('fcidumpfile', kmf, nmp, scaled_kpts, False)
```

<sup>1</sup> The `pyscfdump` module code will be released shortly. For preliminary access contact Alex Thom at `ajwt3@cam.ac.uk`.

Now we are ready to run the CCMC calculation. System definition is read in from the FCIDUMP files. There are two points to notice

- path to files with additional exchange integrals is specified as `ex_int_file`
- to properly exploit translational symmetry in the crystal lattice, the orbitals and hence the integrals must be complex. The complex mode of HANDE is enabled by setting `complex = true`. Consequently, numbers of particles on excitors also have both real and imaginary part, as well as projected energy.

In a non-initiator calculation, we try setting the time step `tau` as big as possible before too many blooms happen. A shoulder plot should be used to determine `target_population`. The `heat_bath` excitation generator [Holmes16] (adapted to HANDE as described in [Neufeld19]) is often a good choice in small systems. The input script used in this tutorial is:

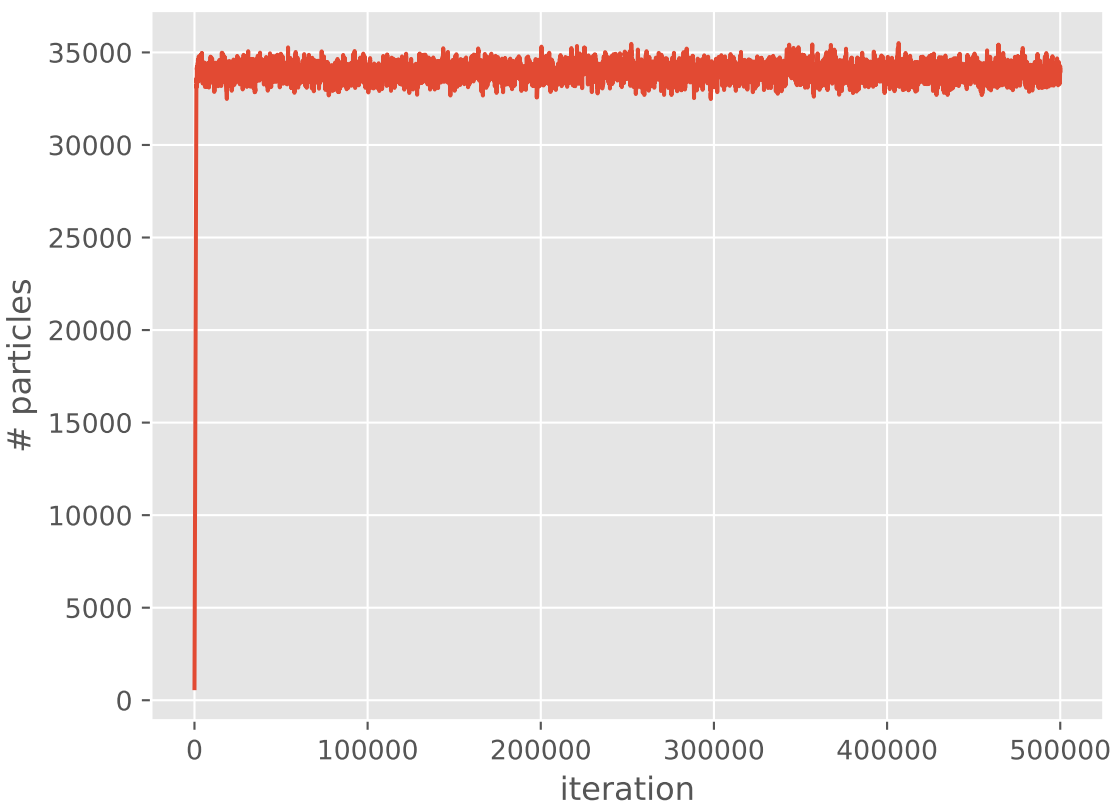
```
sys = read_in {
  int_file = "fcidumpfile",
  complex = true,
  ex_int_file = "fcidumpfile_X",
}
ex_l=2

ccmc {
  sys = sys,
  qmc = {
    tau = 0.02,
    rng_seed = 13086,
    mc_cycles = 10,
    init_pop = 200,
    nreports = 50000,
    target_population = 1e4,
    state_size = -800,
    spawned_state_size = -500,
    excit_gen = "heat_bath",
    real_amplitudes = true,
  },
  ccmc = {
    even_selection = true,
    full_non_composite=true,
  },
  reference = {
    ex_level = ex_l,
  },
  blocking = {
    blocking_on_the_fly = true,
    auto_shift_damping = true,
  },
  restart = {
    write = true,
  },
}
```

The Hilbert space of the system we are dealing with is quite small and so is the target population. The general rule is that in order to use MPI parallelism, each process should contain at least  $10^5$  occupied excitors [Spencer18]. Having fewer excitors on each process is both inefficient and in extreme cases can lead to biased results. This is why we will use only one process here. However, use of openMP shared memory threads is recommended in order to make full use of the available resources.

```
$ hande.x ccmc.lua > diamond_ccmc.out
```

We can now plot the population



and correlation energy:

It is worth noting that the projected energy is in fact a complex quantity, whose imaginary part evaluates to zero in a non-trivial way [Booth13]. For the plot we calculate the result by only using real parts of both  $\sum_j H_{0j} N_j(\tau)$  and  $N_0(\tau)$ , using the fact that

$$E(\tau) = \Re\left(\frac{\sum_j H_{0j} N_j(\tau)}{N_0(\tau)}\right) = \frac{\Re(\sum_j H_{0j} N_j(\tau))}{\Re(N_0(\tau))}$$

where the second equality holds provided that imaginary part of  $E(\tau)$  is zero.

The reblocking analysis uses magnitudes rather than real parts as this prevents problems with potential changes of phase during the calculation. Nevertheless, for a well behaved calculation such as the one presented here, it is found that reblocking using real parts would give identical results.

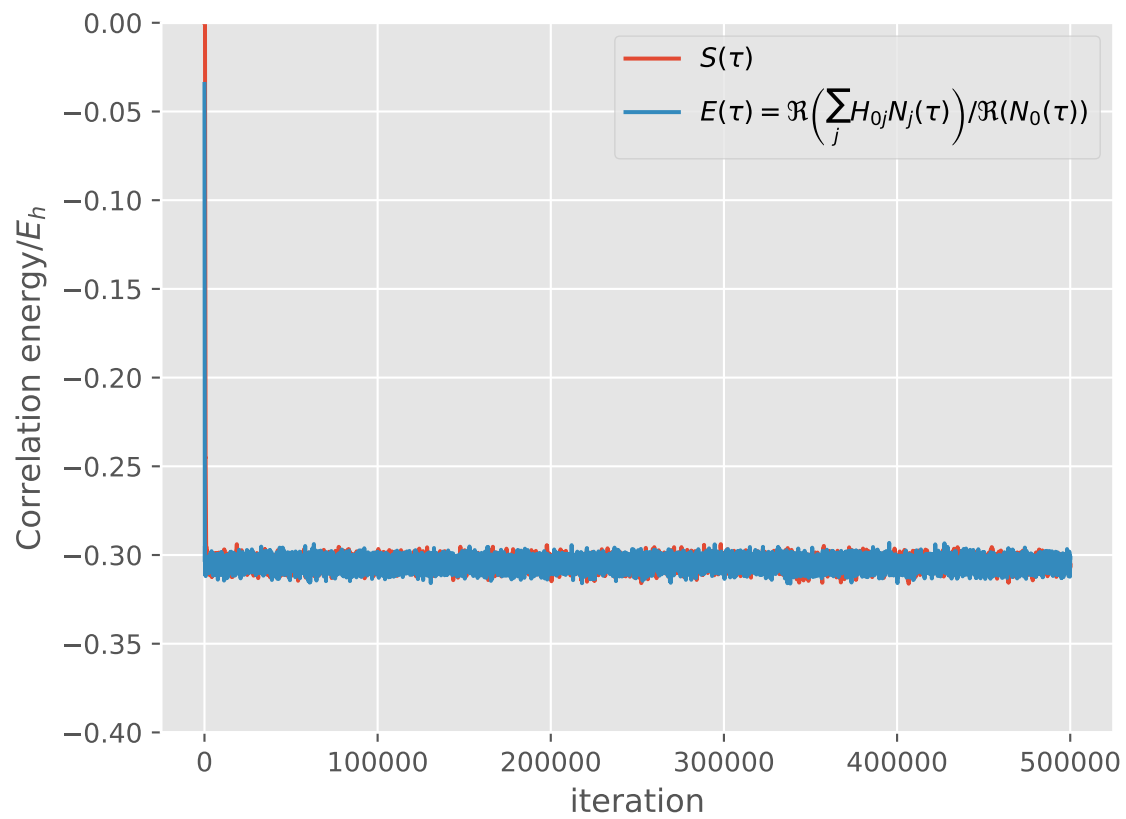
In any case, the shift remains a strictly real measure of the correlation energy<sup>2</sup>.

To analyse the calculation we can use `reblock_hande.py` script:

```
$ reblock_hande.py --quiet diamond_ccmc.out
```

which results in:

<sup>2</sup> As discussed in [Booth13] for FCIQMC - the CCMC case is exactly analogous.



```
Block from: 20790
Recommended statistics from optimal block size:

      Block from # H psips \sum H_0j N_j      N_0      Shift Proj.
↪ Energy
diamond_ccmc_2.out 2.07900000e+04 33940 (10)      -1015 (2) 3328 (6) -0.30485 (8) -0.
↪ 30495 (5)
```

All calculations were analysed using *pyhande* and all graphs were plotted using *matplotlib*. Parts of the plot generation code were adapted from the matplotlib tutorials.





pyhande provides powerful abstractions for analysing HANDE calculations.

HANDE includes many scripts for common analysis tasks which are (typically) thin wrappers around pyhande. More complicated data analysis or examining large numbers of output files can be easily performed by using pyhande directly from a python interpreter or a custom script.

pyhande can extract data from output produced by HANDE and perform a variety of data analysis tasks on the data obtained. See the documentation for each submodule for more details.

**Note:** Sections 2.7-2.11 refer to a new object oriented version of pyhande. Tutorials on how to use this version may be found in `tools/pyhande/tutorials`.

## 2.1 pyhande.analysis

Analysis of data from FCIQMC and CCMC calculations.

`pyhande.analysis.projected_energy(reblock_data, covariance, data_length, sum_key='sum  
H_0j N_j', ref_key='N_0', col_name='Proj. Energy')`

Calculate the projected energy estimator and associated error.

The projected energy estimator is given by

$$E = \frac{\sum H_0 j N_j}{N_0}$$

The numerator and denominator are correlated and so their covariance must be taken into account.

### Parameters

- **reblock\_data** (`pandas.DataFrame`) – reblock data for (at least) the numerator and denominator in the projected energy estimator.
- **covariance** (`pandas.DataFrame`) – covariance at each reblock iteration between (at least) the numerator and denominator in the projected energy estimator.

- **data\_length** (`pandas.DataFrame`) – number of data points in each reblock iteration.
- **sum\_key** (*string*) – column name in `reblock_data` containing  $\sum H_{0j} N_j$ , i.e. the sum of the population weighted by the Hamiltonian matrix element with the trial wavefunction.
- **ref\_key** (*string*) – column name in `reblock_data` containing  $N_0$ , i.e. the population of the trial wavefunction (often/originally just a single determinant).

**Returns** `proje` – The projected energy estimator at each reblock iteration.

**Return type** `pandas.DataFrame`

**See also:**

`pyblock.pd_utils.reblock()`

`pyhande.analysis.qmc_summary` (*data*, *keys*=(`'\sum H_0j N_j'`, `'N_0'`, `'Shift'`, `'Proj. Energy'`), *summary\_tuple*=None)

Summarise a reblocked data set by the optimal block.

#### Parameters

- **data** (`pandas.DataFrame`) – reblocked data (i.e. data with the reblock iteration as the index).
- **keys** (*list of strings*) – columns (by top-level index) of the data table to inspect. Each top-level column must contain an optimal block column.
- **summary\_tuple** ((`pandas.DataFrame`, *list of strings*)) – Optionally append summary data to this tuple. Allows repeated calling of this function.

#### Returns

- **opt\_data** (`pandas.DataFrame`) – Data for each column from the optimal block size of that column.
- **no\_opt** (*list of strings*) – list of columns for which no optimal block size was found.

`pyhande.analysis.extract_pop_growth` (*data*, *ref\_key*=`'N_0'`, *shift\_key*=`'Shift'`, *min\_ref\_pop*=10)

Select QMC data during which the population was allowed to grow.

We define the region of population growth as the period in which the shift is held constant.

#### Parameters

- **data** (`pandas.DataFrame`) – HANDE QMC data. `pyhande.extract.extract_data_sets()` can be used to extract this from a HANDE output file.
- **ref\_key** (*string*) – column name in `reblock_data` containing the number of psips on the reference determinant.
- **shift\_key** (*string*) – column name in `reblock_data` containing the shift.
- **min\_pop** (*int*) – discard data entries with fewer than `min_pop` on the reference.

**Returns** `pop_data` – The subset of data prior to the shift being varied.

**Return type** `pandas.DataFrame`

`pyhande.analysis.plateau_estimator` (*data*, *total\_key*=`'# H psips'`, *ref\_key*=`'N_0'`, *shift\_key*=`'Shift'`, *min\_ref\_pop*=10, *pop\_data*=None)

Estimate the (plateau) shoulder from a FCIQMC/CCMC calculation.

The population on the reference starts to grow exponentially during the plateau, whilst the total population grows exponentially from the start of the calculation before stabilising (perhaps only briefly) during the plateau phase.

As a result, the ratio of the total population to the population on the reference is at a maximum at the start of the plateau.

The shoulder estimator is defined to be mean of the ten points with the smallest proportion of the population on the reference (excluding points when the population drops below `min_pop` excips (psips). The shoulder height is the total population at this point.

Credit to Alex Thom for original implementation.

#### Parameters

- **data** (`pandas.DataFrame`) – HANDE QMC data. `pyhande.extract.extract_data_sets()` can be used to extract this from a HANDE output file.
- **total\_key** (`string`) – column name in `reblock_data` containing the total number of psips.
- **ref\_key** (`string`) – column name in `reblock_data` containing the number of psips on the reference determinant.
- **shift\_key** (`string`) – column name in `reblock_data` containing the shift.
- **min\_ref\_pop** (`int`) – exclude points with less than `min_ref_pop` on the reference.
- **pop\_data** (`pandas.DataFrame`) – The subset of data prior to the shift being varied. Calculated if not supplied from `extract_pop_growth`.

**Returns** `plateau_data` – An estimate of the shoulder (plateau) from a FCIQMC (CCMC) calculation, along with the associated standard error.

**Return type** `pandas.DataFrame`

`pyhande.analysis.plateau_estimator_hist(data, total_key='# H psips', shift_key='Shift', pop_data=None, bin_width_fn=None)`

Estimate the plateau height via a histogram of the population.

The population (approximately) stabilises during the plateau phase. By taking a histogram of the population, the plateau can be estimated from the histogram bin with greatest frequency. Due to the exponential population growth outside of the plateau, we histogram the logarithm of the population.

This tends to give similar numbers to `shoulder_estimator`, though may be less useful for shoulder-like plateaus. Detecting a plateau automatically is tricky so having multiple approaches for comparison helps with corner cases.

Used in [Shepherd14].

Credit to James Shepherd for the idea and original (perl) implementation.

#### Parameters

- **data** (`pandas.DataFrame`) – HANDE QMC data. `pyhande.extract.extract_data_sets()` can be used to extract this from a HANDE output file.
- **total\_key** (`string`) – column name in `reblock_data` containing the total number of psips.
- **shift\_key** (`string`) – column name in `reblock_data` containing the shift.
- **pop\_data** (`pandas.DataFrame`) – The subset of data prior to the shift being varied. Calculated if not supplied from `extract_pop_growth`.
- **bin\_width\_fn** (`function`) – A function which calculates the bin width in the histogram based upon `pop_data`.  $12500/\text{len}(\text{data})^2$  (obtained empirically) is used if not supplied.

**Returns** `plateau` – An estimate of the population at the plateau.

**Return type** `float`

## References

**Shepherd14** J.J. Shepherd et al., Phys. Rev. B 90, 155130 (2014).

```
pyhande.analysis.inefficiency(opt_block, dtau, iterations, sum_key='sum H_0j N_j',
                              ref_key='N_0', total_key='# H psips', proje_key='Proj. En-
                              ergy')
```

Estimate the inefficiency of a calculation from the blocked data.

The statistical error of an ideal FCIQMC calculation decreases with the square-root of number of steps,  $N$ , total number of particles,  $N_p$  and (at sufficiently low values) timestep,  $\delta\tau$ .

We define the inefficiency,  $a$ , as a quantity independent of these, which depends on purely the algorithm and system studied, and can be used to determine the expected runtime to achieve a given error. We provide an estimate of this from the best estimate of the error in the projected energy,  $\sigma_E$ :

$$a = \sigma_E \sqrt{N_p N \delta\tau}$$

Error bars are (over)-estimated with a simple error propagation, but since no information about the covariance of the error estimates is available, this will always be an overestimate.

Used in [Vigor16].

Credit to William Vigor for the original pyhande implementation.

### Parameters

- **opt\_block** (`pandas.DataFrame`) – Optimally blocked HANDE QMC data. `func:pyhande.analysis.qmc_summary` can be used to extract this from reblocked HANDE data.
- **dtau** (`float`) – length of an imaginary time timestep.
- **iterations** (`integer`) – number of iterations (timesteps) in the reblocked data.
- **sum\_key** (`string`) – column name in reblock\_data containing  $\sum H_0jN_j$ , i.e. the sum of the population weighted by the Hamiltonian matrix element with the trial wavefunction.
- **ref\_key** (`string`) – column name in reblock\_data containing  $N_0$ , i.e. the population of the trial wavefunction (often/originally just a single determinant).
- **total\_key** (`string`) – column name in reblock\_data containing the total number of psips.
- **proje\_key** (`string`) – key for projected energy index in `opt_block`.

**Returns** **ineff** – A data frame with index ‘inefficiency’ and columns ‘mean’ and ‘standard error’ or None if the appropriate data is not available.

**Return type** `pandas.DataFrame`

## References

### Vigor16

W. A. Vigor, et al., J. Chem. Phys. 144, 094110 (2016); doi: 10.1063/1.4943113

## 2.2 pyhande.canonical

Analysis of data from canonical thermodynamic calculations.

`pyhande.canonical.analyse_hf_observables` (*means, covariances, nsamples*)

Perform Error analysis for Hartree-Fock estimates which are the ratio of two quantities.

### Parameters

- **means** (`pandas.DataFrame`) – Data frame containing means of various observables.
- **covariances** (`pandas.DataFrame`) – Data frame containing covariances between various observables.
- **nsamples** (`int`) – Number of samples contributing to estimates and standard errors

**Returns** **results** – Averaged Hartree-Fock estimates along with error estimates.

**Return type** `pandas.Series`

`pyhande.canonical.estimate` (*metadata, data*)

Perform error analysis for canonical thermodynamic estimates.

### Parameters

- **metadata** (`dict`) – metadata (i.e. calculation information, parameters and settings) extracted from output files.
- **data** (`pandas.DataFrame`) – HANDE QMC data.

**Returns** **results** – Averaged estimates.

**Return type** `pandas.Series`

## 2.3 pyhande.extract

Extract data from the output of a HANDE calculation.

---

**Note:** All *pyhande* analysis procedures assume data is in the format produced by `extract_data()` and `extract_data_sets()`.

---

`pyhande.extract.extract_data_sets` (*filenames*)

Extract QMC data tables from multiple HANDE calculations.

**Parameters** **filenames** (*list of strings*) – names of files containing HANDE QMC calculation output.

---

**Note:** Files compressed with gzip, bzip2 or xz (python 3 only) are automatically decompressed.

---

**Returns** **data** – Calculation output represented by a tuple for each calculation, consisting of metadata (dict) and a `pandas.DataFrame` (MC calculations) or `pandas.Series` (other calculations) containing the calculation output/results.

**Return type** list of (dict, `pandas.DataFrame` or `pandas.Series`)

See also:

`extract_data()` underlying data extraction implementation.

`pyhande.extract.extract_data(filename)`

Extract QMC data table from a HANDE calculation.

**Parameters** `filename` (*string*) – name of file containing the HANDE QMC calculation output.

---

**Note:** Files compressed with gzip, bzip2 or xz (python 3 only) are automatically decompressed.

---

**Returns** `data_pairs` – Calculation output represented by a tuple for each calculation, consisting of metadata (dict) and a `pandas.DataFrame` (MC calculations) or `pandas.Series` (other calculations) containing the calculation output/results.

**Return type** list of (dict, `pandas.DataFrame` or `pandas.Series`)

## 2.4 pyhande.lazy

Tools for the lazy amongst us: automation of common HANDE analysis tasks.

`pyhande.lazy.find_starting_iteration_mser_min(data, md, start_max_frac=0.9,  
n_blocks=100, verbose=None,  
end=None)`

Find the best iteration to start analysing CCMC/FCIQMC data based on MSER minimization scheme.

**Warning:** Use with caution, check whether output is sensible and adjust parameters if necessary.

This function gives an optimal estimation of the starting iterations based on MSER minimization heuristics. This methods decides the starting iterations  $d$  as minimizing an evaluation function  $MSER(d) = \frac{\sum_{i=1}^{n-d} (X_{i+d} - X_{mean}(d))}{(n-d)^2}$ . Here,  $n$  is length of time-series,  $X_i$  is ‘sum H\_0j N\_j’ / ‘N\_0’ of  $i$ -th step, and  $X_{mean}$  is the average of  $X_i$  after the  $d$ -th step.

### Parameters

- **data** (`pandas.DataFrame`) – Calculation output for a FCIQMC or CCMC calculation.
- **md** (*dict*) – Metadata corresponding to the calculation in *data*.
- **n\_blocks** (*int*) – This analysis takes long time when  $n$  is large. Thus, we pick up  $d$  for every ‘n\_blocks’ samples, calculate  $MSER(d)$ , and decide the optimal estimation of the starting iterations only from these  $d$ .
- **start\_max\_frac** (*float*) –  $MSER(d)$  may oscillate when become unreasonably small when  $n - d$  is large. Thus, we calculate  $MSER(d)$  for  $d < (n * start\_max\_frac)$  and give the optimal estimation of the starting iterations only in this range of  $d$ .
- **verbose** (*int*) – Inactive. This valuable does not change anything.
- **end** (*int or None*) – Last iteration included in analysis. If *None*, the last iteration included is the last iteration of the data set.

**Returns** `starting_iteration` – Iteration from which to start reblocking analysis for this calculation.

**Return type** integer

`pyhande.lazy.lazy_hybrid(calc, md, start=0, end=None, batch_size=1)`

New post-analysis on zero-temperature QMC calcaulations.

---

**Note:** `std_analysis()` is recommended unless custom processing is required before blocking analysis is performed.

---

This scheme is made by hybridizing two different post-analysis methods, AR model and Straatsma. The former (the latter) is comparatively good at estimating the statistic error for smaller (larger) length of time-series, respectively. This method just picks up the larger statistic error from the ones given by both methods. The mathematical details of both methods are explained in an upcoming paper.

#### Parameters

- **calc** (`pandas.DataFrame`) – Zero-temperature QMC calculation output.
- **md** (`dict`) – Metadata for the calculation in *calc*.
- **end** (`start,`) – See `std_analysis()`.
- **batch\_size** (`int`) – The energy time-series is coarse-grained by averaging several sequential samples into just one sample and the statistic error is calculated for the coarse-grained time-series. This variable designates how many sequential samples are averaged together.

#### Returns

- **info** (`collections.namedtuple()`) – See `std_analysis()`.
- *[todo]* - Catch `ValueError` from `statsmodels` when there is too little
- *[todo]* - data.

```
pyhande.lazy.std_analysis(datafiles, start=None, end=None, select_function=None,
                           extract_psips=False, reweight_history=0, mean_shift=0.0,
                           calc_inefficiency=False, verbosity=1, starts_reweighting=None,
                           extract_rep_loop_time=False, analysis_method='reblocking',
                           warmup_detection='hande_org')
```

Perform a ‘standard’ analysis of HANDE output files.

#### Parameters

- **datafiles** (*list of strings*) – names of files containing HANDE QMC calculation output.
- **end** (`start,`) – iteration after which/until which the blocking analysis is performed. The end iteration is included in analysis, the start iteration is not. If start is None, then attempt to automatically determine a good iteration using `find_starting_iteration()`. If end is None, the last iteration included is the last iteration of the data set.
- **select\_function** (*function*) – function which returns a boolean mask for the iterations to include in the analysis. Not used if set to None (default). Overrides start. See below for examples.
- **extract\_psips** (*bool*) – also extract the mean number of psips from the calculation.
- **reweight\_history** (*integer*) – reweight in an attempt to remove population control bias. According to [Umrigar93] this should be set to be a few correlation times.
- **mean\_shift** (*float*) – prevent the weights from becoming too large.
- **calc\_inefficiency** (*bool*) – determines whether inefficiency should be calculated.
- **verbosity** (*int*) – values greater than 1 print out blocking information when automatically finding the starting iteration. 0 and 1 print out the starting iteration if automatically found. Negative values print out nothing from the automatic starting point search.

- **starts\_reweighting** (*list of floats*) – used by the `reweighting_graph` function to pass more than one starting iteration
- **extract\_rep\_loop\_time** (*bool*) – also extract the mean time taken per report loop from the calculation.
- **analysis\_method** (*string*) – determines which post-analysis method is used to estimate the statistic error. Currently ‘reblocking’ and ‘hybrid’ are prepared.
- **warmup\_detection** (*string*) – determines which method is used to decide the starting iterations to be discarded before calculation the statistic error. Currently ‘hande\_org’ and ‘mser\_min’ are prepared.

### Returns

**info** –

raw and analysed data, consisting of:

**metadata, data** from `pyhande.extract.extract_data_sets()`. If data consists of several concatenated calculations, then the only metadata object is from the first calculation.

**data\_len, reblock, covariance** from `pyblock.pd_utils.reblock()`. The projected energy estimator (evaluated by `pyhande.analysis.projected_energy()`) is included in `reblock`.

**opt\_block, no\_opt\_block** from `pyhande.analysis.qmc_summary()`. A ‘pretty-printed’ estimate string is included in `opt_block`.

**Return type** list of `collections.namedtuple()`

### Examples

The following are equivalent and will extract the data from the file called `hande.fciqmc.out`, perform a blocking analysis from the 10000th iteration onwards, calculated the projected energy estimator and find the optimal block size from the blocking analysis:

```
>>> std_analysis(['hande.fciqmc.out'], 10000)
>>> std_analysis(['hande.fciqmc.out'],
...               select_function=lambda d: d['iterations'] > 10000)
```

### References

**Umrigar93** Umrigar et al., J. Chem. Phys. 99, 2865 (1993).

`pyhande.lazy.check_key` (*calc, key*)

Check if this key is present in *calc*, and if not, append “\_1”.

#### Parameters

- **calc** (`pandas.DataFrame`) – Zero-temperature QMC calculation output.
- **key** (*str*) – key name to check in *calc*.

**Returns** `key_`

**Return type**

**str** modified key name.



`pyhande.lazy.zeroT_qmc(datafiles, reweight_history=0, mean_shift=0.0)`

Extract zero-temperature QMC (i.e. FCIQMC and CCMC) calculations.

Reweight information is added to the calculation data if requested.

---

**Note:** `std_analysis()` is recommended unless custom processing is required before blocking analysis is performed.

---

**Parameters** `reweight_history`, `mean_shift` (`datafiles`,) – See `std_analysis()`.

#### Returns

- **calcs** (list of `pandas.DataFrame`) – Calculation outputs for just the zero-temperature/ground-state QMC calculations contained in `datafiles`.
- **metadata** (list of dict) – Metadata corresponding to each calculation in `calcs`.

`pyhande.lazy.lazy_block(calc, md, start=0, end=None, select_function=None, extract_psips=False, calc_inefficiency=False, extract_rep_loop_time=False)`

Standard blocking analysis on zero-temperature QMC calculations.

---

**Note:** `std_analysis()` is recommended unless custom processing is required before blocking analysis is performed.

---

#### Parameters

- **calc** (`pandas.DataFrame`) – Zero-temperature QMC calculation output.
- **md** (dict) – Metadata for the calculation in `calc`.
- **end**, **select\_function**, **extract\_psips**, **calc\_inefficiency**, (`start`,) – `extract_rep_loop_time`: See `std_analysis()`.

**Returns** `info` – See `std_analysis()`.

**Return type** `collections.namedtuple()`

`pyhande.lazy.filter_calcs(outputs, calc_types)`

Select calculations corresponding to a given list of calculation types.

#### Parameters

- **outputs** (list of (dict, `pandas.DataFrame` or `pandas.Series`)) – List of (metadata, data) tuples for each calculation, as created in `pyhande.extract.extract_data_sets()`.
- **calc\_types** (iterable of strings) – Calculation types (e.g. ‘FCIQMC’, ‘CCMC’, etc.) to select.

**Returns** `filtered` – As in `pyhande.extract.extract_data_sets()` but containing only the desired calculations.

**Return type** list of (dict, `pandas.DataFrame` or `pandas.Series`)

`pyhande.lazy.concat_calcs(metadata, data)`

Concatenate data from restarted calculations to analyse together.

#### Parameters

- **metadata** (*list of dicts*) – Extracted metadata for each calculation.
- **data** (*list of `pandas.DataFrame`*) – Output of each QMC calculation.

### Returns

- **calcs\_metadata** (*list of dicts*) – Metadata for each calculation, with duplicates from restarting dropped.
- **calcs** (*list of `pandas.DataFrame`*) – Output of each QMC calculation, with parts of a restarted calculation combined.

```
pyhande.lazy.find_starting_iteration(data, md, frac_screen_interval=300,
                                     number_of_reblockings=30, num-
                                     ber_of_reblocks_to_cut_off=1, pos_min_frac=0.8,
                                     verbose=0, show_graph=False, end=None)
```

Find the best iteration to start analysing CCMC/FCIQMC data.

**Warning:** Use with caution, check whether output is sensible and adjust parameters if necessary.

First, consider only data from when the shift begins to vary. We are interested in finding the minimum in the fractional error in the error of the shift weighted by  $1/\sqrt{\text{number of data points left}}$ . The error in the error of the shift and the error in the shift vary as  $1/\sqrt{\text{number of data points to analyse}}$  with the number of data points to analyse. If we were looking for the minimum in either of these quantities, the minimum would therefore be biased to the lower iterations as then more data points are included in the analysis. However, we have noticed that the error in the shift and its error fluctuate as we have less iterations to analyse which means that our search for the minimum could get trapped easily in a local minimum. We therefore consider their fraction. As they are divided by each other in the fractional error, the  $1/\sqrt{\text{number of data points to analyse}}$  gets removed. It is therefore artificially included as a weight. To be more conservative, we also find the minimum in the weighted fractional error in the error of # H psips,  $N_0$ ,  $\sum H_{0j} N_j$ . We then consider the minimum out of these four minima which is at the highest number of iterations.

The best estimate of the iteration to start the blocking analysis is found by:

1. discard data during the constant shift phase.
2. estimate the weighted fractional error in the error of the shift, # H psips,  $N_0$ ,  $\sum H_{0j} N_j$ , by blocking the remaining data  $n$  times, where the blocking analysis considers the last  $1 - i/f$  fraction of the data and where  $i$  is the number of blocking analyses already performed,  $n$  is `number_of_reblockings` and  $f$  is `frac_screen_interval`.
3. find the iteration which gives the minimum estimate of the weighted fractional error in the error of the shift, numerator of projected energy, reference and total population. We then focus on the minimum out of these four minima which is at the highest number of iterations. If this is in the first `pos_min_frac` fraction of the blocking attempts, go to 4, otherwise repeat 2 and perform an additional `number_of_reblockings` attempts.
4. To be conservative, discard the first `number_of_reblocks_to_cut_off` blocks from the start iteration, where each block corresponds to roughly the autocorrelation time, and return the resultant iteration number as the estimate of the best place to start blocking from.

### Parameters

- **data** (`pandas.DataFrame`) – Calculation output for a FCIQMC or CCMC calculation.
- **md** (*dict*) – Metadata corresponding to the calculation in `data`.
- **frac\_screen\_interval** (*int*) – Number of intervals the iterations from where the shift started to vary to the end are divided up into. Has to be greater than zero.

- **number\_of\_reblockings** (*int*) – Number of reblocking analyses done in steps set by the width of an interval before it is checked whether suitable minimum error in the error has been found. Has to be greater than zero.
- **number\_of\_reblocks\_to\_cut\_off** (*integer*) – Number of reblocking analysis blocks to cut off additionally to the data before the best iteration with the lowest error in the error. Has to be non negative. It is highly recommended to not set this to zero.
- **pos\_min\_frac** (*float*) – The minimum has to be in the first pos\_min\_frac part of the tested data to be taken as the true minimum. Has to be greater than a small number (here 0.00001) and can at most be equal to one.
- **verbose** (*int*) – If greater than 1, prints out which blocking attempt is currently being performed.
- **show\_graph** (*bool*) – Determines whether a window showing the shift vs iteration graph pops up highlighting where the minimum was found and - after also excluding some reblocking blocks - which iteration was found as the best starting iteration to use in reblocking analyses.
- **end** (*int or None*) – Last iteration included in analysis. If None, the last iteration included is the last iteration of the data set.

**Returns** **starting\_iteration** – Iteration from which to start reblocking analysis for this calculation.

**Return type** integer

`pyhande.lazy.reweighting_graph(datafiles, start=None, verbosity=1, mean_shift=0.0)`

Plot a graph of reweighted projected energy vs. reweighted factor W.

Detecting biases by reweighting is described in [Umrigar93] and [Vigor15], see `pyhande.weight` for details. The graph produced by this function is similar to figure 4 in [Vigor15].

A similar function has been published in Neufeld, V., & Thom, A. J. Research data and further information supporting “A study of the dense uniform electron gas with high orders of coupled cluster” [Dataset]. <https://doi.org/10.17863/CAM.14336> under Attribution 4.0 International (CC BY 4.0).

#### Parameters

- **datafiles** (*list of strings*) – names of files containing HANDE QMC calculation output.
- **start** (*int or None*) – iteration from which the blocking analysis is performed. If None, then attempt to automatically determine a good iteration using `find_starting_iteration()`.
- **verbosity** (*int*) – values greater than 1 print out blocking information when automatically finding the starting iteration. 0 and 1 print out the starting iteration if automatically found. Negative values print out nothing from the automatic starting point search.
- **mean\_shift** (*float*) – prevent the weights from becoming too large.

#### References

**Umrigar93** C.J. Umrigar et al., J. Chem. Phys. 99, 2865 (1993)

**Vigor15** W.A. Vigor, et al., J. Chem. Phys. 142, 104101 (2015).

Thanks to Will Vigor for original implementation.

## 2.5 pyhande.utils

Utility procedures for manipulating HANDE data.

`pyhande.utils.groupby_beta_loops(data, name='iterations')`

Group a HANDE DMQMC data table by beta loop.

**Parameters** `data` (`pandas.DataFrame`) – DMQMC data table (e.g. obtained by `pyhande.extract.extract_data()`).

**Returns** `grouped` – GroupBy object with data table grouped by beta loop.

**Return type** `pandas.DataFrameGroupBy`

`pyhande.utils.groupby_iterations(data)`

Group a HANDE QMC data table by blocks of iterations.

**Parameters** `data` (`pandas.DataFrame`) – QMC data table (e.g. obtained by `pyhande.extract.extract_data()`).

**Returns** `grouped` – GroupBy object with data table grouped into blocks within which the iteration count increases monotonically.

**Return type** `pandas.DataFrameGroupBy`

## 2.6 pyhande.weight

Attempt to remove the population control bias by reweighting estimates.

`pyhande.weight.reweight(data, mc_cycles, tstep, weight_history, mean_shift, weight_key='Shift')`

Reweight using population control to reduce population control bias.

Reweight estimators linear in the number of psips by the factor:

$$W(\tau, N) = \prod_{m=0}^{N-1} e^{-A\delta\tau S(\tau - m\delta\tau)}$$

where  $A$  is the number of steps per shift update cycle,  $\delta\tau$  is the time step and  $S(\tau - m\delta\tau)$  is the shift at time  $\tau - m\delta\tau$ , and  $m$  is the number of iterations to reweight over.

See [Umrigar93] Eqs. 14-20 for details and [Vigor15] for use in FCIQMC.

**Parameters**

- **data** (`pandas.DataFrame`) – HANDE QMC data.
- **tstep** (`float`) – The time step used in the weight factor.
- **mc\_cycles** (`int`) – The number of monte carlo cycles per update step.
- **weight\_history** (`integer`) – The number of iterations to reweight over.
- **mean\_shift** (`float`) – The mean shift. Used to prevent weights becoming too big.
- **weight\_key** (`string`) – Column to generate the reweighting data.

**Returns** `weight` – List of weights.

**Return type** `List[float]`

## References

**Umrigar93** C.J. Umrigar et al., J. Chem. Phys. 99, 2865 (1993)

**Vigor15** W.A. Vigor, et al., J. Chem. Phys. 142, 104101 (2015).

## 2.7 pyhande.data\_preparing

Mappings/preparation of output data column names.

### 2.7.1 pyhande.data\_preparing.hande\_ccmc\_fciqmc

CCMC and FCIQMC HANDE data preparation for analysis.

```
class pyhande.data_preparing.hande_ccmc_fciqmc.PrepHandeCcmcFciqmc
    Bases: pyhande.data_preparing.abs_data_preparator.AbsDataPreparator
```

Prepare HANDE CCMC/FCIQMC data for analysis.

#### observables

Access observables, key mapping.

**Raises** `AttributeError` – If data has not been prepared yet.

**Returns** Map of observables property to column/observables name.

**Return type** `Dict[str, str]`

#### data

Access (prepared) data.

**Raises** `AttributeError` – If data has not been prepared yet.

**Returns** QMC Data. Cleaned list over merged calculations.

**Return type** `List[pd.DataFrame]`

#### complex\_data

True if data is complex.

**Raises** `AttributeError` – If preparation has not been done yet.

**Returns**

**Return type** `bool`

#### replica\_data

True if replica tricks were used.

**Raises** `AttributeError` – If preparation has not been done yet.

**Returns**

**Return type** `bool`

```
exe (data: List[pandas.core.frame.DataFrame], make_copy: bool = True)
```

Prepare data; deal with complex, replica and add inst. proje.

#### Parameters

- **data** (`List[pd.DataFrame]`) – List of output data. Should be all of same type (complex/non-complex, replica-tricks/no replica tricks, calc\_type).

- **make\_copy** (*bool*, *optional*) – If true, deepcopy data so that passed in data are not altered by any changes here. The default is True.

## 2.8 pyhande.error\_analysing

Classes for analysis of CCMC/FCIQMC observables.

### 2.8.1 pyhande.error\_analysing.analysis\_utils

Shared helper functions for analysers.

`pyhande.error_analysing.analysis_utils.check_data_input` (*data*:  
*List[pandas.core.frame.DataFrame]*,  
*cols*: *Optional[List[str]]*,  
*eval\_ratio*: *Optional[Dict[str, str]]*,  
*hybrid\_col*: *Optional[str]*,  
*start\_its*: *Union[List[int], str]*, *end\_its*: *Optional[List[int]]*) →  
None

Check data input against other, previous, input.

#### Parameters

- **data** (*List[pd.DataFrame]*) – List of QMC data.
- **cols** (*Union[List[str], Optional[List[str]]]*) – Columns to be analysed when blocking/ finding starting iteration with ‘blocking’.
- **eval\_ratio** (*Optional[Dict[str, str]]*) – Contains information to evaluate ratio (e.g. projected energy) when doing blocking analysis.
- **hybrid\_col** (*Union[Optional[str], str]*) – Column name when doing hybrid analysis/ finding starting iteration with ‘mser’.
- **start\_its** (*Union[List[int], str]*) – Starting iterations for analysis or information on type of find\_starting\_it function.
- **end\_its** (*Optional[List[int]]*) – Last iterations for analysis.

**Raises** `ValueError` – If cols, eval\_ratio, hybrid\_cols are specified but not in data respectively. If start\_its/end\_its are lists of iterations but the list has a different length than data.

`pyhande.error_analysing.analysis_utils.set_cols` (*observables*: *Dict[str, str]*, *it\_key*: *str*,  
*cols*: *Optional[List[str]]*, *replica\_col*:  
*str*, *eval\_ratio*: *Optional[Dict[str, str]]*,  
*hybrid\_col*: *Optional[str]*) → *Tuple[str, Optional[List[str]], str, Optional[Dict[str, str]], str]*

Set various columns and observable names.

Either the input is simply returned or set to observables[input] if input starts with ‘obs:’.

#### Parameters

- **observables** (*Dict[str, str]*) – Map of key to column/observable name, e.g. {‘ref\_key’: ‘N\_0’}

- **it\_key** (*str*) – Key or actual name for iterations.
- **cols** (*Union[Optional[List[*str*]], List[*str*]]*) – Keys or actual names of columns/observables to be analysed in blocking.
- **replica\_col** (*str*) – Key or actual name for replica column.
- **eval\_ratio** (*optional[Dict[*str*, *str*]]*) – Keys or actual names of elements in observable ratio to be evaluated.
- **hybrid\_col** (*Union[Optional[*str*], *str*]*) – Key or actual name of column/observable to be analysed in hybrid analysis.

**Returns**

**Return type** (Set) values from above (except *observables*).

## 2.8.2 pyhande.error\_analysing.blocker

Analyse Monte Carlo correlated output using reblocking.

```
class pyhande.error_analysing.blocker.Blocker (it_key: str, cols: List[str], replica_col:
                                             str, eval_ratio: Optional[Dict[str, str]]
                                             = None, hybrid_col: Optional[str] =
                                             None, start_its: Union[List[int], str] =
                                             'blocking', end_its: List[int] = None,
                                             find_start_kw_args: Dict[str, Union[bool,
                                             float, int]] = None)
```

Bases: `pyhande.error_analysing.abs_error_analyser.AbsErrorAnalyser`

Reblock specified columns from HANDE output using pyblock.

Can be used instead of HybridAnalyser.

This uses pyblock [1] to do reblocking, see Ref. [2] for more details on the reblocking algorithm.

[1] - pyblock, James Spencer, <http://github.com/jsspencer/pyblock> [2] - Flyvbjerg, H., Petersen, H. G., 1989, J. Chem. Phys. 91, 461.

```
classmethod inst_hande_ccmc_fciqumc (start_its: Union[List[int], str] = 'blocking', end_its:
                                     List[int] = None, find_start_kw_args: Dict[str,
                                     Union[bool, float, int]] = None)
```

Return Blocker instance for a HANDE CCMC/FCIQMC calculation.

**Parameters** `__init__()` (See) –

**Returns** Instance of the Blocker class, customised for a HANDE CCMC/FCIQMC calculation.

**Return type** *Blocker*

**start\_its**

Access `_start_its` attribute if available, else error.

**end\_its**

Access `_end_its` attribute if available, else error.

**opt\_block**

Access `_opt_block` attribute if available. Else error.

**no\_opt\_block**

Access `_no_opt_block` attribute if available. Else error.

**reblock**

Access `_reblock` attribute if available. Else raise error.

**data\_len**

Access `_data_len` attribute if available. Else raise error.

**covariance**

Access `_covariance` attribute if available. Else error.

**exe** (*data*: *List[pandas.core.frame.DataFrame]*, *observables*: *Dict[str, str]*) → None

Do reblocking (first finding starting iteration if required).

**Parameters**

- **data** (*List[pd.DataFrame]*) – HANDE calculation Monte Carlo output data.
- **observables** (*Dict[str, str]*) – Mapping of column key to column name, e.g. `'ref_key': 'N_0'`. The default is None. If any of *it\_key*, *cols*, *eval\_ratio*, *hybrid\_col*, *replica\_col* were instantiated as `'obs:key'` to be overwritten with `observables['key']`, `observables` can't be None and those keys have to be present.

**Raises** `ValueError` – If not all columns to be blocked appear in `'data'` or if the length of `'data'` is different to length of `'start_its'` or `'end_its'` if they are defined.

### 2.8.3 pyhande.error\_analysing.find\_starting\_iteration

Functions to find starting iteration for analysis.



```

pyhande.error_analysing.find_starting_iteration.find_starting_iteration_blocking(data:
    pan-
    das.core.frame
    end_it:
    int,
    it_key:
    str,
    cols:
    List[str],
    hy-
    brid_col:
    str,
    start_max_fra-
    float
    =
    0.8,
    grid_size:
    int
    =
    10,
    num-
    ber_of_rebloc-
    int
    =
    1,
    show_graph:
    bool
    =
    False)
    →
    int

```

Find the best iteration to start analysing CCMC/FCIQMC data.

It first excludes data before not all data in all columns specified in *cols* are varying and after *end\_it*. Then it searches for the starting iteration using an adaptive grid search on a log scale since we assume that the starting iteration is closer to the beginning than the end of the available data. During the search, a loss function is minimised. The loss is the fractional error over number of data involved in the blocking for each data column in *cols*.

This implementation is based on an older version in `pyhande/lazy.py`. V. A. Neufeld thanks the EPSRC CDT CMMS cohort 1 in Cambridge for helpful discussions.

**Warning:** Use with caution, check whether output is sensible and adjust parameters if necessary.

### Parameters

- **data** (*pd.DataFrame*) – QMC data, e.g. as extracted by `extract.py`. Has to contain columns with key *it\_key* and columns in *cols*, used for blocking.
- **end\_it** (*int*) – Last iteration to be considered in blocking.
- **it\_key** (*str*) – Key of column containing MC iterations.
- **cols** (*List[str]*) – List of keys of columns involved in blocking.
- **hybrid\_col** (*str*) – Ignored here, for common interface.

- **start\_max\_frac** (*float*, *optional*) – The start iterations found has to be in the first *start\_max\_frac* fraction of the data between the point where all columns in *cols* have started varying and *end\_it*. This prevents finding a starting iteration too close to the end. Has to be between 0.00001 and 1.0. The default is 0.8.
- **grid\_size** (*int*, *optional*) – Number of logarithmically spaced grid points per run. The default is 10.
- **number\_of\_reblocks\_to\_cut\_off** (*int*, *optional*) – To be extra sure, cut off a few reblocks to make sure data after starting iteration is truly in equilibrium. Cannot be negative. The default is 1.
- **show\_graph** (*bool*, *optional*) – If True, show a graph showing the columns with key *cols[0]* as a function of iterations. The suggested starting iteration is highlighted. The default is False.

#### Raises

- `ValueError` – If *start\_max\_frac* or *number\_of\_reblocks\_to\_cut\_off* are out of range.
- `RuntimeError` – If not all columns with keys in *cols* have started varying in *data* or if suitable starting iteration was not found.

**Returns** Suggestion iteration in columns *it\_key* where analysis should start.

**Return type** `int`

```
pyhande.error_analysing.find_starting_iteration.find_starting_iteration_mser_min(data:
    pan-
    das.core.frame,
    end_it:
    int,
    it_key:
    str,
    cols:
    List[str],
    hy-
    brid_col:
    str,
    start_max_fra-
    float
    =
    0.84,
    n_blocks:
    int
    =
    100)
    →
    int
```

Estimate starting iteration with MSER minimization scheme.

**Warning:** Use with caution, check whether output is sensible and adjust parameters if necessary.

This function gives an optimal estimation of the starting iterations based on MSER minimization heuristics. This methods decides the starting iterations  $d$  as minimizing an evaluation function  $\text{MSER}(d) = \sum_{i=1}^{n-d} (X_{i+d} - X_{\text{mean}}(d)) / (n - d)^2$ . Here,  $n$  is length of time-series,  $X_i$  is `eval_ratio['num'] / eval_ratio['denom']` of  $i$ -th step, and  $X_{\text{mean}}$  is the average of  $X_i$  after the  $d$ -th step.

This is a reformatted and altered version of a previous implementation in lazy.py by Tom Ichibha. See Ichibha, T., Hongo, K., Maezono, R., Thom, A. J. W., 2019 arXiv:1904.09934 [physics.comp-ph]

#### Parameters

- **data** (`pandas.DataFrame`) – Calculation output of a FCIQMC or CCMC calculation.
- **end\_it** (`int`) – Last iteration to be considered in blocking.
- **it\_key** (`str`) – Key of column containing MC iterations.
- **cols** (`List[str]`) – Ignored here. Keep for common interface.
- **hybrid\_col** (`str`) – Column in data to be analysed here, e.g. ‘Inst. Proj. Energy’.
- **start\_max\_frac** (`float`) – MSER( $d$ ) may oscillate when become unreasonably small when  $n - d$  is large. Thus, we calculate MSER( $d$ ) for  $d < (n * \text{start\_max\_frac})$  and give the optimal estimation of the starting iterations only in this range of  $d$ . The default is 0.84.
- **n\_blocks** (`int`) – This analysis takes long time when  $n$  is large. Thus, we pick up  $d$  for every ‘n\_blocks’ samples, calculate MSER( $d$ ), and decide the optimal estimation of the starting iterations only from these  $d$ . The default is 100.

**Returns** **starting\_it** – Iteration from which to start reblocking analysis for this calculation.

**Return type** `int`

`pyhande.error_analysing.find_starting_iteration.select_find_start` (`key: str`)  
Select `find_starting_iteration` function to use.

**Parameters** **key** (`str`) – Key linked to `find_starting_iteration`.

**Returns**

**Return type** `Find_starting_iteration` function.

## 2.8.4 pyhande.error\_analysing.hybrid\_ana

Analyse Monte Carlo correlated output with hybrid analyser.

```
class pyhande.error_analysing.hybrid_ana.HybridAna(it_key: str, hybrid_col: str,
                                                    replica_col: str, cols: Optional[List[str]] = None,
                                                    start_its: Union[List[int], str] = 'mser', end_its: List[int] = None,
                                                    batch_size: int = 1, find_start_kw_args: Dict[str, Union[bool, float, int]] = None)
```

Bases: `pyhande.error_analysing.abs_error_analyser.AbsErrorAnalyser`

Analyse ratio observable, such as projected energy.

Can be used instead of Blocker.

This scheme is made by hybridizing two different post-analysis methods, AR model and Straatsma. The former (the latter) is comparatively good at estimating the statistic error for smaller (larger) length of time-series, respectively. This method just picks up the larger statistic error from the ones given by both methods. The mathematical details of both methods are explained in (please cite if you use this):

Ichibha, T., Hongo, K., Maezono, R., Thom, A. J. W., 2019 arXiv:1904.09934 [physics.comp-ph]

```
classmethod inst_hande_ccmc_fcimc (start_its: Union[List[int], str] = 'mser',
                                   end_its: List[int] = None, batch_size: int = 1,
                                   find_start_kw_args: Dict[str, Union[bool, float, int]]
                                   = None)
```

Return HybridAna instance for a HANDE CCMC/FCIQMC calc.

**Parameters** `__init__()` (See) –

**Returns** Instance of the HybridAna class, customised for a HANDE CCMC/FCIQMC calculation.

**Return type** *HybridAna*

**start\_its**

Access `_start_its` attribute if available, else error.

**end\_its**

Access `_end_its` attribute if available, else error.

**opt\_block**

Access `_opt_block` attribute if available. Else error.

**no\_opt\_block**

Access `_no_opt_block` attribute if available. Else error.

**exe** (*data*: List[pandas.core.frame.DataFrame], *observables*: Dict[str, str]) → None

Do analysis (first finding starting iteration if required).

**Parameters**

- **data** (List[pd.DataFrame]) – HANDE calculation Monte Carlo output data.
- **observables** (Dict[str, str]) – Mapping of column key to column name, e.g. 'ref\_key': 'N\_0'. The default is None. If any of *it\_key*, *cols*, *eval\_ratio*, *hybrid\_col*, *replica\_col* were instantiated as 'obs:key' to be overwritten with `observables['key']`, `observables` can't be None and those keys have to be present.

**Raises** `ValueError` – If not all columns to be blocked appear in 'data' or if the length of 'data' is different to length of 'start\_its' or 'end\_its' if they are defined.

## 2.9 pyhande.extracting

Classes for extracting metadata and data from output files.

### 2.9.1 pyhande.extracting.extractor

Extract and merge (meta)data from (multiple) HANDE output files.

```
class pyhande.extracting.extractor.Extractor (merge: Dict[str, Union[List[str], str]] =
                                              None)
```

Bases: `pyhande.extracting.abs_extractor.AbsExtractor`

Extract data/metadata from HANDE output files and merge.

Merge if desired/sensible, e.g. when calculation was restarted. This expands the functionality of `extract.py` and is more compactly represented as a class.

**out\_files**

Access (read only) `out_files` property.

**Raises** `AttributeError` – If data has not been extracted yet, i.e. output files have not been passed yet.

**Returns** List of *out\_files* names the data is extracted from.

**Return type** `List[str]`

#### **data**

Access (extracted) data property.

**Raises** `AttributeError` – If data has not been extracted yet.

**Returns** QMC Data. List over merged calculations.

**Return type** `List[pd.DataFrame]`

#### **metadata**

Access (extracted) metadata property.

**Raises** `AttributeError` – If metadata has not been extracted yet.

**Returns** Metadata. List over merged calculations where each element is a list over the metadata of the calculations that got merged.

**Return type** `List[List[Dict]]`

#### **calc\_to\_outfile\_ind**

Map index of calculation to output file.

This maps what HANDE output file the data and metadata belong to. E.g. `[[0], [0], [1, 2]]` with three output files shows that the first calculations (index 0) contained two calculations and the second and third output file (indices 1 and 2) were merged to the third calculation.

**Raises** `AttributeError` – If data has not been extracted yet.

**Returns** Outer list has length equal the length of the data/metadata lists and contains list of indices of output files containing them (see above).

**Return type** `List[List[int]]`

#### **all\_ccmc\_fciqmc**

Are all calculations extracted either CCMC or FCIQMC.

This will affect what postprocessing can be done.

**Raises** `AttributeError` – If data has not been extracted yet.

**Returns** True if all calculations extracted are either CCMC or FCIQMC. False if at least one is of another type, such as FCI or Hilbert space estimation.

**Return type** `bool`

#### **exe** (*out\_files: List[str]*)

Extract and merge.

The merge code was inspired by an older implementation in deprecated/removed `lazy.py` file. [todo] Test with `calc` where a file has more then one `calc`.

**Parameters** *out\_files* (`List[str]`) – List of HANDE output filenames to be extracted here.

## 2.10 pyhande.helpers

Helpful generic callables.

### 2.10.1 pyhande.helpers.simple\_callables

Simple, useful callables when selecting. *\*args* are ignored.

```
pyhande.helpers.simple_callables.do_nothing(*args)
    Do nothing.
```

```
class pyhande.helpers.simple_callables.RaiseValueError(message)
    Bases: object
    Raise ValueError with message.
```

## 2.11 pyhande.results\_viewer

Further analysis and data viewing.

### 2.11.1 pyhande.results\_viewer.get\_results

Helper functions to run analysis and get results object.

```
pyhande.results_viewer.get_results.define_objects_common(merge_type: str =
    'uuid', analyser: str
    = 'blocking', start_its:
    Union[List[int], str]
    = 'blocking') → Tu-
    ple[pyhande.extracting.extractor.Extractor,
    py-
    hande.data_preparing.hande_ccmc_fcqmc.PrephH
    Union[pyhande.error_analysing.blocker.Blocker,
    py-
    hande.error_analysing.hybrid_ana.HybridAna]]
```

Create extractor, preparator and analyser with common options.

#### Parameters

- **merge\_type** (*str*, *optional*) – how to do merge, ‘uuid’, ‘legacy’ or ‘no’. Note that this is different to fuller options when instantiating extractor object directly, by default ‘uuid’.
- **analyser** (*str*, *optional*) – ‘blocking’ for doing reblocking or ‘hybrid’, by default ‘blocking’
- **start\_its** (*Union[List[int], str]*, *optional*) – Either list of integer for start iterations or ‘blocking’ or ‘hybrid’, defining find starting iteration function to use. by default ‘blocking’

**Returns** Instantiated objects for extracting, preparing and analysing data.

**Return type** `Tuple[Extractor, PrepHandeCcmcFcqmc, Union[Blocker, HybridAna]]`

```
pyhande.results_viewer.get_results.analyse_data(out_files: List[str], extractor: py-
                                                hande.extracting.extractor.Extractor,
                                                preparator: py-
                                                hande.data_preparing.hande_ccmc_fciqmc.PrepHandeCcmcFc
                                                = None, analyser:
                                                Union[pyhande.error_analysing.blocker.Blocker,
                                                pyhande.error_analysing.hybrid_ana.HybridAna]
                                                = None) →
                                                Union[pyhande.results_viewer.results.Results,
                                                pyhande.results_viewer.results_ccmc_fciqmc.ResultsCcmcFc
```

Execute objects to extract data, prepare and analyse it.

#### Parameters

- **out\_files** (*List[str]*) – Output files with data to extract, prepare and analyse.
- **extractor** (*Extractor*) – Instance to extract data from files.
- **preparator** (*PrepHandeCcmcFciqmc*) – Instance to prepare data, e.g. calculate inst. proj. energy or deal with complex/replica tricks. The default is None.
- **analyser** (*Union[Blocker, HybridAna]*) – Instance to analyse data, e.g. blocking. The default is None.

**Returns** Results object to view and further analyse results.

**Return type** *Union[Results, ResultsCcmcFciqmc]*

```
pyhande.results_viewer.get_results.get_results(out_files: List[str], merge_type:
                                                str = 'uuid', analyser:
                                                str = 'blocking', start_its:
                                                Union[List[int], str] = 'blocking') →
                                                Union[pyhande.results_viewer.results.Results,
                                                pyhande.results_viewer.results_ccmc_fciqmc.ResultsCcmcFc
```

Lazy function to combine defining objects and executing them.

**Parameters** **define\_objects\_common** and **analyse\_data** (*see*) –

**Returns**

**Return type** *see analyse\_data*

## 2.11.2 pyhande.results\_viewer.results

Access and investigate generic results from HANDE QMC.

```
class pyhande.results_viewer.results.Results(extractor: py-
                                                hande.extracting.extractor.Extractor)
```

Bases: *object*

Show and allow investigation of HANDE QMC results.

Extraction has already happened. This is a base class, used for now for all non CCMC and non FCIQMC calculations who use a more specific class.

#### **extractor**

Access extractor used to supply these results.

#### **summary**

Access summary.

**get\_metadata** (*meta\_keys*: *Union[str, List[str]]*) → *pandas.core.frame.DataFrame*

Get part(s) of metadata in pandas DataFrame.

**Parameters** **meta\_keys** (*Union[str, List[str]]*) – List of metadata items to put into DataFrame. Each item as ‘keyOuter:keyInner:...’, e.g. [‘qmc:tau’, ‘system:ueg:r\_s’] adds *extractor.metadata[:, ‘qmc’][‘tau’]* as well as *extractor.metadata[:, ‘system’][‘ueg’][‘r\_s’]*.

**Returns** Contains metadata requested for all calculations.

**Return type** *pd.DataFrame*

**add\_metadata** (*meta\_keys*: *List[str]*)

Add metadata to summary. Overwritten in *ResultsCcmcFciqmc*.

**Parameters** **meta\_keys** (*List[str]*) – List of metadata to add in strings where different level keys are separated by colons. E.g. [‘qmc:tau’, ‘system:ueg:r\_s’] adds *extractor.metadata[:, ‘qmc’][‘tau’]* as well as *extractor.metadata[:, ‘system’][‘ueg’][‘r\_s’]* to summary (if they exist).

### 2.11.3 pyhande.results\_viewer.results\_ccmc\_fciqmc

Access and investigate CCMC/FCIQMC results from HANDE QMC.

**class** *pyhande.results\_viewer.results\_ccmc\_fciqmc.ResultsCcmcFciqmc* (*extractor*:

*py-*  
*hande.extracting.extractor.Extractor*  
*prepara-*  
*tor: Optional[pyhande.data\_preparing.hande\_data\_preparing.Preparator]*  
*= None,*  
*analyser:*  
*Union[pyhande.error\_analysing.blas\_error\_analysing.BlasAnalyser,*  
*py-*  
*hande.error\_analysing.hybrid\_analysing.HybridAnalyser]*  
*=*  
*None)*

Bases: *pyhande.results\_viewer.results.Results*

Show CCMC and FCIQMC HANDE results and allow further analysis.

**preparator**

Access preparator used to prepare data for analysis.

**analyser**

Access analyser used to supply the analysed results.

**summary\_pretty**

Access *self.\_summary* but prettify for viewing data.

Combine value in “value/mean” column with “standard error” columns for easy viewing, e.g. ‘0.123(4)’. If not possible, due to type or not present values, fill in value in “value/mean”.

**Returns** Prettified summary table for viewing (not further analysis).

**Return type** *pd.DataFrame*

**compare\_obs** (*observables*: *List[str]*) → *pandas.core.frame.DataFrame*

Compare observables from *.summary* where obs are columns.

**Parameters** **observables** (*List[str]*) – Observables from *.summary* to compare.



**Returns** DataFrame where easier comparisons are possible.

**Return type** pd.DataFrame

#### **shoulder**

Access shoulder. For now, not hist shoulder [todo].

See J. S. Spencer and A. J. W. Thom (2016), J. Chem. Phys. 144, 084108.

#### **add\_shoulder()**

Add shoulder to summary. [todo]: allow hist shoulder.

#### **inefficiency**

Access inefficiency.

See W. A. Vigor et al. (2016), J. Chem. Phys. 144, 094110.

#### **add\_inefficiency()**

Add inefficiency to summary.

#### **add\_metadata(meta\_keys: List[str])**

Overwritten version of Results.add\_metadata.

**Parameters meta\_keys** (*List[str]*) – List of metadata to add in strings where different level keys are separated by colons. E.g. ['qmc:tau', 'system:ueg:r\_s'] adds extractor.metadata[:,['qmc']]['tau'] as well as extractor.metadata[:,['system']]['ueg']['r\_s'] to summary (if they exist).

#### **do\_reweighting(max\_weight\_history: int = 300) → None**

Do reweighting to check for population bias if done blocking.

For each independent shift value, this shows a graph of *weight\_history* against (weighted) projected energy/*eval\_ratio*. If the (weighted) projected energies (*eval\_ratio['name']*) do not agree with each other, this is a sign of population control bias. Note that this is only tested if *eval\_ratio['name']* contains the projected energy. See references. Very first implementation credit to Will Vigor.

**Parameters max\_weight\_history** (*int, optional*) – The maximum value of *weight\_history*. *Weight\_history* is done in steps of  $2^{**}n$  with  $2^{**}n < \text{'max\_weight\_history'}$ . The default is 300.

#### **Raises**

- `TypeError` – If analyser is not the blocking analyser.
- `ValueError` – *eval\_ratio* not specified when analysing.

## **References**

**Umrigar93** C.J. Umrigar et al. (1993), J. Chem. Phys. 99, 2865.

**Vigor15** W.A. Vigor, et al. (2015), J. Chem. Phys. 142, 104101.

#### **plot\_shoulder(inds: List[int] = None, show\_shoulder: bool = True, log\_scale: bool = True) → None**

Plot shoulder.

#### **Parameters**

- **inds** (*List[int]*) – Indices of calculations to plot. If None, plot all. The default is None.
- **show\_shoulder** (*bool*) – Show positions of shoulder height with vertical lines.
- **log\_scale** (*bool*) – Set x and y axis on log scale.



Compiled from various email threads on (and before) the nascent hande-dev list. The HANDE project's paper [Spencer14] for the 2nd Workshop on Sustainable Software for Science: Practice and Experiences (WSSSPE2) at SC14 contains a summary of working practices and our approach for developing software in an academic environment.

## 3.1 Git

### 3.1.1 git repository

HANDE can be downloaded by cloning the repository from github:

```
$ git clone https://github.com/hande-qmc/hande
```

We periodically tag releases

A private git repository, where much of the day-to-day development work takes place, is currently located at a private repository at github and can be cloned using:

```
$ git clone https://github.com/hande-qmc/hande-dev
```

or if using ssh keys,

```
$ git clone git@github.com:hande-qmc/hande-dev
```

If you would like access, please speak to one of the developers. The rest of this guide assumes you used the default remote name during the clone (i.e. `origin`). If this is not the case, we assume you are capable of appropriately adjusting the commands given in the rest of the guide.

---

**Note:** Bug fixes and similar work are applied to both public and private repositories. New features are often developed in the private repository (which hooks into our buildbot server for regression testing), whilst we iron them out. Once

we are happy that new features are ready for production use, they will also be migrated to the public repository.

---

### 3.1.2 Precepts

- All development happens in branches.
- Branches belong to a relevant namespace (feature/XXX indicates XXX is a branch (name) for a new feature, he/XXX for a HANDE enhancement (he), bug\_fix/XXX for a bug fix, config/XXX for a new config file, etc).
- Branches are merged into master after review. Merging between development branches should be avoided.
- Branches should be reviewed by one other person (at least) before merging into master.
- To review, send a pull request email (see [git request-pull](#)) to all developers (perhaps including a summary of work in the branch, which is not generated by request-pull!). This should be viewed as starting a conversation on the work.
- Make changes prompted by the review and resend the pull request. (This might take a few iterations.)
- After a happy conclusion to the review, merge into master.

Notes:

- We would like each commit to at least compile but don't expect each commit to be perfect in its own right! This is extremely useful for using `git-bisect` when investigating regression errors.
- New functionality should be incorporated by new tests. I intend to spend a day soon creating new tests and checking the code coverage (`lcov` is a wonderful tool) of the test suite.

See <http://nvie.com/posts/a-successful-git-branching-model/> for a popular variant on this approach.

The hope is that this approach will lead to better code and also (with a little work) everyone will be more familiar/comfortable with the code that they're not directly working on themselves.

### 3.1.3 Branch namespaces

A (non-exhaustive!) list of namespaces we use for branches:

**he/XXX** for an enhancement to HANDE (usually a modification to existing algorithms).

**bug\_fix/XXX** for a bug fix to a specific area of the codebase.

**opt/XXX** for optimisation work (please include performance details in the commit message!).

**feature/XXX** for a new feature (generally bigger than an enhancement).

**doc/XXX** for fixes/enhancements solely to the documentation. (Often this kind of work is coupled to feature/enhancement development work and the documentation is updated directly in the relevant branches consisting mainly of changes to the source code.)

**config/XXX** for new configuration file(s)/updates to existing configurations.

Obviously there is some overlap between the `he`, `feature` and (to a lesser extent) `opt` namespaces. Broadly speaking, new algorithms or changes to existing algorithms which require a new input options are best suited to the `feature` namespace, speed/memory improvements to `opt/` and other improvements (code tidying, logging, etc.) to the `he` namespace.

### 3.1.4 How to generate a pull request

First push your work to the relevant branch on the git sever and then generate template text for the pull request:

```
$ git request-pull startref origin [endref]
```

where startref (endref) is the commit you want to be reviewed from (to) and origin is the name of remote configured to the git sever. startref and endref can be any way of referring to a specific commit and endref defaults to HEAD if not given. Usually the branch would have been created from master, in which case you can simply do (even if master has been committed to since the branch was created):

```
$ git request-pull master origin
```

which generates (for example):

```
$ git request-pull master origin
The following changes since commit 7a58a8d1a8f2e8af15df1c9946e7596078649d79:

    Updated the config files for cx2. (2013-12-09 11:07:52 +0000)

are available in the git repository at:

    git@tyc-svn.cmth.ph.ic.ac.uk:hubbard_fcigmc config/cx2

for you to fetch changes up to 1a5522648378f406d3e5fbd87e22e3768da490bc:

    Fixed typo cx2 config comment (2013-12-13 14:35:42 +0000)

-----
William Vigor (1):
    Fixed typo cx2 config comment

config/cx2 |      2 +-
1 file changed, 1 insertion(+), 1 deletion(-)
```

Copy and paste this text into your email client and send the pull request to [hande-dev@imperial.ac.uk](mailto:hande-dev@imperial.ac.uk) (possibly with some additional text describing motivation/benchmark results/etc). If sendmail/exim4/other MTA is set up properly (naturally the CMTH ones are) then

```
$ git request-pull master origin | mail -s "Pull request" hande-dev@imperial.ac.uk
```

works as one would expect.

### 3.1.5 Merging to master

Here's a workflow to make merging to master simple. Remember that with git it's extremely difficult to make permanently destructive changes so if it goes wrong it can be fixed.

Before you start make sure your code compiles and passes the test suite. Do not merge broken code into master.

Now make sure your master branch is up to date. Here I do this in a fetch then a pull just to see what else has changed. I do a diff to be sure I'm the same as the origin master.

```
[master]$ git fetch
remote: Counting objects: 340, done.
remote: Compressing objects: 100% (182/182), done.
```

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```

remote: Total 200 (delta 137), reused 47 (delta 16)
Receiving objects: 100% (200/200), 96.89 KiB, done.
Resolving deltas: 100% (137/137), completed with 58 local objects.
From tyc-svn.cmth.ph.ic.ac.uk:hubbard_fcigmc
   c17ef9e..2d8e130  master    -> origin/master
   ...

[master]$ git pull
Updating c17ef9e..2d8e130
Fast-forward
 lib/local/parallel.F90      |    9 ++-----
src/full_diagonalisation.F90 |   30 ++++++++-----
2 files changed, 14 insertions(+), 25 deletions(-)

[master]$ git diff origin/master

```

The blank output from this indicates we're at origin/master.

I'm going to merge the branch `bug_fix/rdm_init`. Crucially we use the `--no-ff` flag to ensure that the merge creates a commit on master; this keeps the history clean (by keeping development work in logical chunks after merging) and also makes it very easy to roll-back and revert an entire feature if problems are encountered.

```

[master]$ git merge --no-ff bug_fix/rdm_init
Merge made by the 'recursive' strategy.
 src/fcigmc_data.f90 |    2 +-
 1 file changed, 1 insertion(+), 1 deletion(-)

[master]$ git log --graph --oneline --decorate | head
*   647b7dd (HEAD, master) Merge branch 'bug_fix/rdm_init'
| \
| * 3c67d81 (bug_fix/rdm_init) Fix uninitialised doing_exact_rdm_eigv breaking fci
* |   2d8e130 (origin/master, origin/HEAD) Merge branch 'bug_fix/small_fci_mpi'
| \ \

```

This shows that a new commit has been created on master.

At this point it's possible that the merge needed some manual intervention. It's fine to make these changes directly and commit them in the merge to your local master. If the merge is starting to get messy it might be best to rebase first to make it easier.

Very importantly, you should now compile the code and run the tests, even if the merge completed without any problems — there might be unintended effects. Only continue if the code compiles and the tests pass. If you need to make changes at this point, you can modify your local existing merge commit with

```
[master]$ git commit --amend
```

Now we've made sure that the code works, all we do is push to the main repo

```

[master]$ git push origin master
Counting objects: 12, done.
Delta compression using up to 12 threads.
Compressing objects: 100% (7/7), done.
Writing objects: 100% (7/7), 705 bytes, done.
Total 7 (delta 5), reused 0 (delta 0)
To git@tyc-svn.cmth.ph.ic.ac.uk:hubbard_fcigmc.git
   2d8e130..647b7dd  master -> master

```

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```
[master]$ git log --graph --oneline --decorate | head
* 647b7dd (HEAD, origin/master, origin/HEAD, master) Merge branch 'bug_fix/rdm_
↪init'
| \
| * 3c67d81 (bug_fix/rdm_init) Fix uninitialised doing_exact_rdm_eigv breaking fci
* | 2d8e130 Merge branch 'bug_fix/small_fci_mpi'
| \ \
```

Almost there. We now ought to clean up the namespace to avoid old branch names hanging around (the code of course will always stay).

```
[master]$ git branch --delete bug_fix/rdm_init
[master]$ git push origin --delete bug_fix/rdm_init
```

The list of branches merged into HEAD can be found by doing

```
[master]$ git branch --all --merged
```

All done!

### 3.1.6 Unwanted experimental branches

Occasionally (frequently?!) we have tried something which didn't work out. If we don't want to keep any of the history, we can simply delete the local (and if necessary) remote branches:

```
$ git branch --delete unwanted_branch
$ git push origin --delete unwanted_branch
```

But what about branches that we don't intend to continue working on in the near future, would like to keep around but without cluttering up the main repository, making it unclear which branches need some TLC before merging? We have a separate repository where such branches can be sent, to be resurrected if desired later. The repository is at [ch-hande@git.uis.cam.ac.uk:hande\\_graveyard.git](https://git.uis.cam.ac.uk:hande_graveyard.git). To push a local branch there:

```
$ git remote add graveyard ch-hande@git.uis.cam.ac.uk:hande_graveyard.git
$ git push remote graveyard unwanted_branch
```

and then delete the branch (both local and remote) from the main repository using the same commands as before. If the branch is not local, then you can either check it out and then do the push and delete (easier) or use a refspec:

```
$ git push graveyard refs/remotes/origin/unwanted_branch:refs/heads/unwanted_branch
```

where origin/unwanted\_branch is the remote branch to be moved to the graveyard repository. The branch on origin can then be deleted as before.

## 3.2 Adding a new test

1. Ensure the test suite passes with the master on your system.
2. Now checkout the branch you're working on where you'd like to add the test.
3. Rebuild HANDE so that the HANDE binary prints out the SHA1 hash of the current commit. Make sure that there are no uncommitted changes to the source directory so that the benchmarks can be reproduced at a later date using the same binary.

4. Inside test\_suite find the appropriate directory in which to add your test, or create a new directory, appropriately named, if necessary.
5. Inside this directory create a new directory with a sensible name describing your test, and change to it.
6. Place the input files for your test in the directory. You can have multiple input files in a single directory.
7. git add your directory (this avoids having to separate out files generated during the tests).
8. If you created a directory for a new category of tests then you will probably need to add the directory name in [ ] to the jobconfig file. If not, then the test should already be included through the globbing in jobconfig.
9. If required, pick some appropriate categories to add your test to in jobconfig.
10. Run testcode.py make-benchmarks to create new benchmarks e.g.

```
$ ../../testcode2/bin/testcode.py make-benchmarks
Using executable: /home/Alex/code/HANDE/master/test_suite/../../bin/hande.x.
Test id: 09042014-2.
Benchmark: 288ad50.

...

Failed tests in:
  /home/Alex/code/HANDE/master/test_suite/H2-RHF-cc-pVTZ-Lz
Not all tests passed.
Create new benchmarks? [y/n] y
Setting new benchmark in userconfig to be 6d161d0.
```

Hopefully the only failed tests are your new tests (which you've checked).

Alternatively, a better method is to make a benchmark for the new test only:

```
$ ../../testcode2/bin/testcode.py make-benchmarks -ic fciqmc/H2-RHF-cc-pVTZ-Lz

...

Setting new benchmark in userconfig to be: 6d161d0 288ad50.
```

The use of the 'i' flag tells testcode2 to insert the new benchmark at the start of the existing list of benchmarks, as can be seen in this example.

If you leave the 'i' flag out then it will remove all old benchmarks, which we do not want.

11. Now remember to add the benchmark files and the jobconfig and userconfig files to the repository.

```
$ git add userconfig jobconfig fciqmc/*/benchmark.out.6d161d0.inp*
```

where 6d161d0 is the hash of the newly-created benchmark.

12. Do a quick git status to make sure you haven't missed anything important out, and then you're ready to commit the tests:

```
$ git commit -m "Added new test H2-RHF-cc-pVTZ-Lz and benchmark 6d161d0."
```

Remember you're committing to a branch not the master.

13. Push this to the main repository and send round a pull request for review before its to be merged with master.



### 3.3 Debugging options

There are a couple of compilation options to help with debugging HANDE.

- The `-g` option to `tools/mkconfig.py` enables compiler options for warnings and run-time checking.
- The `-DDEBUG` preprocessor flag enables additional debugging output. Currently this is stack traces when `stop_all` is called to terminate with an error - the addresses given can be converted to `file:line` number information with `addr2line`. For example:

```
$ /path/to/hande.x test.lua
[...]
/usr/lib/libasan.so.4(+0x55c60) [0x7fc1c5000c60]
./bin/hande.x(+0x609e80) [0x5614f6742e80]
./bin/hande.x(+0x469177) [0x5614f65a2177]
./bin/hande.x(+0x1aa839) [0x5614f62e3839]
./bin/hande.x(+0x1aa8f1) [0x5614f62e38f1]
/usr/lib/libc.so.6(__libc_start_main+0xea) [0x7fc1c17e1f4a]
./bin/hande.x(+0xa93ca) [0x5614f61e23ca]

ERROR.
HANDE stops in subroutine: run_hande_lua.
Reason: File does not exist:test.lua
EXITING...
```

The addresses are not conserved between builds, compilers, optimisation levels and so on. The filenames can be included if `-rdynamic` is included in the linker flags:

```
/usr/lib/libasan.so.4(+0x55c60) [0x7f1943b93c60]
./bin/hande.x(__errors_MOD_stop_all+0x1c2) [0x55bf6aae5d30]
./bin/hande.x(__lua_hande_MOD_run_lua_hande+0x6e1) [0x55bf6a945027]
./bin/hande.x(+0x1c66e9) [0x55bf6a6866e9]
./bin/hande.x(main+0x36) [0x55bf6a6867a1]
/usr/lib/libc.so.6(__libc_start_main+0xea) [0x7f1940374f4a]
./bin/hande.x(_start+0x2a) [0x55bf6a58527a]

ERROR.
HANDE stops in subroutine: run_hande_lua.
Reason: File does not exist:test.lua
EXITING...
```

The actual source (file and linenumber) can be found using either `addr2line` or `gdb` (easier). With `addr2line`:

```
$ addr2line +0x469177 -e /path/to/hande.x
/home/james/hande/src/hande-bug-fix/src/lua_hande.F90:92
```

and with `gdb`:

```
$ gdb /path/to/hande.x
(gdb) list *__lua_hande_MOD_run_lua_hande+0x6e1
0x485027 is in lua_hande::run_lua_hande (src/lua_hande.F90:92).
 87
 88             ! Read input file on parent and broadcast to all other_
 89             ↪processors.
 89             if (parent) then
 90                 call get_command_argument(1, inp_file)
 91                 inquire(file=inp_file, exist=t_exists)
```

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```

92             if (.not.t_exists) call stop_all('run_hande_lua','File_
↳does not exist: '//trim(inp_file))
93
94             write (6,'(a14,/,1X,13("-"),/)') 'Input options'
95             call read_file_to_buffer(buffer, inp_file)
96             write (6,'(A)') trim(buffer)

```

where `__lua_hande_MOD_run_lua_hande+0x6e1` was the address of interest from the stacktrace. Note the `*` prefix. The same can be done with just the bare address if `-rdynamic` isn't used.

`addr2line` is a little more involved if `-rdynamic` is used – one needs to find the offset for the function of interest and hence find the line address by adding the address relative to the function start. For example, in:

```
./bin/hande.x(__errors_MOD_stop_all+0x1c2) [0x55bf6aae5d30]
```

the function is `__errors_MOD_stop_all` (`stop_all` in the `errors` module). The start address can be found from `objdump`:

```

$ objdump -T /path/to/hande.x | grep __errors_MOD_stop_all
0000000000625b6e g    DF .text    0000000000000c0c Base      __errors_MOD_stop_
↳all

```

The first field is the address in **hexadecimal**. Hence:

```

$ python -c 'print(hex(0x0000000000625b6e+0x1c2))'
0x625d30
$ addr2line -e /path/to/hande.x 0x625d30
/path/to/hande/lib/local/error_handling.F90:60

```

Note the explicit `0x` prefix for the start address of `__errors_MOD_stop_all`.

## 3.4 FAQ

- Is it ever ok to commit directly to master?

Yes, but only under very restricted circumstances! If in doubt make a branch and let someone else do the merge.

- I've got a quick bugfix which I've tested - can I commit it to master?

Well done on the testing. A bugfix should go in a `bugfix/XXX` branch. It's a single command to create this. Another few commands and you'll have an pull request email to the `hande-dev` list for review.

- But it's a really quick fix! Surely it won't hurt?

If it will affect functionality (and potentially someone else's jobs) then it probably ought to be reviewed! If it's a very minor corner case of which you're certain, then commit to a bugfix branch and then do the merge yourself. Always do this via a branch - don't commit directly to master. It's sensible to ask the original author if you're fixing their code however.

- But I need to use this fix to make my runs work.

You can always run from a bugfix branch. Because you've committed it to the central git repository, you'll have access to it everywhere.

- What if I need this bugfix to develop a new feature?

I don't know. Ask James! One option is to base your subsequent feature branch off the bug fix branch before it's merged into master (git handles merges very well!) or to cherry-pick the bug fix into your feature branch or make enough noise to get the bug fix merged quickly.

- I've added some comments to clear up something.

This might be ok to commit to master. If you designed the feature/documentation then you're effectively reviewing yourself. If it's somebody else's code it's polite to have consulted someone on this (either by email, or a review branch).

- But I've modified a feature that only I'm using...

It sounds like this should be in an enhancement branch `he/XXX`. If only you're using it it's even more important than someone else review it.

- I've accidentally committed some changes to my local master. What do I do?

Remember that you can always push to a different branch on the main server.

```
$ git push origin master:he/XXX
```

would push your changes to the `he/XXX` branch. It's probably better, however to checkout your changes locally to a branch, and then roll back your master, and then commit the branch:

```
$ git checkout -b he/XXX
$ git push --set-upstream origin he/XXX
$ git checkout master
$ git reset --hard origin/master
```

Note the last command resets your local master to the same state as that on origin. You should adapt the reset command to set your master to point to the desired commit (ie the first commit shared with the new branch `he/XXX`).

- Ok - I've gone through the review process and I'd like to try to merge to master myself. Is it easy?

Easy as pie. There's a workflow in the section [Merging to master](#)

- I've got a local branch which I've been working on for some time, but I don't want the pain of a large merge at the end.

This sounds like a workflow problem. Some comments on this:

- We need to lose the idea of personal branches (note the branch namespace is organised by topic rather than person), even though a branch might be written entirely/mostly by one person. In that sense, long-running development work should be split into small, logical chunks, each of which is attached one-at-a-time in its own branch. We have always regretted having (multiple) long-running branches.
- When wrenched away from a WIP with only a distant prospect of future free time, a commit and push with light notes is a very worthwhile thing. It's probably even worthwhile committing a plan before committing any actual code. If these are fast and flexible enough they will hopefully not discourage, but actually encourage organization. It might also encourage (*gasp*) collaboration. Perhaps you could create a directory in documentation as a place for such notes/roadmaps, somewhere between Python's PEP system and informal topic-based TODO lists?
- We are pretty happy for development branches to be regularly rebased against master (*note*: not merged in either direction), to lessen the pain of one final merge between two very disparate branches.

- This is all very well (and I enjoy the Socratic method), but I'm stuck with a huge branch I don't have time to merge. What do I do?

Commit it as a `feature/XXX` or `he/XXX` and ask for help from the `hande-dev` list.

- How do I review code?

We're working on a workflow for this. One method is to make a branch (if you're not already in one) and just add comments to the source. It's helpful if the review is part of the git history (even if the comments never actually make it to the master). We currently are using [watson-style](#) tags in comments for code review and discussion, for example:

```
! [review] - JSS: How about doing it this way?  
! [reply] - AJWT: I thought about it but that causes problems due to X.
```

where JSS and AJWT are the initials of the reviewer and code author respectively.

Documentation can also be reviewed, and in rst has the format

```
Some Documentation in RST format.  
  
..  
    [review] - AJWT: I don't see how this works.
```

- Will *my* code actually get reviewed?

We're all usually terribly busy and have very little time, but in a group effort a little from each person goes a long way. If you review others' code then they're more likely to review yours. Make it easy to review, by keeping it clean and the features short. Remember, this kind of review is far more lightweight than peer review of publications, and should be able to slot into people's 'free' time. (Each branch is far more lightweight than a paper.) A simple pull-request should be enough to get people to review. This is rather intricately tied in with the idea of project management. Prodding/cajoling/bullying emails are all possible to aid the review

- What happens if no-one replies to the pull request?

Here are some opinions:

- I suggest that after an agreed upon time (X working days?) without even a "I'll review but am too busy until next week" reply, the author is free to merge it into master (but should be open to fixes/improvements to that work that others subsequently suggest).
- Having been burdened with years-long old dirty branches from other projects, merging is certainly vital. I don't think lack of review should stop merging, but it should prompt someone to ask why.
- I would view it as a sign that the work is stable and relatively complete (for the time being) and is ready to be used by others/in production calculations.

- What about major (long-term) development work? Perhaps anyone engaged in major projects should send out 'pull-requests' to request review of ongoing work periodically?

Yes.

- Why are we bothering with review? Surely it makes life more difficult?

In an attempt to avoid heaps of

1. completely redundant code
2. untested code
3. buggy code

all ending up in master. The main reason is to encourage something resembling a coherent design and prevent someone going off in a (technical) direction others don't agree with/can see major problems with. A big plus is that it helps everyone become familiar with code that they didn't write (which is why doing code review is good for newcomers).

- PhD students are going to be working on this. How do you see the work they produce on a single project over the course of 3 years going? How often should their code be subject to review?

PhD projects are never one single monolithic project (or at least shouldn't be!). The amount and frequency of review is probably a function of how experienced a developer is (in general and with HANDE). Remember a pull request can simply be an indication that the developer would like to start a conversation rather than presenting the final result. Developers should also be encouraged to consider how a development task can be broken down into smaller projects, which might well aid design and testing, as well as reducing horrible merge conflicts from attempting to merge long-standing branches.

- How do I signify a 'fine - no need to comment' commit?

We suggest a pull request to the email list followed immediately by an email announcing that the requester had also merged into master (or perhaps just the latter email).



## 4.1 Release notes for v1.6

### 4.1.1 Added

- **DMQMC**
  - Piecewise IP-DMQMC, where IP-DMQMC is used to sample the density matrix for a given target beta, and thereafter the Bloch equation is used to sample a temperature range from the target beta to a user defined final beta (see W. Z. Van Benschoten and J. J. Shepherd. Piecewise Interaction Picture Density Matrix Quantum Monte Carlo. *J. Chem. Phys.* **156**, 184107 (2022). <https://doi.org/10.1063/5.0094290>)
  - Asymmetric propagation using the Bloch equation in DMQMC.
  - Symmetric propagation for systems defined by an FCIDUMP in IP-DMQMC.
  - A population scaling factor for the initial distribution of particles on the density matrix in DMQMC.
- Ability to generate and print out only the diagonal FCI matrix elements.
- FCIQMC RDM's and simple analysis scripts for the associated RDM files and energy estimates.
- Statehistogram code, analysis scripts and unit tests of analysis scripts for FCIQMC and DMQMC.
- Harmonic population control.
- Wall-Chebyshev propagator for FCIQMC/CCMC.
- Utility script that generates  $L_z$ -transformed FCIDUMPs for  $D_{\infty h}$  and spherically symmetric systems.
- Davidson algorithm for FCI.
- Unitary CCMC (UCCMC) algorithm and Trotterized Unitary CCMC algorithm (tUCCMC) (see M.-A. Filip and A. J. W. Thom. A stochastic approach to unitary coupled cluster. *J. Chem. Phys.* **153**, 214106 (2020). <https://doi.org/10.1063/5.0026141>)
- **CCMC**

- Deterministic MPI initialisation of CCMC calculations.
- Metric-tree based multi-reference CCMC acceptance algorithm.
- Reading in of multi-reference CCMC secondary references.
- Symmetry screening of multi-reference CCMC secondary references.
- Discard threshold for (U)CCMC for discarding clusters with large amplitude/ $p_{gen}$  ratios. This has been empirically shown to alleviate blooms and have small effect on the final energy, and is in principle extrapolatable to the exact energy.

### 4.1.2 Changed

- New options for analysis of DMQMC data with pyHANDE.
- **Several grand canonical initialization amendments:**
  - More robust population counting to reduce the severity of over/under initialization of the initial particle population for certain systems.
  - Arbitrary spin configurations (Previously only  $M_s = 0$  or  $M_s = N_{el}$  were possible)
  - Reference configuration checks to ensure the lowest energy configuration is used in the normalization procedure.
- Canonical estimates can now handle arbitrary spin configurations due to the changes mentioned for grand canonical initialization.
- Language changes for defining the propagators symmetry in DMQMC methods.

### 4.1.3 Removed

### 4.1.4 Bug Fixes

- Various intent(inout) compatibility issues with new compilers.
- Fix time reporting for OpenMP, now wall clock time instead of CPU time are reported per report loop. Language changes in final timings report to make clear whether wall clock or CPU times are reported.
- Fix an CCMC OpenMP bug where reference populations are sometimes undersampled.
- Fix edge cases in the real-space Hubbard model where self-interactions in more than one dimension were not correctly accounted for; and where nearest-neighbour interactions through the PBC are undercounted.

## 4.2 Release notes for v1.5

### 4.2.1 Added

- New hybrid analysis of output files implemented in pyhande. (T. Ichibha, K. Hongo, R. Maezono and A. J. W. Thom, arXiv:1904.09934)
- Unit tests for pyhande.
- Revised, object-oriented python analysis code for FCIQMC/CCMC/FCI implemented in pyhande.



### 4.2.2 Changed

- pyhande updated for pandas 1.0 compatibility.
- Multireference CCMC updated to enable use of multiple secondary references (M-A. Filip, C. J. C. Scott and A. J. W. Thom, J. Chem. Theory Comput., 15, 12, 6625-6635) (2019)
- Quasi-Newton propagation algorithm updated for compatibility with 3D UEGs. Automatic thresholds have also been added. (V. A. Neufeld and A. J. W. Thom, J. Chem. Theory Comput., 16, 3, 1503-1510)

### 4.2.3 Removed

- Iterative Lanczos algorithm for FCI calculations.

### 4.2.4 Bug Fixes

- Various minor memory and parallelism bugs.
- Unused variables removed from a series of functions.

## 4.3 Release notes for v1.4

### 4.3.1 Added

- Modified exchange integrals for complex read in systems for CCMC and FCIQMC solids calculations as mentioned in HANDE-QMC developers/J. S. Spencer et al., J. Chem. Theory Comput., published online (2019)
- Functionality for multireference stochastic coupled cluster, as implemented by M-A. Filip, C. J. C. Scott and A. J. W. Thom (unpublished)
- Weighted excitation generators for CCMC and FCIQMC called “Heat-Bath/Uniform Cauchy-Schwarz” excitation generators in V.A. Neufeld, A.J.W. Thom, J. Chem. Theory Comput., 15, 1, 127-140 (2019), related to S. D. Smart, G. H. Booth, and A. Alavi, unpublished (whose excitation generators are mentioned in L. R. Schwarz, PhD thesis, Cambridge (2017)) for molecular read in systems.

### 4.3.2 Changed

n/a

### 4.3.3 Removed

n/a

### 4.3.4 Bug Fixes

- When using `pattempt_update` and OpenMP simultaneously, there were potential race conditions when updating `pattempt_single` which have been fixed now.
- Previously, the k-points were printed off incorrectly in the symmetry table when doing solids CCMC/FCIQMC calculations.

- Fixed problems when using Quasi-Newton and k space lattice model systems (Hubbard model).

## 4.4 Release notes for v1.3

### 4.4.1 Added

- Weighted excitation generators for CCMC and FCIQMC as published in V. A. Neufeld, and A. J. W. Thom, arXiv:1808.05093 and A. A. Holmes, H. J. Changlani, and C. J. Umrigar, J. Chem. Theory Comput. 12, 1561 (2016) and S. D. Smart, G. H. Booth, and A. Alavi, unpublished.
- Complex DMQMC.
- CMake-based build system also available.
- Ability to restart the state of the dSFMT RNG stream, allowing for restarted calculations to have the same Markov chain as single calculations. Enabled by default. Can be disabled in the *restart options*.
- Quasi-Newton propagation for complex particles.
- Shared memory MPI with the integrals.
- Pyhande: reweighting plot to check for population bias as published in W. A. Vigor, J. S. Spencer, M. J. Bearpark, and A. J. W. Thom, J. Chem. Phys, 142, 104101 (2015).

### 4.4.2 Changed

- `write_frequency` now is in units of report loops rather than Monte Carlo cycles.

### 4.4.3 Removed

n/a

### 4.4.4 Bug Fixes

- Even selection weighting had an initialization bug affecting any calculation with more than one MPI process where one process has no single excitations. The effect is that for those cycles without singles, the even\_selection probability for the singles will be uninitialized, and possibly not zero. For a sufficiently large calculation there will be a low probability that this is the case, and if there are ever single excitations on the processor, that number will be used, and will continue to be used if there are no singles at some later date. It is expected that there will be no notable effect after equilibration. Incorrect even selection weightings only affect the efficiency of the selection, and will not in general introduce a bias. Effects on systems without single excitations (e.g. UEG and Hubbard models) are undefined. The bug-fix changes Markov chains.
- Even selection also had a bug that caused integer overflow when the number of MPI processes raised to the power of (coupled cluster level - 1) is bigger than a 32 bit integer.

## 4.5 What's new in version 1.2? (not an exhaustive list)

- We are now on restart file version number 2.

### 4.5.1 Features

- Auto-shift-damping
- Blocking-on-the-fly
- Complex CCMC
- DMQMC structure factor
- DMQMC momentum distribution
- Logging of CCMC stochastic selection
- Lua “cookbook”
- Reduced Density Matrices
- Replica Tricks for CIQMC
- Semi stochastic quasi-Newton
- Truncated and Even Selection
- Use of real cumulative populations in CCMC
- Write to arbitrary output file

### 4.5.2 Bug Fixes

- Storing projected energy in restart file to avoid estimation based on configuration interaction when restarting coupled cluster. Once we allow the rng state to be stored as well, this means continuous Markov chains across restarting in CCMC. Before this bug fix, the initial projected energy when restarting was (usually) different from what it should have been.
- Reading in semistochastic restart files.

### 4.5.3 Improvements to Stability and Robustness and Version Updates

- Move to LUA 5.3.3
- Removed support for GCC 4.7 and below
- Improve HDF5 support
- Improve broadcasting of integrals
- Alter how HANDE decides whether the shift should be varied or not when restarting.
- Improve direct LANCZOS hamiltonian memory handling.
- Improve dealing with HANDE.COMM in multi node calculations.
- Fix logging of death step
- Correctly convert 32 and 64 bit strings in restart files.

#### 4.5.4 Pyhande Updates

- Compatibility with Pandas 0.20
- Extend lazy.py to deal with Simple FCIQMC and fix how QMC calculations are detected.
- Allow multiple canonical calculations to be averaged.

## CHAPTER 5

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### Bibliography

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- search



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## Bibliography

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### p

- `pyhande`, [133](#)
- `pyhande.analysis`, [133](#)
- `pyhande.canonical`, [137](#)
- `pyhande.data_preparing`, [145](#)
- `pyhande.data_preparing.handc_ccmc_fcqmc`,  
[145](#)
- `pyhande.error_analysing`, [146](#)
- `pyhande.error_analysing.analysis_utils`,  
[146](#)
- `pyhande.error_analysing.blocker`, [147](#)
- `pyhande.error_analysing.find_starting_iteration`,  
[148](#)
- `pyhande.error_analysing.hybrid_ana`, [151](#)
- `pyhande.extract`, [137](#)
- `pyhande.extracting`, [152](#)
- `pyhande.extracting.extractor`, [152](#)
- `pyhande.helpers`, [153](#)
- `pyhande.helpers.simple_callable`, [154](#)
- `pyhande.lazy`, [138](#)
- `pyhande.results_viewer`, [154](#)
- `pyhande.results_viewer.get_results`, [154](#)
- `pyhande.results_viewer.results`, [155](#)
- `pyhande.results_viewer.results_ccmc_fcqmc`,  
[156](#)
- `pyhande.utils`, [144](#)
- `pyhande.weight`, [144](#)



## A

`add_inefficiency()` (py-hande.results\_viewer.results\_ccmc\_fciqmc.ResultsCcmcFciqmc method), 157

`add_metadata()` (py-hande.results\_viewer.results.Results method), 156

`add_metadata()` (py-hande.results\_viewer.results\_ccmc\_fciqmc.ResultsCcmcFciqmc method), 157

`add_shoulders()` (py-hande.results\_viewer.results\_ccmc\_fciqmc.ResultsCcmcFciqmc method), 157

`all_ccmc_fciqmc`

(py-hande.extracting.extractor.Extractor attribute), 153

`analyse_data()` (in module py-hande.results\_viewer.get\_results), 154

`analyse_hf_observables()` (in module py-hande.canonical), 137

`analyser` (py-hande.results\_viewer.results\_ccmc\_fciqmc.ResultsCcmcFciqmc attribute), 156

## B

`Blocker` (class in py-hande.error\_analysing.blocker), 147

## C

`calc_to_outfile_ind` (py-hande.extracting.extractor.Extractor attribute), 153

`check_data_input()` (in module py-hande.error\_analysing.analysis\_utils), 146

`check_key()` (in module py-hande.lazy), 140

`compare_obs()` (py-hande.results\_viewer.results\_ccmc\_fciqmc.ResultsCcmcFciqmc method), 156

`complex_data` (py-hande.data\_preparing.hande\_ccmc\_fciqmc.PrepHandeCcmcFciqmc attribute), 145

`concat_calcs()` (in module py-hande.lazy), 141

`covariance` (py-hande.error\_analysing.blocker.Blocker attribute), 148

## D

`data` (py-hande.data\_preparing.hande\_ccmc\_fciqmc.PrepHandeCcmcFciqmc attribute), 145

`data` (py-hande.extracting.extractor.Extractor attribute), 153

`data_len` (py-hande.error\_analysing.blocker.Blocker attribute), 148

`define_fciqmc_projects_common()` (in module py-hande.results\_viewer.get\_results), 154

`do_nothing()` (in module py-hande.helpers.simple\_callables), 154

`do_reweighting()` (py-hande.results\_viewer.results\_ccmc\_fciqmc.ResultsCcmcFciqmc method), 157

## E

`end_fciqmc` (py-hande.error\_analysing.blocker.Blocker attribute), 147

`end_its` (py-hande.error\_analysing.hybrid\_ana.HybridAna attribute), 152

`estimates()` (in module py-hande.canonical), 137

`exe()` (py-hande.data\_preparing.hande\_ccmc\_fciqmc.PrepHandeCcmcFciqmc method), 145

`exe()` (py-hande.error\_analysing.blocker.Blocker method), 148

`exe()` (py-hande.error\_analysing.hybrid\_ana.HybridAna method), 152

`exe()` (py-hande.extracting.extractor.Extractor method), 153

`extract_data()` (in module py-hande.extract), 138

`extract_data_sets()` (in module py-hande.extract), 137

`extract_pop_growth()` (in module py-hande.canonical), 134

`Extractor` (class in py-hande.extracting.extractor), 152

extractor (*pyhande.results\_viewer.results.Results* attribute), 155

## F

filter\_calcs() (in module *pyhande.lazy*), 141

find\_starting\_iteration() (in module *pyhande.lazy*), 142

find\_starting\_iteration\_blocking() (in module *pyhande.error\_analysing.find\_starting\_iteration*), 148

find\_starting\_iteration\_mser\_min() (in module *pyhande.error\_analysing.find\_starting\_iteration*), 150

find\_starting\_iteration\_mser\_min() (in module *pyhande.lazy*), 138

## G

get\_metadata() (*pyhande.results\_viewer.results.Results* method), 155

get\_results() (in module *pyhande.results\_viewer.get\_results*), 155

groupby\_beta\_loops() (in module *pyhande.utils*), 144

groupby\_iterations() (in module *pyhande.utils*), 144

## H

HybridAna (class in *pyhande.error\_analysing.hybrid\_ana*), 151

## I

inefficiency (*pyhande.results\_viewer.results\_ccmc\_fcimc.ResultsCcmFcimc* attribute), 157

inefficiency() (in module *pyhande.analysis*), 136

inst\_hande\_ccmc\_fcimc() (*pyhande.error\_analysing.blocker.Blocker* class method), 147

inst\_hande\_ccmc\_fcimc() (*pyhande.error\_analysing.hybrid\_ana.HybridAna* class method), 151

## L

lazy\_block() (in module *pyhande.lazy*), 141

lazy\_hybrid() (in module *pyhande.lazy*), 138

## M

metadata (*pyhande.extracting.extractor.Extractor* attribute), 153

## N

no\_opt\_block (*pyhande.error\_analysing.blocker.Blocker* attribute), 147

no\_opt\_block (*pyhande.error\_analysing.hybrid\_ana.HybridAna* attribute), 152

## O

observables (*pyhande.data\_preparing.hande\_ccmc\_fcimc.PrepHande* attribute), 145

opt\_block (*pyhande.error\_analysing.blocker.Blocker* attribute), 147

opt\_block (*pyhande.error\_analysing.hybrid\_ana.HybridAna* attribute), 152

out\_files (*pyhande.extracting.extractor.Extractor* attribute), 152

## P

plateau\_estimator() (in module *pyhande.analysis*), 134

plateau\_estimator\_hist() (in module *pyhande.analysis*), 135

plot\_shoulders() (*pyhande.results\_viewer.results\_ccmc\_fcimc.ResultsCcmFcimc* method), 157

preparator (*pyhande.results\_viewer.results\_ccmc\_fcimc.ResultsCcmFcimc* attribute), 156

PrepHandeCcmFcimc (class in *pyhande.data\_preparing.hande\_ccmc\_fcimc*), 145

projected\_energy() (in module *pyhande.analysis*), 133

*pyhande* (module), 133

*pyhande.analysis* (module), 133

*pyhande.canonical* (module), 137

*pyhande.data\_preparing* (module), 145

*pyhande.data\_preparing.hande\_ccmc\_fcimc* (module), 145

*pyhande.error\_analysing* (module), 146

*pyhande.error\_analysing.analysis\_utils* (module), 146

*pyhande.error\_analysing.blocker* (module), 147

*pyhande.error\_analysing.find\_starting\_iteration* (module), 148

*pyhande.error\_analysing.hybrid\_ana* (module), 151

*pyhande.extract* (module), 137

*pyhande.extracting* (module), 152

*pyhande.extracting.extractor* (module), 152

*pyhande.helpers* (module), 153

*pyhande.helpers.simple\_callable* (module), 154

*pyhande.lazy* (module), 138

*pyhande.results\_viewer* (module), 154

`pyhande.results_viewer.get_results(module)`, 154  
`pyhande.results_viewer.results (module)`, 155  
`pyhande.results_viewer.results_ccmc_fcqmc (module)`, 156  
`pyhande.utils (module)`, 144  
`pyhande.weight (module)`, 144

## Q

`qmc_summary()` (in module `pyhande.analysis`), 134

## R

`RaiseValueError` (class in `pyhande.helpers.simple_callables`), 154  
`reblock (pyhande.error_analysing.blocker.Blocker attribute)`, 147  
`replica_data (pyhande.data_preparing.hande_ccmc_fcqmc.PrepHandeCcmcFcqmc attribute)`, 145  
`Results` (class in `pyhande.results_viewer.results`), 155  
`ResultsCcmcFcqmc` (class in `pyhande.results_viewer.results_ccmc_fcqmc`), 156  
`reweight()` (in module `pyhande.weight`), 144  
`reweighting_graph()` (in module `pyhande.lazy`), 143

## S

`select_find_start()` (in module `pyhande.error_analysing.find_starting_iteration`), 151  
`set_cols()` (in module `pyhande.error_analysing.analysis_utils`), 146  
`shoulder (pyhande.results_viewer.results_ccmc_fcqmc.ResultsCcmcFcqmc attribute)`, 157  
`start_its (pyhande.error_analysing.blocker.Blocker attribute)`, 147  
`start_its (pyhande.error_analysing.hybrid_ana.HybridAna attribute)`, 152  
`std_analysis()` (in module `pyhande.lazy`), 139  
`summary (pyhande.results_viewer.results.Results attribute)`, 155  
`summary_pretty (pyhande.results_viewer.results_ccmc_fcqmc.ResultsCcmcFcqmc attribute)`, 156

## Z

`zeroT_qmc()` (in module `pyhande.lazy`), 140