Unravelling the mysteries of NECI

The n-Electron Configuration Interaction solver

Simon Smart, Nick Blunt and George Booth

September 1, 2015

1 Using NECI

1.1 Getting into the game

1.1.1 Getting the code

The NECI repository is stored on bitbucket. To gain access you need to be invited. Contact one of the repository administrators [Simon Smart (simondsmart@gmail.com), George Booth (george.booth24@gmail.com) and Nick Blunt (nsb37@cam.ac.uk)] who will invite you. If you already have a bitbucket account let the repository administrators know the email address associated with your account.

You will receive an invitation email. Please accept this invitation, and create a bitbucket account as prompted if necessary.

To gain access to the NECI repository, an ssh key is required. This can be generated on any linux machine using the command[1]

```
ssh-keygen -t rsa -b 2048
```

This will create a private (`~/.ssh/id_rsa`) and a public key file (`~/.ssh/id_rsa.pub`).

The private key must be kept private. On the bitbucket homepage, go to account settings (accessible from the top-right of the main page), and navigate to "SSH keys". Click "Add key" and add the contents of the public key. This will give you access to the repository.

You can now clone the code into a new directory using the command

```
git clone git@bitbucket.org:neci_developers/neci.git [target_dir]
```

1.1.2 Required libraries

NECI requires some external software and library support to operate:

MPI
> For builds of NECI intended to be run in parallel, an implementation of MPI is required. NECI has been heavily tested with OpenMPI, and MPICH2 and its derivatives (IBM MPI, Cray MPI, and Intel MPI).

Linear algebra
> NECI makes use of the linear algebra routines normally contained in BLAS/LA-PACK. There are a number of different packages which provide these routines, and are optimised for different compilers and platforms. NECI has been built and tested with either the AMD Core Math Library (ACML), the Intel Math Kernel Library

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[1] `ssh-keygen` can also generate DSA keys. Some ssh clients and servers will reject DSA keys longer than 1024 bits, and 1024 bits is currently on the margin of being crackable. As such 2048 bit RSA keys are preferred. Top secret this code is. Probably. Apart from the master branch which hosted for all on github. And in molpro. And anyone that wants it obviously.

(MKL), or the more general Basic Linear Algebra Subprograms (BLAS)/Linear Algebra Package (LAPACK) combination.

HDF5

To make use of the structured HDF5 format for reading/writing POPSFILES (files storing the population of walkers, and other information, to restart calculations). This library should be built with MPI and fortran support (`--enable-parallel --enable-fortran --enable-fortran2003`).

FFTW

A small number of options in NECI, which are not enabled by default, require Fast Fourier Transforms. If these are re-enabled then the Fastest Fourier Transform in the West (FFTW3) library is required.

If combinations of these choices are made other than those most commonly used then either the configuration files, or the resultant Makefile, will need to be modified.

On the majority of machines available to the Alavi group and department, the compilation environment is managed using the `module` command. Documentation for that command is available from the command `module help`. The most commonly used command is to load a module, using the command

```
module load <module_name>
```

Installing and configuring the module system on private machines is far beyond the scope of this document. Configuring your user account to use modules may required modifications to your `.bashrc` file, depending on the local machine configuration. Please contact the local IT administrators or Simon Smart for further advice.

A number of standard combinations of modules present themselves. Where an asterisk is presented, any version of the module can be used. Where the version is under specified, the latest module should be used. This will occur by default.

gfortran (Cambridge)

```
mpi/mpich2/gnu/1.4.1p1 acml/64/gfortran/*/up
```

ifort (Cambridge)

```
ifort/64 mpi/openmpi/64/intel12 acml/64/ifort/*/up
```

PGI (Cambridge)

```
pgi/64 mpi/openmpi/64/pgi12 lapack/64/pgi
```
The lapack module might not be available to all users. Please contact Simon Smart if required.

ifort (Max Planck FKF)

```
ifort mpi.intel
```
Note that the MKL library is included in the ifort module.

ifort (hydra)

```
git intel mkl mpi.ibm hdf5-mpi cmake
```


1.1.3 Building the code (using CMake)

There are two ways of building NECI. The recommended approach is to use the cmake build system. For legacy purposes, and for more explicitly customised build configura-

tions, the older Makefile system may also be used.

CMake allows building the code in a separate directory. One directory should be used per configuration that is to be built. This module can be a subdirectory of the NECI directory, or otherwise. With the `build` directory as the current working directory, execute

```
cmake [path_to_neci}
```

pointing CMake at the root directory of the cloned NECI repository.

At this point CMake will automatically configure NECI according to the currently loaded modules, and available compilers and libraries. If a different set of modules or compilers are to be used a fresh directory should be initialised (or equivalently

> If there is an available HDF5 library, which is compiled with support for MPI and for the Fortran compiler in use, then CMake will happily make use of it. Otherwise support for HDF5 POPSFILES will be disabled by default.
>
> The CMake configuration for NECI contains the functionality to download, compile and use HDF5. To do this just run
>
> ```
> make [-j] hdf5
> ```
>
> in the `build` directory and then re-run `cmake`.

The code is then built using the command

```
make [-j [n]] [neci|kneci|dneci|mneci]
```

The optional flag `-j` specifies that the build should be performed in parallel (with up to an optional number, `n`, threads).

The final argument specifies whether the normal code (`neci`) should be built, the complex code (`kneci`) the double run code (`dneci`) or the multi run code (`mneci`) are built. If not specified, all targets are built.

1.1.4 Configuring builds (Makefile system)

A specific configuration for building NECI is initialised by using the command

```
./tools/mkconfig.py config_name [-g]
```

The configuration names correspond to the configuration files contained in the config directory. If the flag `-g` is used, then a debug configuration will be created, and otherwise an optimised one.

There are a number of different configurations for differing systems, library and compiler setups. The following are some of the more important, and most likely to be used.

gfortran_simple, ifort_simple
> These are the basic configurations, set up for the gfortran and ifort compilers. For development these are the most likely configurations to be used. On personal machines the easiest environment to install is gfortran and openMPI, using the `gfortran\_simple` - see note regarding libraries below.

`fkf_ifort`
> The MPI and ifort installation at the FKF in Stuttgart is different to that available in most locations. Use this config file to compile there.

`PC-ifort64-MPI-TARDIS, PC-ifort64-MPI-HYDRA`
> The ifort compiler supports additional (expensive) optimisations during the link stage. For production runs on supercomputers these should be used. The -TARDIS config file is the normal one to use, with the -HYDRA for the differing environment available on HYDRA.

To specify a default configuration file to use on a particular machine, create a symbolic link called `.default` in the config directory to the appropriate configuration file. This allows `mkconfig.py` to be usedwithout specifying the configuration name.

To compile NECI, a number of linear algebra routines are required. The relevant routines are available in the AMD Core Math Library (ACML), the Intel Math Kernel Library (MKL) and in the more widely available combination of Basic Linear Algebra Subprograms (BLAS) and the Linear Algebra Package (LAPACK). The configuration files above make some assumptions about which packages are available, which are not always correct.

In particular, the elements of the linker lines

```
-lacml
-lmkl_intel_ilp64 -lmkl_core -lmkl_sequential
-lblas -llapack
```

are in principle interchangeable. On personal development machines it is easiest to install BLAS and LAPACK, but these are generally less performant so are not used by default. These lines can be substituted in the generated `Makefile` before compilation.

1.1.5 Building the code (Makefile system)

The code is built using the command

```
make [-j [n]] [neci.x|kneci.x|dneci.x|mneci.x|both|all]
```

The optional flag `-j` specifies that the build should be performed in parallel (with up to an optional number, `n`, threads).

The final argument specifies whether the normal code (`neci.x`) should be built, the complex code (`kneci.x`), the double run code (`dneci.x`), the multiple run code (`mneci.x`) or both the normal and complex codes (`both`) or all of the above and various extra utilities (`all`).

1.1.6 Git overview

It is essential if you plan to do developmental work to get familiar with the source-code management software 'git'. The code will get unusable exponentially quickly if all development and new ideas are hacked into the master branch of the code. The nature of research is that most things probably won't work, but you want to implement them and test relatively quickly, without requiring a standard of code that will remain usable in perpetuity. To avoid an inexorable increase in code 'clutter', it is essential to work in 'branches' off the main code. For a more detailed introduction to the git package,

see git-scm.com/book/en/v2/getting-started-git-basics. In short, the workflow should be:

1. Branch off a clean master version to implement something

2. Test and develop in the branch

3. Regularly merge the new code from the master branch into your personal development branch

4. Once satisfied with the development, and that it is an improvement in scope or efficiency of the existing code, ensure it is tidy, commented, documented, as bug-free as possible, and tests added to the test suite for it. This may involve reimplementing it from a clean version of master if it can be done more efficiently

5. Merge code back into master branch

A few potentially useful git commands in roughly the workflow described above:

`git branch`
> See what branch I am on. -a flag for all (inc. remote) branches.

`git pull origin master`
> Update the master branch into the current local repository

`git checkout -b newbranchname`
> Fork off current branch to a new branch called 'newbranchname'

`git commit -a -m 'Commit message'`
> Commit a set of changes for the current branch to your local repository.

`git push origin branchname`
> Push your current local branch called branchname to a new remote branch of the same name to allow access to others and secure storage of the work

`git checkout -b newbranchname --track origin/remotebranch`
> Check out a branch stored on the remote repository, and allow pushing and pulling from the remote repository for that branch.

`git push`
> Push the current branch to the remote branch that it is tracking.

`git merge master`
> Merge the recent changes in master into your local branch (requires a pull first)

`git checkout master`
> Switch branches to the master branch

`git merge newbranch`
> Merge your code in 'newbranch' into your current branch (potentially master)

Each commit should contain one logical idea and the commit message should clearly describe *everything* that is done in that commit. It is fine for one commit to only contain a very minor change. Try and commit regularly and avoid large commits. It is also a good idea to make sure that code compiles before commiting. This helps catch errors that you may be introducing and also allows the use of debugging tools such as git bisect.

It should be noted that the 'stable' branch of the code, automatically merged into from master upon successful completion of nightly tests, is hosted on github on a public repository, and also pushed to the molpro source code. The molpro developers will quickly send us angry emails if poor code gets pushed into it from NECI, and I will be sure to forward complaints onto the relevant parties!

1.2 Calculation inputs

```
title

system read
freeformat
electrons 10
(nonuniformrandexcits 4ind-weighted)
(hphf 0)
(molpromimic)
endsys

calc

methods
method vertex fcimc
endmethods

time 2000.0
memoryfacspawn 1.5
memoryfacpart 0.3
totalwalkers 100000
(tau 0.001)
(tau 0.001 search)
(max-tau 0.01)
startsinglepart 50
shiftdamp 0.02
stepsshift 10
diagshift 0.1
truncinitiator
addtoinitiator 3
allrealcoeff
(realcoeffbyexcitlevel 4)
realspawncutoff 0.01
semi-stochastic 500
(doubles-core)
(pops-core 1000)
trial-wavefunction 500
(doubles-trial)
(pops-trial 1000)
(readpops)
(readpops-changeref)
jump-shift
proje-changeref 1.5
maxwalkerbloom 1
(nmcyc 1000000) Necessary with molpromimic...
(definedet 1 2 3 4 5 6 7 8 9)
endcalc

integral
(freeze 2, 0)
(partiallyfreeze 6 2)
(partiallyfreezevirt 10 2)
endint

logging
popsfile
```

```
(popsfile -1)
popsfiletimer 10.0
incrementpops
binarypops
(calcrdmonfly ...)
(fcimcdebug 5)
write-core
endlog
end
```

1.3 Useful References Containing Technical Details

Original FCIQMC method:

- Fermion Monte Carlo without fixed nodes: a game of life, death, and annihilation in Slater determinant space.
  GH Booth, AJ Thom, A Alavi The Journal of chemical physics (2009) 131, 054106

Quite a bit of symmetries some stuff on the initiator method that is actually implemented:

- Breaking the carbon dimer: the challenges of multiple bond dissociation with full configuration interaction quantum Monte Carlo methods. GH Booth, D Cleland, AJ Thom, A Alavi The Journal of chemical physics (2011) 135, 084104

Linear scaling algorithm, (uniform) excitation generation and overall algorithm of FCIQMC:

- Linear-scaling and parallelisable algorithms for stochastic quantum chemistry GH Booth, SD Smart, A Alavi Molecular Physics (2014) 112, 1855

Density matrices, real walker weights and sampling bias:

- Unbiased Reduced Density Matrices and Electronic Properties from Full Configuration Interaction Quantum Monte Carlo. Catherine Overy, George H. Booth, N. S. Blunt, James Shepherd, Deidre Cleland, Ali Alavi, http://arxiv.org/abs/1410.6047

KP-FCIQMC:

- Krylov-projected quantum Monte Carlo N. S. Blunt, Ali Alavi, George H. Booth, http://arxiv.org/abs/1409.2420

1.4 Real walker coefficients

Real walker coefficients can be turned on in NECI in one of two ways. The recommended method is to use the 'RealCoeffByExcitLevel' option. If one adds 'RealCoeffByExcitLevel 4' to the Calc block then real coefficients will be used for all determinants up to 4 excitations of the reference determinant.

The following options relate to real coefficients, and all should be inserted in the Calc block.

`RealCoeffByExcitLevel n`
> Use real walkers on all determinants which are up to n excitations of the reference determinant.

`AllRealCoeff`
    Use real walkers for all determinants.

`RealSpawnCutoff x`
    Continuous real spawning will be performed, unless the spawn has weight less than x. In this case, the weight of the spawning will be stochastically rounded up to x or down to zero, such that the average weight of the spawning does not change. This is a method of removing very low weighted spawnings from the spawned list, which require extra memory, processing and communication. A reasonable value for x is 0.01.

`SetOccupiedThresh x`
    Set the value for the minimum walker weight in the main walker list. If, after all annihilation has been performed, any determinants have a total weight of less than x, then the weight will be stochastically rounded up to x or down to zero such that the average weight is unchanged.

    Default: x=1.0. This value should usually be used, and should only be changed if you have a good reason.

1.5 Semi-stochastic

To use semi-stochastic in NECI, the `semi-stochastic` option should be added to the Calc block, along with a further option to specify what core space to use. The following options are available and should be added to the Calc block.

`semi-stochastic`
    Turn on the semi-stochastic adaptation.

`doubles-core`
    Use the reference determinant and all single and double excitations from it to form the core space.

`cas-core cas1 cas2`
    Use a CAS space to form the core space. The parameter cas1 specifies the number of electrons in the cas space and cas2 specifies the number of virtual spin orbitals (the cas2 highest energy orbitals will be virtuals).

`ras-core ras1 ras2 ras3 ras4 ras5`
    Use a RAS space to form the core space. Suppoose the list of spatial orbitals are split into three sets, RAS1, RAS2 and RAS 3, ordered by their energy. ras1, ras2 and ras3 then specify the number of spatial orbitals in RAS1, RAS2 and RAS3. ras4 specifies the minimum number of electrons in RAS1 orbitals. ras5 specifies the maximum number of electrons in RAS3 orbitals. These together define the RAS space used to form the core space.

`optimised-core`
    Use the iterative approach of Petruzielo *et al.* (see PRL, 109, 230201). One also needs to use either optimised-core-cutoff-amp or optimised-core-cutoff-num with this option.

`optimised-core-cutoff-amp` $x1, x2, x3...$

    Perform the optimised core option, and in iteration i, choose which determinants to keep by choosing all determinants with an amplitude greater than xi in the ground state of the space (see PRL 109, 230201). The number of iterations is determined by the number of parameters provided.

`optimised-core-cutoff-num` $n1, n2, n3...$

    Perform the optimised core option, and in iteration i, choose which determinants to keep by choosing the ni most significant determinants in the ground state of the space (see PRL 109, 230201). The number of iterations is determined by the number of parameters provided.

`fci-core`

    Use all determinants to form the core space. A fully deterministic projection is therefore performed with this option.

`pops-core` n

    When starting from a POPSFILE, this option will use the n most populated determinants from the popsfile to form the core space.

`read-core`

    Use the determinants in the CORESPACE file to form the core space. A CORESPACE file can be created by using the write-core option in the Logging block.

The following semi-stochastic related options should be added to the Logging block.

`write-core`

    When performing a semi-stochastic calculation, adding this option to the Logging block will cause the core space determinants to be written to a file called CORESPACE. These can then be further read in and used in subsequent semi-stochastic options using the read-core option in the Calc block.

`write-most-pop-core-end` n

    At the end of a calculation, output the n most populated determinants to a file called CORESPACE. This can further be read in and used as the core space in subsequent calculations using the read-core option.

1.6 Trial wave functions

By default, NECI uses a single reference determinant, $|D_0\rangle$, in the projected energy estimator, or potentially a linear combination of two determinants if the the HPHF code is being used.

$$E_0 = \frac{\langle D_0|\hat{H}|\Psi\rangle}{\langle D_0|\Psi\rangle}. \tag{1.1}$$

This estimator can be improved by using a more accurate estimate of the true ground state, a trial wave function, $|\Psi^T\rangle$,

$$E_0 = \frac{\langle \Psi^T|\hat{H}|\Psi\rangle}{\langle \Psi^T|\Psi\rangle}. \tag{1.2}$$

Such a trial wave function can be used in NECI using by adding the `trial-wavefunction` option to the Calc block. You must also specify a trial space. The trial wave function used will be the ground state of the Hamiltonian projected into this trial space.

The trial spaces available are the same as the core spaces available for the semi-stochastic option. However, you must replace `core` with `trial`. For example, to use all single and double excitations of the reference determinant, one should use the 'doubles-trial' option.

1.7 Davidson RAS code

NECI has an option to find the ground state of a RAS space using a direct CI davidson approach, which does not require the Hamiltonian to be stored. This code is particularly efficient for FCI and CAS spaces, but is less efficient for CI spaces.

To perform a davidson calculation, put

```
davidson ras1 ras2 ras3 ras4 ras5
```

in the Methods block, inside the Calc block. The parameters ras1-ras5 define the RAS space that will be used. These are defined as follows. First, split all of the spatial orbitals into theree sets, RAS1, RAS2 and RAS3, so that RAS1 contains the lowest energy orbitals, and RAS3 the highest. Then, ras1, ras2 and ras3 define the the number of spatial orbitals in RAS1, RAS2 and RAS3. ras4 defines the minimum number of electrons in RAS1. ras4 defines the maximum number of electrons in RAS3. These 5 parameters define the ras space.

This method will allocate space for up to 25 Krylov vectors. It will iterate until the norm of the residual vector is less than 10^{-7}. If this is not achieved in 25 iterations, the calculation will simply stop and output whatever the current best estimate at the ground state is.

This code should be able to perform FCI or CAS calculations for spaces up to around 5×10^6 or so, but will probably struggle for spaces much larger than this.

The method has only been implemented with RHF calculations and with $M_s = 0$.

1.8 KP-FCIQMC

The Krylov-projected FCIQMC (KPFCIQMC) method is available on the master branch of NECI. The theory behind the method is described in the article, currently available on arXiv (arXiv:1409.2420). Here we simply describe the main input options available.

KP-FCIQMC is accessed via its own block in the input file. This block is started with 'kp-fciqmc' and ended with 'end-kp-fciqmc'. The methods block should be removed.

KP-FCIQMC is only implemented with the linear scaling algorithm. It should be run in double-run mode.

The main options are:

`num-krylov-vecs` N
> N specifies the total number of Krylov vectors to sample.

`num-iters-between-vecs` N
> N specifies the (constant) number of iterations between each Krylov vector sampled. The first Krylov vector is always the starting wave function.

`num-iters-between-vecs-vary` i_{12}, i_{23}, i_{34}...

   $i_{n,n+1}$ specifies the number of iterations between the nth and (n+1)th Krylov vectors. The number of parameters input should be the number of Krylov vectors asked for minus one. The first Krylov vector is always the starting wave function.

`num-repeats-per-init-config` N

   N specifies the number repeats to perform for each initial configuration, i.e. the number of repeats of the whole evolution, from the first sampled Krylov vector to the last. The projected Hamiltonian and overlap matrix estimates will be output for each repeat, and the averaged values of these matrices used to compute the final results.

`averagemcexcits-hamil` N

   When calculating the projected Hamiltonian estimate, an FCIQMC-like spawning is used, rather than calculating the elements exactly, which would be too computationally expensive. Here, N specifies the number of spawnings to perform from each walker from each Krylov vector when calculating this estimate. Thus, increasing N should improve the quality of the Hamiltonian estimate.

`finite-temperature`

   If this option is included then a finite-temperature calculation is performed. This involves starting from several different random configurations, whereby walkers are distributed on random determinants. The number of initial configurations should be specified with the num-init-configs option.

`num-init-configs` N

   N specifies the number of initial configurations to perform the sampling over. An entire FCIQMC calculation will be performed, and an entire subspace generated, for each of these configurations. This option should be used with the finite-temperature option, but is not necessary for spectral calculations where one always starts from the same initial vector.

`memory-factor` x

   This option is used to specify the size of the array allocated for storing the Krylov vectors. The number of slots allocated to store unique determinants in the array holding all Krylov vectors will be equal to ABx, where here A is the length of the main walker list, B is the number of Krylov vectors, and x is the value input with this option.

`num-walker-per-site-init` x

   For finite-temperature jobs, x specifies the number of walkers to place on a determinant when it is chosen to be occupied.

`exact-hamil`

   If this option is specified then the projected Hamiltonian will be calculated exactly for each set of Krylov vectors sampled, rather than randomly sampling the elements via an FCIQMC-like spawning dynamic.

`fully-stochastic-hamil`

   If this option is specified then the projected Hamiltonian will be estimated without using the semi-stochastic adaptation. This will decrease the quality of the estimate, but may be useful for debugging or analysis of the method.

`init-correct-walker-pop`

> For finite-temperature calculations on multiple cores, the initial population may not be quite as requested. This is because the quickest (and default) method involves generating determinants randomly and sending them to the correct processor at the end. It is possible in this process that walkers will die in annihilation. However, if this option is specified then each processor will throw away spawns to other processors, thus allowing the correct total number of walkers to be spawned.

`init-config-seeds seed1, seed2...`

> If this option is used then, for finite-temperature calculations, at the start of each calculation over an initial configuration, the random number generator will be re-initialised with the corresponding input seed. The number of seeds provided should be equal to the number of initial configurations.

`all-sym-sectors`

> If this option is specified then the FCIQMC calculation will be run in all symmetry sectors simultaneously. This is an option relevant for finite-temperature calculations.

`scale-population`

> If this option is specified then the initial population will be scaled to the populaton specified with the 'totalwalkers' option in the Calc block. This is relevant for spectral calculations when starting from a perturbed POPSFILE wave function, where the initial population is not easily controlled.

In spectral calculations, one also typically wants to consider a particular perturbation operator acting on the ground state wave functions. Therefore, you must first perform an FCIQMC calculation to evolve to the ground state and output a POPSFILE. You should then start the KP-FCIQMC calculation from that POPSFILE. To apply a perturbation operator to the POPSFILE wave function as it is read in, use the pops-creation and pops-annihilate options. These allow operators such as

$$\hat{V} = \hat{c}_i \hat{c}_j + \hat{c}_k \hat{c}_l \hat{c}_m \tag{1.3}$$

to be applied to the POPSFILE wave function. The general form is `pops-annihilate n_sum orb1 orb2... ...` where n_{sum} is the number of terms in the sum for $\hat{V}$ (2 in the above example), and *orbi* specify the spin orbital labels to apply. The number of lines of such orbitals provided should be equal to n_{sum}. The first line provides the orbital labels for the first term in the sum, the second line for the second term, etc...

1.9 RDM generation

Currently the 2-RDMs can only be calculated for closed shell systems. However, calculation and diagonalisation of only the 1-RDM is set up for either open shell or closed shell systems.

The original theory behind the calculation of the RDMs (including details of parallelisation) can be found in the paper: http://arxiv.org/abs/1410.6047. The most accurate RDM method (which is also unbiased) is the double-run approach, which requires the code to be compiled with the `-D__DOUBLERUN` flag in `CPPFLAGS` in the Makefile.

This propagates two completely independent populations of walkers, and calculates an unbiased RDM by taking cross-terms between the two populations.

The calculation of the diagonal elements is done by keeping track of the average walker populations of each occupied determinant, and how long it has been occupied. The diagonal element from Di is then calculated as ¡Ni¿(pop1) x ¡Ni¿(pop2) x [No. of iterations in this block], and this is included every time we start a new averaging block, which can occur when a determinant becomes unoccupied in either population, or when we require the calculation of the RDM energy during the simulation. As such, the exact RDM accumulated is dependent on the interval of RDM energy calculations, but in an unbiased way.

The off diagonal elements are sampled through spawning events, and use instantaneous walker populations. Subtle details in the code are:

1. RDMs take contributions to diagonal elements and HF connections whenever the RDM energy is calculated. As the averaging blocks are now reset at this point too, this change is unbiased. 2. The off-diagonal contributions (both HF connections and other contributions sampled through spawning events) contain contributions from both cross-terms. I.e $N_i(pop1) * N_j(pop2)$ as well as $N_i(pop2) * N_j(pop1)$.

There is also the facility to do a single-run calculation of the RDM. This method is BIASED, so should not be used for high accuracy calculations. However, it is cheaper than the double run method, both in memory and in simulation time, so may be useful for rough-and-ready calculations. Reducing the effect of the bias in the SR method can be done by applying a cutoff to the diagonal contributions, such that contributions are only added in if the average sign of the determinant at the time of adding in the contribution exceeds some preset parameter. (See THRESHOCCONLYRDMDIAG)

To perform a calculation, use

```
calcrdmonfly RDMLevel RDMIterStart RDMEnergyIter
```

It requires 3 integers. The first refers to the type of RDMs to calculate. A value of 1 will calculate only the 1-RDM. Any other value will calculate the 2-RDM (which contains the information of the 1-RDM). The second integer is the number of iterations after the shift has begun to change that we want to begin filling the RDMs. Finally, if the 2-RDMs are being calculated, the RDM energy will be automatically obtained at the end of the calculation. The 3rd integer refers to how often (every RDMEnergyIter iterations) we want to additionally calculate and print the energy during the calculation. This will be ignored if only calculating the 1-RDM. Clearly making RDMEnergyIter very large will mean the energy is only calculated with a softexit, or this can also be achieved by using `CalcRdmEnergy OFF`.

The RDM energy is one measure of the accuracy of the RDMs. Also printed by default are the maximum error in the hermiticity (2-RDM(i,j;a,b) - 2-RDM(a,b;i,j)) and the sum of the absolute errors.

1.9.1 Reading in / Writing out the RDMs for restarting calculations

Two types of 2-RDMs can be printed out. The final normalised hermitian 2-RDMs of the form `TwoRDM_a***`, or the binary files `TwoRDM_POPS_a***`, which are the unnormalised RDMs, before hermiticity has been enforced. The first are the `2-RDM(i,j;a,b)` matrices,

which are printed in spatial orbitals with $i < j$, $a < b$ and $i, j < a, b$. The second are the ones to read back in if a calculation is restarted (they are also printed in spatial orbitals with $i < j$ and $a < b$, but for both i, j, a, b and a, b, i, j because they are not yet hermitian). These are the matrices exactly as they are at that point in the calculation. By default the final normalised 2-RDMs will always be printed, and the `TwoRDM_POPS_a***` files are connected to the `popsfile/binarypops` keywords - i.e. if a wavefunction popsfile is being printed and the RDMs are being filled, a RDM `POPSFILE` will be also. If only the 1-RDM is being calculated, `OneRDM_POPS/OneRDM` files will be printed in the same way. The following options can override/modify these defaults.

`writerdmstoread off`
>   The presence of this keyword overrides the default. If the OFF word is present, the unnormalised `TwoRDM_POPS_a***` files will definitely not be printed, otherwise they definitely will be, regardless of the state of the `popsfile/binarypops` keywords.

`readrdms`
>   This keyword tells the calculation to read in the `TwoRDM_POPS_a***` files from a previous calculation. The restarted calc then continues to fill these RDMs from the very first iteration regardless of the value put with the `calcrdmonfly` keyword. The calculation will crash if one of the `TwoRDM_POPS_a***` files are missing. If the `readrdms` keyword is present, but the calc is doing a `StartSinglePart` run, the `TwoRDM_POPS_a***` files will be ignored.

`nonormrdms`
>   This will prevent the final, normalised `TwoRDM_a***` matrices from being printed. These files can be quite large, so if the calculation is definitely not going to be converged, this keyword may be useful.

`writerdmsevery iter`
>   This will write the normalised `TwoRDM_a***` matrices every `iter` iterations while the RDMs are being filled. At the moment, this must be a multiple of the frequency with which the energy is calculated. The files will be labelled with incrementing values - `TwoRDM_a***.1` is the first, and then next `TwoRDM_a***.2` etc.

1.10 Outputs of NECI

TODO

1.11 Performing error analysis

Data from an FCIQMC calculation is usually correlated. As a result, standard error analysis for uncorrelated data cannot be used. Instead we perform a so-called blocking analysis (JCP 91, 461). In this, data is grouped into blocks of increasing size until the data in subsequent blocks becomes uncorrelated, to a good approximation.

A blocking analysis can be performed in NECI in one of two ways. Firstly, a rough blocking analysis is performed automatically after a job is finished. The final result is output to standard output and further information about the blocking analysis at various block sizes is output to separate files, such as `Blocks_num` and `Blocks_denom`. This should only be

used as a rough and quick estimate as there are issues with this approach. For example, the analysis starts as soon as the shift is turned on. This is before the population has stabilised, and so unusual results can occur in the analysis of the denominator and numerator. Also, data is not taken from the optimal block size.

A better approach for a more careful analysis is to use the blocking script in the utils directory, called blocking.py. The key command is

```
./blocking.py -f start_iter -d24 -d23 -o/ FCIMCStats
```

This will perform a blocking analysis starting from iteration `start_iter`. The analysis should be started only once the energy estimate, (column 11 in `FCIMCStats`) and the numerator and denominator (columns 24 and 25) have stabilised and are fluctuating about some final value. Just because the energy looks stable, it does not mean that the populations is not still growing!

`-d24 -d23`' tells the script to perform the blocking on columns 25 and 24 of the `FCIMCStats` file, which correspond to the numerator and denominator of the energy estimator, respectively. `-o/` tells the script to also provide data for the results of dividing columns 25 and 24, which gives the energy estimate that we want.

Running this will produce a graph of the errors for both the numerator and denominator as a function of the number of blocks (and therefore of the block size). As the block size increases, the error estimates should increase, tending towards the true values. Eventually the estimates will plateau. This indicates that, at this block length, the data in the blocks are uncorrelated to a good approximation, and the error estimate calculated is accurate. The data from this block length should therefore be used.

Each estimate of the error will also have an error on it. As the block length increases this 'error on the error' will increase. One should therefore use the *first* block length where the plateau is reached, so as to minimise the error on the final error estimate.

If no plateau is seen in the plot then the simulation has not been run for long enough, and needs to be continued by restarting from the POPSFILE. It can take on the order of $10^5 - 10^6$ iterations to perform an accurate blocking analysis.

The `blocking.py` script will also output the final estimates on the energy at the different block lengths. You should find the blocking length where the errors plateau and read of the final estimates (the rightmost columns) from here.

More information (including example plots, similar to those that `blocking.py` produces) is available at JCP 91, 461.

1.12 Anatomy of an FCIQMC calculation

1.13 Useful tools

- Tools for post-processing (e.g. blocking)
- Tools for pre-processing (e.g. for Lz pure FCIDUMPS)
- Model calculations?
- Tools for processing POPSFILES?

2 Working in NECI

In many ways, NECI is a fairly hostile environment to code, especially for inexperienced software developers, or those who are not familiar with the ideosynchrasies of different versions of FORTRAN/Fortran.

In the following sections we aim to give some general guidance for working in the NECI codebase, and

GHB, NSB: For many of these sections it is arguable whether they belong in an overall about-the code description, or a walkthrough of the code itself. Feedback would be good!

As a general guideline, programs should be written to fail as loudly and as early as possible. This pushes the job of finding errors and debugging up the tree.

1. Just "looks wrong" to the programmer.
2. Syntax highlighting in the editor makes a mistake stand out.
3. Error detected by compiler.
4. Error detected by linker.
5. Runtime error detected by debug sanity checks through code.
6. Runtime error caused in code at a different location to the bug.
7. Runtime error only occurs when running in parallel, or in bigger calculations.
8. Simulation appears to run correctly, but gives obviously wrong output.
9. Simulation appears to run correctly, but gives subtly wrong output.

We strongly aim to be at the top of the list.

2.1 Code conventions

The code in NECI has been developed over a number of years by many different developers, and has very little standardisation of approach or code appearance. This is not an example to copy!

We are trying to (gradually) normalise sections of code, and isolate those sections which are old and generally unredemable from the rest of the code base. As such there are a number of restrictions we place on code in NECI, and a range of other guidelines.

Fortran standard

Due to the use of procedure pointers, a reasonably up to date compiler supporting (at least some of) the Fortran 2003 standard is *required* to compile NECI. The C-interoperability and procedure pointer features of Fortran 2003 should be used. Other features of this standard should be used sparingly, as Fortran 2003 support in compilers is patchy at best.

Otherwise, code should be written to the Fortran 90/95 standard. In particular, several features of FORTRAN 77 should be avoided at all costs:

- `DO` statements using `REAL` type loop variables.
- Assigned `GOTO` statements
- Cray pointers (declared with the format `pointer` (`ptr, pointee`))
- Implicit variables. `implicit none` MUST appear in every module, or interface statement.
- Implicitly typed routines and subroutines. See section on modules and interfaces.
- `COMMON` blocks for sharing data between files.

All of these features do, or have appeared, in NECI at some point. It is also highly advised that `intent` arguments should be used for all argument declarations. This both improves performance, and the ability of others to quickly identify what the routine is attempting to do.

CAPITAL letters

Fortran is a case insensitive programming language.

For historical reasons a large proportion of FORTRAN 77 code was written entirely in CAPITAL LETTERS (with the exception of displayable strings). This is extremely bad practice.

Humans generally read by recognising word shape. This is obliterated in fully capitalised text, making code much harder to read, and typos especially difficult to identify.

Indentation

Indentation of sections of code should use spaces (and not tabs). The Fortran 95 standard explicitly rejects the use of tabs, and tabs in source code will elicit warnings from the compiler.

All indentations should be multiples of 4 characters.

Source code in *.F files (old-style FORTRAN 77) has specific layout restrictions. In particular an initial indent of 7 spaces. This style should not be mimicked elsewhere.

Code line length

The Fortran 90/95 standard restricts line lengths to a (hard) maximum of 132 characters. Code with lines longer than this *may* work on *some* compilers, but this limit should be avoided.

This limit applies after preprocessing has been applied. A number of our macros in `macros.h` can create lines of considerably longer length if not used carefully. These may require using temporary variables with shorter names to control the line length.

The fixed-format FORTRAN 77 code is restricted to 72 characters per line.

On a 19″monitor at standard resolution, two columns of code vertically split and side by side use 79 characters each. This is a convenient soft-limit to use - although it is not trivially achievable in all code, and overall readability should be prioritised.

Variable name conventions

There are a number of competing conventions for variable and function names within NECI. Insisting on following any specific one would be highly hypocritical for anyone in the Alavi group. That said, there are a number of existing conventions that it is *useful* to be aware of.

- `CamelCase` or `snake_case` should be used to provide descriptive variable names. The wider the scope of a variable, the longer and more descriptive the name should be. Trivial local variables (loop indices, etc.) can and should be trivially named. Variables should not, ever, be used entirely in capital letters.
- `tVariableName` is a logical control variable. Normally globally declared in a module for switching on (or off) an overall feature, or signalling overall calculation state.
- `nVariableName` is an integer containing a count of a number of a given entity.
- `Varible`, `AllVariable` are paired sets of variables tracking an extensive property of a simulation. That is properties which can be accumulated on an individual node, but that the system-relevant property needs to be collected from all nodes and amalgamated. This is done once per iteration or once per update cycle as appropriate.

Fortran 95 restricts variable names to 31 characters. Although Fortran 2003 extends this to 63, making use of this extension can cause problems with some compilers, and this should be avoided.

Subroutine decoration (especially intent statements)

Subroutine and function declarations should be decorated to the greatest extent feasible. This should restrict the variables to only their expected role in a function.

In particular, all function arguments should be decorated with either `intent(in)`, `intent(out)`, or `intent(inout)` as appropriate. The additional decorations `optional` and `target` can be used with care.

The supplied arguments should be as restrictive as possible, to maximise the likelihood of the compiler catching programming errors.

The single exception to this rule is for routines that are to be stored in procedure pointers. These routines must exactly match the definition of the relevant `abstract interface`, which may be more general than is required for the specific case.

Data types

With the exception of small integers being directly assigned to known integer variables, or used in loop counters, all constants should have their types explicitly specified. The available types are described in section 3.1.

Most specifically, the `*D*` specifier and the floating point type `double precision` should never be used. Examples such as `1.D0` should be replaced with `1.0_dp`, and the data types `real(dp)` and `complex(dp)` should be used.

As compilers have moved between 16-bit, 32-bit and 64-bit, there is ambiguity about whether `double precision` should mean a 32-bit, 64-bit or 128-bit floating point value, depending on the age of the compiler and which compiler is used. This can cause chaos and difficult to track runtime bugs that appear only on certain machines.

For Hamiltonian matrix elements (that may be real or complex depending on build configuration) the custom (preprocessor defined) data type `HElement_t` should be used, which resolves to either `real(dp)` or `complex(dp)`.

Array declarations

Fortran arrays can be declared in multiple ways. In particular, the dimensionality of an array can be declared on the variable itself, or as part of the type declaration;

```
integer, dimension(10, 20) :: arr1
integer :: arr2(10, 20)
```

In general the latter declaration is preferred for two reasons:

1. It is clear that the array property is attached to the variable, and not to the type. When scanning data declarations it is not possible to mistake a scalar for an array.

2. Multiple different arrays can be declared in the same data declaration with different bounds.

The only exception to this is in templated code, where the bounds of arrays need to be varied.

Where arrays are passed as arguments to a routine, they can be passed in three ways

```
integer, intent(inout) :: arr(*)
integer, intent(inout) :: arr(10)
integre, intent(inout) :: arr(:)
```

The first form should be avoided wherever practical, as it prevents any knowledge of the array dimensions being carried into the code. This means that whole-array manipulations will no longer work.

The second two types can be used in different circumstances. The first essentially overrides the array dimensions passed in. This can be useful for re-indexing arrays (e.g. treating a zero-based array as one-based).

The last approach allows a receiving routine to inspect the array bounds as passed in by the calling routine. This maximises the extent to which the compiler and debugging tools can assist in finding errors in the code, and should be used wherever possible.

Use statements

Globally declared symbols can be shared between modules using `use` statements. Generally, specific symbols should be included rather than all symbols in a module using the notation `use module_name, only: symbol, ...`.

Modules which are templated (see section 2.6) should be included in full (no `only` statements). This includes `sort_mod`, `util_mod` and `Parallel_neci`.

Modules containing only data that have been separated for the purposes of dependency resolution can be fully included into their related modules (e.g. `CalcData` and `Calc`).

The module `constants` should also be fully included everywhere to reduce the likelihood of data types conflicting.

Use statements should (where possible) be located in the module header, and not in individual subroutines - this avoids some serious issues associated with compilers resolving conflicting dependencies. If the same thing is included in multiple places in a file, the compilers dependency resolution tree can become very large, and use a lot of time and memory to resolve unambiguously.

`ASSERT` **statements**

`ASSERT` is a macro, defined in `macros.h`. In an optimised build these statements are entirely removed, and in a debug build they will cause execution to be aborted with an error message if the condition specified is not met.

In NECI, the error message contains the current file and line number. It also includes the current function, which must be manually supplied in a constant named `this_routine`.

An example assert statement, in a function that takes an array with the same number of elements as there are basis functions, would be:

```fortran
subroutine foo(arr)
    integer, intent(inout) :: arr(:)
    character(*), parameter :: this_routine = 'foo'
    ASSERT(len(arr) == nBasis)
    ...
end subroutine
```

> ☞ Be careful not to use tests with side effects in `ASSERT` statements. In the optimised build the tests will not be called, and this can introduce bugs that appear in only one of the optimised or debug builds.

Modules and interfaces

-

Example module layout

A sample module layout is given below:

```fortran
#include "macros.h" ! This enables use of our precompiler macros.
module module_name

    ! To the extent possible, include statements should be at the
    ! beginning of a module, and not elsewhere.
    use SystemData, only: nel, tHPHF
    use module_data
    use constants
    implicit none

    ! Add an interface to an external (non-modularised) function
    interface external_fn
        function splat_it(in_val) result(ret_val) &
                                    bind(c, name='symbol_name')
            ! n.b. interface statements shield from modular includes
            use constants
            implicit none
            integer, intent(in) :: in_val
            real(dp) :: ret_val
        end function
    end interface

contains
```

```
[pure|elemental] subroutine sub_name(in_val, out_val)

    ! This is a description of what the subroutine does

    integer, intent(in) :: in_val
    real(dp), intent(out) :: out_val

end subroutine [sub_name]


[pure|elemental] function fn_name(in_val) result(ret_val)

    ! This is a description of what the function does does

    integer, intent(in) :: in_val
    real(dp) :: ret_val

end function [fn_name]

end module
```

2.2 Important modules and common (global) variable names

2.2.1 `CalcData`

2.2.2 `SystemData`

2.2.3 Inexplicable names and anachronisms

A number of the variable names in NECI are largely inexplicable, or confusing, outside of their origin in historical accident. This section tries to clarify some of these.

ARR, BRR

`ARR(:,1)` contains a list of spin orbital (Fock) energies in order of increasing energy.

`ARR(:,2)` contains a list of spin orbital (Fock) energies indexed by the spin-orbital indices used in the calculation.

`BRR` contains a list of spin orbital indices in increasing (Fock) energy order. Where multiple degenerate orbitals have the same symmetry, they are clustered so that spin orbitals with the same symmetry are adjacent to each other, and within that ordered by m_s value.

TotWalkers and TotParts

`TotWalkers` refers to the number of determinants or sites that must be looped over in the main list. This may include a number of blank slots if the hashed storage is being used.

The number of particles (walkers) on a core is stored in `TotParts`. The total number of particles in the system (including all nodes) is stored in `AllTotParts`.

InitWalkers

The number of particles *per processor* before a simulation will enter variable shift mode.

G1

The variable name `G1` is a historical anachronism. It is an array containing symmetry information about given basis functions. In particular `G1(orb)` contains information about the one electron orbital `orb`.

The data is of type `BasisFN`:

```fortran
type symmetry
    sequence
    integer(int64) :: S
end type
type BasisFn
    type(symmetry) :: sym ! Spatial symmetry
    integer :: k(3)       ! K-vector
    integer :: Ms         ! Spin of electron. Represented as +/- 1
    integer :: Ml         ! Angular momentum quantum number (Lz)
    integer :: dummy      ! Padding for alignment
end type
```

Not all of these values are required for all simulations. The `sym` element points at a padded 64-bit integer. This is done for memory alignment reasons that are no longer important.

2.3 Don't Repeat Yourself (DRY)

When information becomes duplication in software, eventually the people that knew about the duplication will forget. And then the information will be changed — but at least one of the duplicates won't be. This introduces bugs that are extremely difficult to track down.

The Don't Repeat Yourself (DRY) principle is one that say a developer should systematically, and always, avoid duplication of information.

NECI is a terrible example of this, but it has been improved over time with a lot of effort.

Information is a very broad term. There are many types of duplication that can occur. A non exhaustive list of some types of duplication (and what can be done about them) follows.

Algorithm duplication across data types

There are many algorithms that are either the same, or similar, across many different data types. The logic involved in these should be written once.

Major examples are the sorting routines in `sort_mod`, general utilities in `util_mod`, shared memory in `shared_alloc` and MPI routines in `Parallel_neci`. Prior to implementing a generalised quicksort there were 37 different sort routines in NECI, using different sort methods, and containing different bugs.

This duplication should be controlled using templating, as described in section 2.6.

Logic duplication across source files

If the same chain of decision making is recurring in different regions of the code, these should be abstracted into their own subroutine which is called from each location. This prevents the logic being duplicated, and then diverging.

Numerous bad examples of this still persist in NECI.

Duplication of data

Compile time constants should only be specified in one place. A large proportion of these are found in the `lib/cons_neci.F90` source file. Other examples include the layout of the bit representations (`BitReps.F90`). A significant proportion of these vary depending on the compile configuration, and prior to collecting them here the code was extremely fragile.

Ongoing cases which are problematic include the use of the literal constant 6 to specify output to stdout in statements such as `write`(6,*), which doesn't interact well with `molpro`.

Duplication of representations in memory

It is important to have a well defined canonical representation of data in memory. The same data should not be allowed to become duplicated in multiple places.

Temporary arrays, with working data copied into them, should be clearly temporary and discarded as soon as not necessary. If the primary data shifts to a new location, the old storage should be deallocated (if possible), or damaged so that attempts to use it fail loudly (such as putting a value of -1 into a variable that would normally hold an index).

Avoid situations where code might work by accident.

An ongoing situation of this type is the array variable `nBasisMax`. It shadowed a large number of global control variables, and there are still locations in the code where its value is used in preference to the global control value as these values diverge, and its value is the one that works in some obsolete code.

There is one, major, exception to this rule. Code that only exists for testing purposes (such as the contents of `ASSERT` statements, or unit tests if they are ever added) may be as explicitly duplicated as desired. Their *purpose* is to explicitly flag up when anything elsewhere changes - so the risk of them getting out of sync with the code base is their purpose.

2.3.1 Procedure pointers (function pointers)

One issue that becomes immediately obvious when repeated logic has been abstracted into specific functions is that conditional logic is executed *every* time certain actions are taken.

In many cases this is not very important, as it occurs high up the call hierarchy, and the controlled code consumes the vast majority of the execution time. However, the closer we get to the inner most tight loops, the more expensive repeated conditional logic becomes. This is particularly frustrating if the decision making is based on global control parameters, and thus always results in the same code path being taken in a simulation. If the decision lies against the branch prediction metrics, then this is especially bad.

The canonical example of this is accessing the 4-index integrals, which is performed very frequently.

In these case, it is a good idea to separate the decision making logic from the execution, so that the conditional logic is only executed at runtime. This can be done using *procedure pointers* (called function pointers, or similarly functors in other programming languages.

These require defining the "shape" of a function call (i.e. its arguments, and return values) in an `abstract interface`. A variable can then be set to point at which of a range of functions with this signature should be executed.

In NECI the global controlling procedure pointers are located in the module `procedure_pointer`, which contains both the abstract interface definitions, and the actual pointer variables. These variables can then be used as functions throughout the code.

These procedure pointers are largely initialised in the routine `init_fcimc_fn_pointers`, where decisions are made between types of excitation generator, matrix element evaluation, etc. The procedure pointers involved in integral evaluation are set in `init_getumatel_fn_pointers`.

The use of procedure pointers generates a strict Fortran 2003 dependency for NECI. We used to make use of a hacky abuse of the linker and templating system to implement function pointers without language support, but this was deprecated once compiler support for procedure pointers was reasonably widespread.

2.4 Don't optimise prematurely

Obviously, good algorithm design is important. If an algorithm scales badly, then no implementation will be able to salvage it.

However, there are many tricks and optimisation that can be made to eek out small and large performance gains in the implementation of a particular algorithm. It is important not to optimise too early for a number of reasons.

- Good optimisation is extremely time intensive. On the whole time is better spent getting the code to work, and making the algorithm efficient. Once an implementation works, then code can be profiled and performance improved.

- Optimisations are often highly non-obvious, involving storing information in unexpected ways and places, leading to code that is hard to write, harder to read and extremely bug prone.

- The compiler is very good. The obvious 'tricks' that you see will be done by the compiler anyway.

- One place where performance gains can legitimately be made is in avoiding conditional switching. In many cases this would involve duplicating code paths, and horrifically breaking the DRY principle above. There are occasions that this is worthwhile, but this should be actively justified by profiling data rather than just a hunch.

2.5 Tracking memory usage

NECI contains automated tracking of memory usage. This enables output statistics to indicate which memory uses are dominating during a calculation.

The `MemoryManager` module keeps track of all units of memory, and assigns a tag value to each of them. It is the responsibility of the developer to store this tag, and pass it when the memory is deallocated. This tag is an `integer`.

Memory should always be allocated using error checking. That is, an allocate statement should always be passed an error value as follows

```
integer, allocatable :: arr1(:)
real(dp), allocatable :: arr2(:,:)
integer :: ierr
allocate(arr1(10), arr2(20, 30), stat=ierr)
```

This value will be zero if the allocation was successful, and non-zero otherwise. The memory logging routines check this value, and report an error if the memory allocation failed.

Memory is logged using the functions `LogMemAlloc` and `LogMemDealloc`.

2.6 Code templating

NECI has an additional build step in comparison with most Fortran code. Prior to running the C preprocessor, the custom script `tools/f90_template.py` converts all of the files with filenames `*.F90.template` into files with the corresponding names `*.F90`.

This mechanism exists to allow general code to be written, and reused for different types, and combinations of types. While this is largely a combinatorial pattern-matching and substitution problem, the templater contains specific additional features to facilitate dealing with array types in Fortran. There are also a number of specific considerations that need to be made.

The templated code in NECI has been written largely by Simon Smart and Alex Thom, who should be able to help with any particularly nasty issues arising.

2.6.1 How it works

Fortran permits multiple routines to be referenced by the same name through the use of interface blocks such as

```
interface sub_name
    module procedure actual_name_1
    module procedure actual_name_2
end interface
```

which allows either of the routines `actual_name_1` or `actual_name_2` to be called using the Fortran symbol `sub_name`. Note that these procedure constructs can be used directly in the code for a hard-coded set of routines which can be called from one interface name if desired (see section 2.6.7).

It is perfectly acceptable to have multiple interface blocks for a specific routine name, so long as all of the referenced routines have different calling signatures. That is, they must accept differently typed arguments so that it is possible for the compiler to determine *at compile time* which of the routines should be called. In principle the actual routine names can always be used.

The Fortran templater creates one module per specified configuration, each with a unique module name. It then performs substitutions on a specified template model to create routines for all of the specified combinations of input types. These routines have their names adjusted to make them unique for each configuration, and an interface block is created to make them accessible under their original name. Finally all of these newly

created modules are collected, with `use` statements, into a macroscopic module which can be used from elsewhere.

2.6.2 Overall structure

A sample templated module structure is given here for reference. The different sections are explained below.

```
# This is the configuration block. Note that it has *.ini syntax,
# and that comments are preceeded by hashes.
[int]
type1=integer(int32)

[float]
type1=real(dp)

====================
#include "macros.h"

module module_name

    ! This is the module which is templated to generate the ensemble
    ! of routines with differing types
    use constants
    implicit none

contains

    elemental function test_fn(arg) result(ret)

        %(type1)s, intent(in) :: arg
        %(type2)s :: ret

    end function

end module


supermodule module_name
    !
    ! Here we include code that should be included in the module but
    ! does not need to be templated.
    !
end supermodule
```

2.6.3 Configuration names and substitution

The top section of the file defines the templated configurations. It has the structure of an INI file, and is processed by the standard python ini file parser.

Configurations are defined by a name, contained in square brackets, and then by a series of key-value pairs. All values are treated as strings for the purpose of substitution in the main body of the routine.

Configurations are *inherited*. That is to say that all key-value pairs (with the exception of `conditional_enable`) are carried forward to the next configuration in the file unless they are overridden. This permits quite sparse configuration files, at the expense of being a bit more tricky to modify.

The length of configuration names must be considered. They will be appended to module names and the subroutine and function names contained therein. The templater does not have a magic means to circumvent the Fortran 95 limit of 31 characters in any symbol. Therefore it makes sense to use highly abbreviated configuration names.

The templater modifies the names of subroutines and functions as it processes the module. As such, it is a little pick about syntax. Normal routine decoration specifiers such as `pure` and `elemental` are supported, but functions *must* be declared using the `result()` specifier to define the return type.

If the special key `conditional_enable` is present, this is used to wrap the generated module in `#if` `#endif` elements. See `lib/quicksort.F90.template` for examples.

Values from the key-value pairs are directly substituted into the templated module below, where they replace the element `%(key)s`. (This specifier is the standard python named-string specifier). Keys named beginning with `type` are treated specially, as described in the following section.

The templater cannot circumvent Fortran line length limits. If necessary a value to substitute can be extended over multiple lines by ensuring the first character on a new line is a space, and then just continuing. Make sure you remember the Fortran line continuation characters, as in this example from the MPI wrapper code:

```
mpilen=((ubound(v,1)-lbound(v,1)+1)*(ubound(v,2)-lbound(v,2)+1)*&
 (ubound(v,3)-lbound(v,3)+1))
```

There is a special variable, which can be accessed using `%(name)s`. This contains the name of the current configuration.

2.6.4 Variable substitution

The templater has extremely powerful mechanisms to manipulate the types of variables. Variable manipulation is enabled by using a key in the key-value pair section that begins with `type`. In particular, the code is able to manipulate the number of dimensions that different arrays have.

As an example, take a routine which is passed an array, and a value that could be an element of that array (such as is necessary for a binary search), such that

```
    subroutine example(arr, elem)
        %(type1)s :: arr(:)
        %(type1)s :: elem()
        ...
    end subroutine
```

If `type1` is a scalar value, this does a substitution exactly as would be expected:

```
    [int]                        subroutine example_int(arr, elem)
                                     integer(int32) :: arr(:)
    type1=integer(int32)   ⟹      integer(int32) :: elem
                                     ...
                                 end subroutine
```

However, it may be necessary for the value which is being considered in the array to itself be an array. An example of this would be the bit representations used in NECI — a list of of these is a two dimensional array, and any intermediate values would be arrays themselves.

In this case, an array type should be specified using the `dimension` keyword, and the code will be automatically adjusted as follows:

```
[arr_int64]
type1=integer(int64), dimension(:)
```
$\implies$
```
subroutine example_int(arr, elem)
    integer(int64) :: arr(:,:)
    integer(int64) :: elem()
    ...
end subroutine
```

Essentially the number of : delimiters appearing in the variable definition is combined with the number of dimensions specified in the type.

As a special case, temporary variables can be created of an appropriate size which are either scalars, or have one dimension. For the definition

```
%(type1)s :: arr(:)
%(type1)s :: tmp(size(arr(1)))
```

then adjustment occurs as follows

```
[int]
type1=integer(int32)
```
$\implies$
```
integer(int32) :: arr(:)
integer(int32) :: tmp
```

```
[arr_int64]
type1=integer(int64), dimension(:)
```
$\implies$
```
integer(int64) :: arr(:,:)
integer(int64) :: tmp(size(arr(1)))
```

In a similar way, the references made to these variables within the routines must be adjusted. This is to ensure that correct sized array slices are used at all times. For the original templated code

```
arr1(j) = arr2(i)
```

the following will result in the the templated output if the variable is of an adjustable type and declared at the top of the function:

```
[int]
type1=integer(int32)
```
$\implies$
```
arr1(j) = arr2(i)
```

```
[arr_int64]
type1=integer(int64), dimension(:)
```
$\implies$
```
arr1(:,j) = arr2(:,i)
```

2.6.5 The supermodule

In many modules, there are routines that do not need to be templated for different variable types. As an example, within the MPI wrapper routines, the code to initialise MPI is not variable type specific.

Code which is placed in the supermodule is not templated, and is included directly in the final generated module.

2.6.6 Optional parameters and lines of code

It is good practice to write templated routines as generally as possible. This likely involves adding more functionality than is needed in all cases, and switching this functionality on and off in some way.

For example, the sorting routine can sort multiple arrays in parallel, according to the order in the first array (such as sorting a list of determinants into energy order, where

the energies are stored in a separate array). It also needs to have comparison functions defined for scalars as well as arrays.

The extent to which interesting features can be developed is limited only by the developers imagination in using the template substition. But two tricks are generally useful.

Additional optional arguments

Subroutines can easily be given flexible numbers of arguments. This is useful for adding additional functionality (and allows multiple templated routines to use the same `type` values). The templated subroutine definition

```
subroutine example(arg%(extra_args)s)
```

will generate the following code

```
[simple]
extra_args=
```
$\implies$ `subroutine example(arg)`

```
[extended]
extra_args=, arg2, arg3
```
$\implies$ `subroutine example(arg, arg2, arg3)`

The next trick is useful for adding the type definitions of these additional arguments, and enabling the code which uses them.

Switching off lines of code

Lines of code in Fortran are trivially disabled when they are commented out. Prefixing lines with a switch-value allows it to be disabled. For example

```
%(use_type2)%(type2) :: val()
```

will allow an additional type to be used in a routine depending on the configuration:

```
[unused]
type2=
use_type2=!
```
$\implies$ `! :: val()`

```
[arr_real]
type2=real(dp), dimension(:)
use_type2=
```
$\implies$ `real(dp) :: val(:)`

2.6.7 Manual renaming of routines

The user can additionally manually create interface blocks for the templated routines. This is useful where there is more than one possible function to call for each of the variable types.

An example of this is given in the MPI wrapper functions, where there are versions of routines that require manually specifying the lengths of various parameters, and automatic versions which take the lengths from the sizes of the arrays passed in. At the top of the templated module definiton lie interfaces blocks such as

```
interface MPIReduce
    module procedure MPIReduce_len_%(name)s
    module procedure MPIReduce_auto_%(name)s
end interface
```

which makes use of the special `%(name)s` element to reference the generated routines after templating.

In this case, the templated routines `MPIReduce_len` and `MPIReduce_auto` will be available to the user as usual, but the routines can both be called by the more generic name of `MPIReduce` with the appropriate arguments supplied.

2.6.8 Examples

All of the features of the templating code have been heavily used the Shared Memory code, in `lib/allocate_shared.F90.template`, the sorting code in `lib/quicksort.F90.template` and the MPI wrapper code in `lib/Parallel.F90.template`. Other less aggressively used case can be found elsewhere.

2.7 Testing

2.8 Interfacing C (and C++) code

Developers have always mixed Fortran code with external routines implemented in other languages, especially C. This has generally been done on an ad-hoc basis by exploiting the naivety of the linker — in particular that the linker will resolve dependencies with any symbol of the specified name. This is useful, but introduces a number of potential problems:

Name clashes
Different compilers follow different naming conventions. In particular Fortran compilers often (but not always) append or prepend one or two underscores to symbols in the object files. This is fine when resolving against other Fortran generated symbols, but requires coordination with the symbol names produced in C.

A solution with an array of compile flags controlling the naming in the Fortran compiler, and underscores liberally scattered through C files is fragile and unreliable. It also makes it difficult to call library routines written in C.

No checking of parameters
The linker is extremely stupid - it only matches by parameter name. If this method is used, absolutely no checking is done on the parameters passed to the C routine from Fortran. This is a recipe for disaster, and will generate only runtime errors.

Calling
By default C passes arguments by value, whereas Fortran passes them by pointer. This requires writing wrappers for almost any non-trivial C library routine to access it from Fortran. Some constructs simply cannot be emulated.

Variable types
As an extension of the lack of checking of parameters, there is no checking of argument types across the Fortran/C interface. This relies on the Fortran and C code using the same types - in particular the same size of floating point and integer variables. This is extremely hard to guarantee, and these can fluctuate according to compiler flags. This can result in compiler and computer specific runtime errors that are extremely difficult to track.

All of these problems can be solved using structured interfacing, at the cost of introducing a dependency on the Fortran 2003 standard.

All access to C routines in NECI must be through a declared interface. This should be declared only once, in a module. An example is given here:

```
interface
    ! Note that we can define the name used in fortran code, and the C
    ! symbol that is linked to independently.
    subroutine fortran_symbol(arg1, arg2) bind(c, name="c_symbol")
        ! The module iso_c_hack is a wrapper for iso_c_binding. This
        ! contains some workaround for incomplete Fortran 2003 support
        ! across compilers.
        use iso_c_hack
        integer(c_int), intent(inout) :: arg1      ! Passed by pointer
        integer(c_bool), intent(in), value :: arg2 ! Passed by value
    end subroutine
end interface
```

A good summary of the rules and procedures for using this interoperability are given in this Stack Overflow answer: http://stackoverflow.com/tags/fortran-iso-c-binding/info

C++ routines can be made suitable for access from Fortran by prepending symbol declarations in the C++ code with `extern "C"`.

2.9 Debugging tips

Code breaks. Sometimes it appears to rot with time. Finding bugs takes the majority of most programmers time, and practices which make this quicker are invaluable!

Obviously, the techniques you will use will depend on the nature of the problem (tracking down small numerical changes in output is generally much harder than finding what causes a segfault), but there are number of tricks which can help!

2.9.1 Build configurations

As soon as you have a problem, build a debug rather than an optimised version of the code. This cause a large array of changes to the compiled code:

Array bounds checking
All Fortran arrays have well defined bounds on all of their dimensions. In debug mode the compiler will insert code to check that all memory accesses are within these bounds. If not, execution will be terminated with a message indicating at what line of what file the error occurred. If running in a debugger (see later) execution will be interrupted at this point.

Disable optimisations
Hopefully this will not make the bug go away! If it does, you are almost certainly looking at either an uninitialised variable, or access beyond the end of an array.

The primary purpose of disabling optimisations is to make the mapping between the source code and the executable more linear. This results in any error messages, and the output of any tools, being easier to interpret.

Adds debugging symbols

When your code crashes it is really useful to know what routine was running, and what the stack trace (list of routines that have been called to get to this point in the code) is. Adding debugging symbols provides the information to convert the memory addresses into files and lines of source code. This makes error messages useful.

Enables the ASSERT macro

There are many consistency checks internally in NECI that can be turned on in debug mode. Particularly for difficult-to-find bugs, these are likely to fail substantially earlier in a run than it is possible to view the problems in the normal output.

Defines __DEBUG

Any blocks contained inside `#ifdef __DEBUG` sections are only enabled in debug mode. Most of these contain either additional output specifically targetted to make debugging easier, or additional consistency checks.

2.9.2 ASSERT statements are your friend

Generally the time to add ASSERT statements to your code is when you are writing it. Debugging will make you acutely aware of their benefit. If you have a suspicion in which bits of code a bug might lie, liberally sprinkling it with ASSERT statements can help to find bugs.

More usefully, when you find the bug, add ASSERT statements to the code to catch similar errors in the future.

2.9.3 Learn to use your tools

Most of the programming tools in existence are for the purposes of debugging. Learn to use them! Practice using them. The really work.

Debuggers

The debugger is the most powerful tool you have. Essentially you run your code in a harness, with the debugger hooked into everything important. On most Linux systems, the most readily available debugger is `gdb`.

The debugger can trap any execution errors, and will interrupt (break) execution of your program at this point — while preserving all of the memory and execution state. You can examine the call stack (the nested list of functions that have been called), and the status of all of the memory. You can also change the contents of any relevant memory and continue execution to see the effects.

Break points can be added to the code at any line of any function, and execution interrupted at that point. If your bug is only showing late in execution, you can interrupt on the n-th time a function is called. You can step through the execution line by line in the source code, examining all variables, and watch precisely what goes wrong.

The debugger is the swiss-army sledgehammer of tools.

Valgrind

Valgrind is a tool for memory debugging. In essence it replaces most of the memory manipulation primitives provided by the operating system with instrumented versions. It will track what happens to memory, where it is created, where it is destroyed, and what code (in)correctly accesses it.

Intel Inspector XE

If you have access to Intel tools, the Intel Inspector is an extremely powerful debugger, memory analysis tool, performance enhancement and problem tracking tool. An top of a good interface to normal debugging tools, it can apply a lot of analysis to your code's execution, and then filter through it to find where things go wrong.

2.9.4 Machete Debugging

When bugs are particularly non-obvious, a good first step is to reduce the complexity of the problem. Try and remove as much code as possible. A good rule of thumb is to remove half of the code, and retest. If the bug has gone away, then it required interacting with the other half of the code.

This technique can very quickly isolate a test case (that still fails) into something of manageable size. In doing so, the bug normally becomes obvious. You can then revert to the original code, and fix the problem there.

In a complex code, this process can be tricky. Lots of the sections of code are coupled to each other. This can require some creative thinking. Choose the domain of your problem carefully (it may only be necessary to apply the machete to one file), and aggressively decouple sections by commenting out function calls.

Remember — it doesn't matter if you break functionality doing this (you obviously will) so long as you retain the buggy behaviour in the code that is left.

This is really good for finding strange memory interactions — left with the two routines that are trampling on each others toes.

2.9.5 `fcimcdebug 5`

For bugs that change the trajectory of simulations, turning on the maximum debug output level in NECI (by adding `fcimcdebug 5` to the logging section of the input file in a debug build) can often give a quick insight into where the problem is located.

Many problems will exhibit with obviously pathological behaviour. For example trying to spawn `NaN` particles, or an extremely large number, generally indicates a problem in either Hamiltonian matrix element generation or calculating the generation probabilities. Similarly walkers being spawned with repeated or zeroed orbitals are a give away.

Similarly, if the bug is recently introduced and a prior version functioned correctly (such as a test code failure)

2.9.6 Look at the git logs

If you are chasing down a regression (such as a testcode failure), then there is certainly a version that used to work, and a version which now does not. Frequently there are not many commits between these two versions — have a look at what they are. Often the failure is really obvious!

If there are a large number of commits between the last known good commit and the first known bad commit, then using `git bisect` is a very efficient way to locate the first bad commit and the last good commit.

3 Guide to specific code in NECI

3.1 Important modules and common (global) variable names

3.1.1 Inexplicable names and anachronisms

A number of the variable names in NECI are largely inexplicable, or confusing, outside of their origin in historical accident. This section tries to clarify some of these.

ARR, BRR

> `ARR(:,1)` contains a list of spin orbital (Fock) energies in order of increasing energy.
>
> `ARR(:,1)` contains a list of spin orbital (Fock) energies indexed by the spin-orbital indices used in the calculation.
>
> `BRR` contains a list of spin orbital indices in increasing (Fock) energy order. Where multiple degenerate orbitals have the same symmetry, they are clustered so that spin orbitals with the same symmetry are adjacent to each other, and within that ordered by m_s value.

TotWalkers and TotParts

> `TotWalkers` refers to the number of determinants or sites that must be looped over in the main list. This may include a number of blank slots if the hashed storage is being used.
>
> The number of particles (walkers) on a core is stored in `TotParts`. The total number of particles in the system (including all nodes) is stored in `AllTotParts`.

InitWalkers

> The number of particles *per processor* before a simulation will enter variable shift mode.

G1

> The variable name `G1` is a historical anachronism. It is an array containing symmetry information about given basis functions. In particular `G1(orb)` contains information about the one electron orbital `orb`.
>
> The data is of type `BasisFN`:
>
> ```fortran
> type symmetry
>     sequence
>     integer(ints64) :: S
> end type
> type BasisFn
>     type(symmetry) :: sym ! Spatial symmetry
>     integer :: k(3)       ! K-vector
>     integer :: Ms         ! Spin of electron. Represented as +/- 1
>     integer :: Ml         ! Magnetic quantum number (Lz)
>     integer :: dummy      ! Padding for alignment
> end type
> ```

Not all of these values are required for all simulations. The `sym` element points at a padded 64-bit integer. This is done for memory alignment reasons that are no longer important.

3.2 Parallelism

FCIQMC is a highly parallelisable algorithm. Implementationally this is achieved through the use of independent MPI processes that communicate using MPI.

The raw `MPI_*` routines, provided by MPI should not be used directly inside NECI for a couple of reasons:

- Depending on the build configuration and compiler, many variables may change their size or alignment, leading to code which only works on some compilers, and
- Naming conventions for linking vary between compilers.

The `Parallel_neci` module abstracts these implementational details away, presenting a consistent interface.

3.2.1 Usage

The relevant MPI functions are accessible through wrapper functions with the underscore in the name removed. For example, the MPI routine `MPI_AllReduce` is available as `MPIAllReduce`.

The arguments to the wrapper routines are a subset of those specified in the MPI standard, and the explanations of those values may be found there.

Many of the routines have versions which require specifying the array dimensions manually (`*_len`) or automatically (`*_auto`). The latter obtain the dimensions of the arrays to communicate by analysis of the array bounds and are preferred, as they are less prone to user error.

If communication is desired between subsets of the available processors (as is used in the CCMC code), the MPI communicator may be specified through the `Node` parameter. No further detail is provided here about how to construct these objects.

If the necessary MPI routine is not present in the `Parallel_neci` module it will be necessary to add it. This can be awkward as discussed below.

☞ The `inplace` MPI functionality is present (although disabled) in NECI. For the time being it should not be used due to serious bugs in the interaction between ifort and OpenMPI.

☞ Different implementations of MPI are not interchangeable at runtime, even if they initially appear to be. For instance, code compiled using OpenMPI on the ifort compiler will run on MPICH built with the gnu toolset, but no communication will occur, and `nProcessors` independent (identical) simulations will run.

> ☞ In keeping with the notion of failing early, and failing loudly, outside of the initialisation and cleanup code, most of the templated MPI routines do not quietly report errors in status variables, but will kill the entire simulation with a runtime error.

3.2.2 Important variables

A number of important control variables are available for use within NECI.

`nProcessors`
> The total number of processors initialised in the MPI calculation.

`iProcIndex`
> The (zero based) index of the current processor. This will be between 0 and `nProcessors-1`.

`root`
> The (zero based) index of the root (head) processor. This should be tested in code using: `if (iProcIndex == root)`.

`nNodes`
> The number of nodes initialised in the MPI calculation. In most cases this will equal `nProcessors`. These values will only differ if the MPI space is being subdivided into smaller nodes.

`iNodeIndex`
> This (zero based) index gives the position of the processor in the current node. For most calculations this will be zero on all processors.

`bNodeRoot`
> This specifies if the current processor is the root processor of a node. I.e. that this processor is responsible for macroscopic communication. For most simulations this is `.true.` on all processors.

3.2.3 Implementation

The current implementation of the `Parallel_neci` module works extremely well. It may, however, be necessary to modify it, either to deal with changes in the available compilers, or (more likely) to add support for additional MPI functions.

Fortunately, the latter is much more straightforward than the former! A modified version of a currently implemented routine is likely to be the best approach.

Much of the complication introduces is the requirement that NECI interoperate with MOLPRO, which uses C based MPI libraries. In order to function correctly in this environment, it is necessary to wrap the MPI routines in a C-wrapper, and interface this with our templated library.

As such, the MPI wrapper implementation has a number of layers and non-obvious facets. This results in the behaviour being relatively opaque, and the code scattered with a large number of `#ifdef` statements.

C-wrapper initialisation

The constants required for operation of the C MPI libraries are not necessarily of a form compatible with Fortran. The C wrapper code (in `lib/parallel_helper.cpp`) contains lookup tables of the values defined in the C MPI headers. The module `ParallelHelper`, which is included in `Parallel_neci` contains Fortran definitions of these values which are the indices to the lookup tables.

The C types required for MPI communicatiors and groups `MPI_Comm` and `MPI_Group` are not Fortran compatible. Fortunately the MPI standard provides inbuilt converters to integer types (`MPI_comm_2cf`, etc.). The c wrapper code mimcs the normal Fortran MPI code, returing Fortran compatible values, but internally converting them to the required types.

Determination of parameter sizes

The code to determine the lengths of the input (`v`) and output (`ret`) arrays is passed to the code a template parameters `mpilen` and `mpilen2`. These make use of the `lbound` and `ubound` intrinsics to determine the number of elements in each array.

Conversion to pointers

Fortran, by default, passes values by pointer. In the case arrays, this passes a pointer to the array structure, rather than the data. This structure includes a pointer to the data and information about the data type and the array bounds.

If the code is to be passed to the C wrapper, the actual data pointer needs to be extracted.

When the C wrapper layer is being used, a value of type `c_ptr_t` is declared. If compiler support is present this is equal to `type(c_ptr)`, but otherwise is a raw 32 or 64 bit integer as appropriate.

The memory address of the array (strictly of its first element) is obtained using either the standardised `c_loc`, or the non-standard `loc` intrinsics.

> ☞ Due to a bug in some versions of gfortran an extra level of indirection is used which hides the type of the array being passed using a routine called `g_loc`. This code circumvents normal interfacing.

Calls to MPI

In the normal case (when the C-wrapper is not being used), the `MPI_*` routines are then called directly. After the return values are checked for errors, the routine returns the output data as normal.

C wrapper layer

Interfaces to each of the C mpi wrappers are defined in the `ParallelHelper` module. These accept the pointers discussed earlier. The Fortran symbols for these wrappers are named so that they coincide with the normal `MPI_*` routines, so that no change to the calling code is required.

3.3 Shared memory

In principle, when using MPI all of the processes are entirely independent except for the explicit communication made through the MPI library. Within NECI, as all of the particles are entirely independent between annihilation steps this is a good thing.

However, we have a large amount of read-only data. The integrals which are read in from the FCIDUMP files can consume a non-trivial proportion of the available system memory, and are duplicated on each of the processes. On modern multi-processor and multi-core systems this is an outrageous waste of system memory — which is made worse by the fact that if the same regions of this memory are requested on multiple different processors the computer will not know these are the same, and will not be able to make use of the L1, L2 and L3 cache to speed memory access.

The shared memory provisions in NECI substantially abuse the MPI specification by mixing the available memory address space between the different processes. This is extremely useful when done careful, but there are some caveats to be aware of.

3.3.1 How to use shared memory provisions

The shared memory provisions have been designed to be as interchangeable with the normal Fortran memory allocation provisions. Essentially memory is allocated largely as usual, but all of the processes on the same physical node will end up with pointers to the same block of memory.

Memory is allocated with a call to

```
subroutine shared_allocate(name, ptr, dims)
```

This is a templated routine, and so will work for a wide variety of data types and array dimensions. The `name` parameter specifies a unique name for this array. This name is used to identify the particular block of shared memory between the processes (there may be an arbitrary number). The `ptr` parameter is a Fortran `pointer` with the relevant data type and the correct array shape. `dims` is an array of integers indicating the size of each dimension of the array to be allocated.

As an example,

```
real(dp), pointer :: real_arr(:,:)
...
call shared_allocate("example", real_arr, (/6, 13/))
```

will allocate a 2-dimensional array named "example" with the array bounds (`1:6, 1:13`), equivalent to `allocate(real_arr(6,13))`.

The read only data should now be written. In principle, the data only needs to be written from one of the processors per node — in practice it is easiest to get all of the nodes to write the read only data. It is important that data is only written at this stage — any processing that needs to be done on this data must not happen in the shared memory, as it could be disrupted by the other processes. This scheme only works because all of the processes write exactly the same data.

After data initialisation, the processes must be synchronised with a call to `MPIBarrier`. This will ensure that the read-only data is in the same state in all of the threads.

☞ The POSIX memory model makes few guarantees about *when* memory that is shared between processes gets updated (as opposed to between threads). This shared memory **must not** be used for communicating between the MPI processes. That is what MPI is for.

☞ There are no synchronisation primitives provided for use with these shared memory blocks. No assumptions can be made about the order of access between the processes. All actions that are carried out **must** be inherently thread-safe, or errors will eventually (and unexpectedly) occur.

The data should be deallocated using the routine `shared_deallocate`.

3.3.2 Quirks and limitations

Customising data types

The shared memory routines are templated so that they can be used with a wide variety of plain-old-data types and array sizes. For any data types outside of those already templated, new configuration options will be needed in `lib/allocate_shared.F90.template`. The information required is the number of bytes per element of the array.

If custom `types` are desired, this may be quite tricky. It is difficult to guarantee the size, memory alignment and packing of the data in a custom type — the compiler is free to choose how it wishes to do this, and as such it varies from compiler to compiler. It is necessary to use the `sequence` keyword must be used to force the compiler to store data contiguously. If there are `pointer` or `allocatable` elements in the custom type, it cannot be used with shared memory, as the size of these elements is highly variable between compilers.

Storing bit representations

There is a special allocate routine `shared_allocate_iluts` which can be used for storing bit representations — these differ in that the lower bound of the first array index must be 0, rather than 1.

Non-uniform memory architectures

Modern chip architectures (in particular the intel i3, i5 and i7 series of processors) move the memory controller onto the processor. This dramatically improves memory access speeds.

The cost is that on multi-processor (as opposed to multi-core) architectures the memory is segmented into regions that are controlled by the different processors. Memory access within the region controlled by the current processor is faster than that between them.

A performance increase could be obtained by only sharing memory between processes which are hosted on the same physical processor. This will require using the processor affinity options of MPI, which is not routinely done currently with NECI. Further, it will require subdividing the processes on each physical node into sub-nodes — support for this exists in the code in NECI, but the processor specific

information required to correctly subdivide the processes is not included, and this facility is currently switched off.

For processor topology, see the Intel documentation at https://software.intel.com/en-us/articles/intel-64-architecture-processor-topology-enumeration.

Disabling shared memory

Shared memory is enabled by the pre-processor define `__SHARED_MEM`. This can be found in the config files for platforms that support it. If necessary, this can be removed from relevant config files and Makefiles, which will disable inter process memory sharing, and fall back on the normal Fortran `allocate` mechanism.

3.3.3 How it works

The way that inter-process memory sharing works is system specific, and depends on operating system primitives being used directly.

The code templating functionality in NECI is used to make the shared memory wrapper work for a wide range of data types, with differing numbers of dimensions in the arguments. From this the size of memory required in bytes is calculated, and this is passed to a C helper function that allocates the memory. The returned raw pointer is converted to a Fortran one through the Fortran 2003 intrinsic `c_f_pointer`.

The C helper library contains a number of utility functions to help it interface with Fortran. In particular wrapper so it can print to the same output, and a mapping to store additional data about the allocated memory to assist in deallocating without the Fortan code requiring knowledge of how the operating system intrinsics work.

Beyond that, there are three main code paths:

POSIX

A unique file name is created, based on the current working directory. The function call `shm_open` with the control parameter `O_CREAT` will open, or create, a POSIX shared memory object. As a result, one of the processes on a node will create the mapping, and the others will join it — it is unknown in advance which will do the creating.

The returned descriptor acts as a file, and so is set to the desired length with `fdtruncate`, and then mapped into memory as if it were a memory-mapped file using `mmap`. The file descriptor is then closed as it is no longer needed.

Once all of the processes have mapped the memory, the shared memory object is unlinked, ensuring that the memory will be deallocated by the operating system when all of the processes stop (preventing a memory leak if the processes crash).

The memory can then be manually deallocated using `munmap`.

System V

A unique file name is generated, based on the current working directory, and the file is created. A System V Inter Process Communication Key is created and obtained from this file using the routine `ftok`.

Using this key, a shared memory object of the correct size is created using `shmget`, and this region is mapped into memory using `shmat`.

Once all of the processes have reached this point, the shared memory control object is destroyed using `shmctl` to ensure the operating system will deallocate the memory in case of a crash.

The memory can be manually deallocated using `shmdt`.

Windows

The memory mapped file provisions in Windows are used to generate a shared memory region. A unique file name is created, based on the current working directory, and then a non-filesystem backed file is created with `CreateFileMappingW`. This can be opened by all of the other processors on the same node using `OpenFileMappingW`, and this "file" is mapped into memory on all of the processes using `MapViewOfFile`.

The memory can be manually deallocated using `UnmapViewOfFile` followed by `CloseHandle`.

The subroutine `iluts_pointer_jig`, which is used when allocating bit representations which start from an index of 0 rather than 1, is an interesting demonstration of how to manipulate the bounds of arrays declared in Fortran in compilers that do not support the array reshaping assignments described in Fortran 2003 (most compilers).

3.4 Integral retrieval

Integral retrieval is found in the tightest of the tightest loops within NECI. Calculating each Hamiltonian matrix element may require a number of different two- and four-index integrals, and at least one Hamiltonian matrix element is required for each generated excitation.

As a result, the normal approach taken to prevent code repetition introduces a bottleneck. If there is a `get_umat_el` function, this will have to contain the logic as to which type of integral is being obtained, and where this should be located. This conditional logic will be executed for every required integral.

As such, access to the integrals is through a procedure pointer, with the interface

```
abstract interface
    function get_umat_el(i, j, k, l) result(hel)
        use constants
        implicit none
        integer, intent(in) :: i, j, k, l
        HElement_t :: hel
    end function
end interface
```

This function pointer can then be called from anywhere in the code (after it is initialised) and this will call the correct routine.

3.4.1 FCIDUMP files

The most commonly usedintegrals routines store their integrals in memory after reading them in from a `FCIDUMP` file.

These routines support FCIDUMP files produced by various codes, including MOLPRO, PSI3 and VASP (hacked versions of Dalton and QChem also support this - I believe MOLCAS as well now). Certain (generally legacy) FCIDUMP files have a strictly fixed

format, which can result in adjacent columns of indices merging. As such, they are read via an explicit format. To use MOLPRO or other FCIDUMP files the `MOLPROMIMIC` option should be supplied in the `SYSTEM` block of the input file. Other sources of FCIDUMP file should use the `FREEFORMAT` option. In general, this should *always* be used.

The FCIDUMP files can be briefly summarised by

Header

The header is specified as a Fortran namelist, with the following possible elements:

NORB

Specifies the number of spatial orbitals in the system if RHF, or the number of spin-orbitals if UHF.

NELEC

Specifies the number of electrons the Hartree–Fock determinant should have.

MS2

Specifies twice the total projected spin of the system (such that it is always an integer)

ORBSYM

A list of spatial symmetries of the orbitals specified in (??? Check name with Giovanni) format in orbital order. Note that the structure of the reference determinant will be visible here if the `MOLPROMIMIC` option is used, and the reference is to be determined by the order of the orbitals.

ISYM

The symmetry of the reference determinant specified in the same format.

UHF

T if the file contains a UHF basis, otherwise F.

SYML, SYMLZ

The total and projected orbital angular momentum for systems with an axis of rotation. Currently FCIDUMP files which use this option can only be generated using QChem, and the resultant file must be pre-processed using the TransLz utility.

PROPBITLEN, NPROP

These parameters are used to describe the behaviour of k-point symmetries. For more details contact George Booth.

4-index integrals

Following the header, all of the integral and energy lines may follow in arbitrary order.

The 4-index integrals are specified with the format `z i j k l`, where `z` is the `real` or `complex` element, and the indices are integers. All indices are one-based. Indices are in **chemical notation**!

2-index integrals

The 2-index integrals are specified in the same way with the final two indices equal to zero.

Fock energies

The Fock energies are specified in the same way, with the final three indices equal to zero.

These values are used for determining the initial (Hartree–Fock) determinant, which is constructed from the lowest energy spin-orbitals. They are strictly optional. If the `MOLPROMIMIC` option is supplied then the order of the orbitals determines the reference determinant.

Core energy

The core energy is specified in the same way, but with all four indices set to zero.

3.4.2 Generation on the fly

A number of schemes exist for generating integrals on the fly. In particular the Uniform Electron Gas and Hubbard model have integrals that can be trivially calculated, and so FCIDUMP files are not used.

3.4.3 Nested schemes

There exist two function pointers with the same abstract interface, `get_umat_el` and `get_umat_el_secondary`. Once the primary method of determining integrals has been selected, then this be moved to the secondary pointer, and another wrapper routine used instead. This allows additional filtering logic to be applied.

The wrapper routine should then call `get_umat_el_secondary` internally.

3.4.4 Fixed Lz and complex orbitals

If either projected angular momentum (Lz) symmetry, or complex orbitals are being used, the pattern of restricted zeros in the integrals changes. Wrappers around the normal `get_umat_el` routine are used to supply these zeros.

These are examples of the nested schemes above.

3.4.5 Further schemes

It is likely that further schemes will be required in the future. In particular, approximate, and interpolating schemes are likely to be required to reduce the $\mathcal{O}(M^4)$ memory dependence on the number of orbitals. These should be implemented as new routines to be pointed at using the function pointers.

3.5 Hamiltonian matrix element evaluation

The two- and four-index integrals are the primary input to a FCIQMC calculation. However, they are used via Hamiltonian matrix elements. There are a number of considerations for the way that Hamiltonian matrix elements are used in NECI.

3.5.1 Different ways to obtain Matrix elements

Certain pieces of information are required in order to calculate Hamiltonian matrix elements. The Excitation level (the number of differing orbitals between the determinants), the corresponding excitation matrix and the parity of the excitation are necessary. Depending on the excitation level, the decoded list of occupied orbitals is required.

Depending on where in the execution path the Hamiltonian matrix elements are required, different information is readily availabile. As some of this is relatively expensive to calculate (in particular the parity) it is important that as much information as is available is used.

As part of the spawning and particle generation process, there is a function pointer called `get_spawn_helement`. This is passed the natural integer and bit representations of the determinant, the excitation level, excitation matrix, parity and (potentially) precalculated matrix element. Depending on the initialisation options, the routine which is selected will make use of the correct subset of these. It is important that the excitation generator and the choice of Hamiltonian matrix element generation here are tightly coupled.

Elsewhere in the code, the routine `get_helement` is used to obtain matrix elements.[1] This routine comes in a number of flavours. The available options are

`nI, nJ`
> This routine will return the matrix element between any two, arbitrary, decoded determinants.

`nI, nJ, ic`
> This version is provided the excitation level of the determinant in addition.

`nI, nJ, ic, ilutI, ilutJ`
> The bit representations of the two determinants are provided, which greatly enhances calculating the parity if needed.

`nI, nJ, ilutI, ilutJ`
> If both the bit representations and the decoded versions are present but no further information is known then this form should be used.

`nI, nJ, ilutI, ilutJ, ic_ret`
> This version is the same as the above, but returns the excitation level of the pair of determinants in addition to the matrix element.

`nI, nJ, ic, excitMat, tParity`
> When everything about the relationship between the two determinants is fully known, this form should be used. It is used implicitly after excitation generation when the excitation level, matrix and parity are known. The second decoded determinant is not used in determinental calculations, but is provided to support systems such as CSFs.

For calculating diagonal Hamiltonian matrix elements, the routine `get_diag_helement`

---

[1]As an exception, some old code makes use of `gethelement` or `gethelement2`. These should not be used in new code. Some of the initialisation code also uses `gethelement` as the prerequisites for `get_helement` have not yet been met.

should be used[2]

The cost of the parity

The overall sign of the returned Hamiltonian matrix element is modulated by the parity of the excitation — that is, the whether the number of pairwise swaps of orbitals required to maximimally align the two determinants according to the standard order of the first is odd or even.[3]

The parity may be obtained by actively aligning the decoded representations, or by examination of the bit representations. The latter is much faster than the former, but is still the rate limiting factor for calculating Hamiltonian matrix elements.

Where this factor is known (i.e. after excitation generation) it should be used. It is worth noting that the weighted excitation generation scheme is only viable because only the absolute value of the matrix elements is modelled, so the parity generation step can be entirely ignored.

Slater–Condon rules implementations

The Slator–Condon rules are implemented in the file `sltcnd.F90`, in the routines `sltcnd` and then more specifically `sltcnd_0`, `sltcnd_1` and `sltcnd_2`. There is a certain amount of duplication both of code paths and of conditional testing in these routines — which is a clear violation of the DRY principle.

Access to matrix elements is inside the smallest of the tight loops in NECI. The provision of duplicated logical pathways, rather than conditional switching, has a measurable performance benefit in this case.

HPHF matrix elements

In most cases the HPHF matrix elements are trivially obtained from the normal determinental matrix elements through multiplication by a factor of $\sqrt{2}$ in all cases where the determinant is not closed shell.

If the excitation level is less than or equal to 2, then the elements are a little more complicated. It is possible that both the target determinant and its spin pair are connected to the source determinant, and so the resultant matrix elements will require two calls to the Slater–Condon routines.

Spin eigenfunctions

Spin eigenfunctions may be expressed as linear combinations of all determinants with a given spatial structure. The Hamiltonian matrix elements may be expressed as a two

---

[2]This general routine is not implemented at the time of writing, but will added shortly.

[3]Note that for double excitations, in principle there are two alignments that work. The two new orbitals could be either way around and the parity of these versions are inverted relative to each other. A convention for the ordering of the new orbitals (in NECI they are required to be numerically increasing) is required but arbitrary. The overall simulation will give the same results either way.

index sum over all the determinants with each of the involved spatial configurations.

Given that the number of configurations increases permutationally with the number of unpaired electrons, this scheme scales extremely badly. NECI has some aggressive optimisation to slightly improve this scaling (see Simon's thesis), but ultimately it is a dead end for big calculations.

See the SPINS branch for Hamiltonian matrix element calculation between other types of spin eigenfunctions. These can scale extremely well, but introduce other problems.

3.6 Excitation generation

Excitation generation is the most complicated and intricate part of NECI. Not only must random moves be made, but they must be made in a manner which is efficient (taking account of symmetry, and in terms of implementation). They must also correctly compute the generation probabilities, taking into account multiple possible selection routes to the same determinant.

A failure to generate all of the connected determinants, or mistakes made in calculating the generation probabilites will lead to silent errors that manifest themselves only through (potentially subtly) incorrect energies being produced by the simulation.

There are a large number of factors that must be considered when writing an excitation generator. This section aims to give an overview of some of them, and a brief outline of the two most commonly used excitation generators.

The Alavi group collectively has a large amount of experience writing excitation generators, and anybody intending to write or modify them would be advised to speak to Simon Smart or George booth first.

3.6.1 Interface

Excitation generation is accessed through a procedure pointer. As such, all excitation generators *must* have the same signature. It is described by

```fortran
subroutine generate_excitation_t (nI, ilutI, nJ, ilutJ, exFlag, ic, &
                                  ex, tParity, pGen, hel, store)

    use SystemData, only: nel
    use bit_rep_data, only: NIfTot
    use FciMCData, only: excit_gen_store_type
    use constants
    implicit none

    integer, intent(in) :: nI(nel), exFlag
    integer(n_int), intent(in) :: ilutI(0:NIfTot)
    integer, intent(out) :: nJ(nel), ic, ex(2,2)
    integer(n_int), intent(out) :: ilutJ(0:NifTot)
    real(dp), intent(out) :: pGen
    logical, intent(out) :: tParity
    HElement_t, intent(out) :: hel
    type(excit_gen_store_type), intent(inout), target :: store

end subroutine
```

`nI` and `ilutI` describe the natural integer and bit representations of the source determinant for the excitation. `nJ` and `ilutJ` will store the generated excitation. `exFlag` specifies the type of excitation — this is generally unused, but in some excitiaton generators permits selecting between single and double excitations for the purposes of testing.

`store` provides a location for the excitation to store information that is specific to the source determinant. This information is available for further excitations from the same site.

`ex` will contain the excitation matrix; `ex(1,:)` contains the *spin-orbitals* of the source electrons in `nI`, and `ex(2,:)` contains the *spin-orbitals* that have replaced these values.

`ic` is used to return the excitation level of the resultant site relative to the source site, `pGen` returns the generation probability for the generated determinant, `tParity` returns the parity of the excitation (is the number of pairwise swaps required to align `nI` and `nJ` even or odd), and `hel` can return the Hamiltonian matrix element for this excitation so that it need not be calculated later (this is only really of interest for HPHF calculations, where it can be easier to calculate this matrix element in the excitation generator for technical reasons).

> ☞ Note that the determinant returned in `nJ` *must* be sorted in the same fashion as the source determinant `nI`. This normally means in order of ascending spin-orbital number. This can result in substantial reshuffling of the internal order of the detrminant.

> ☞ It is possible that to implement a sensibly efficient excitation generator, the simulation may make choices which leave no possible excitations remaining. An excitation may be aborted by setting the first element of `nJ` to zero, so long as the calculated generation probabilites for successful excitations are correct.

3.6.2 Symmetry handling

The excitation generator must always preserve the symmetry of the determinant. The way in which this is done depends on the excitation generator, but will involve measuring the symmetry of the source orbitals and selecting the target orbitals appropriately.

The symmetry of a specific orbital, `orb`, may be found in the array `G1`. The spatial symmetry is found at `G1(Orb)%Sym%S`, the k-vector (if appropriate) at `G1(orb)%k`, and the projected spin and orbital angular momentum values at `G1(orb)%Ms` and `G1(orb)%Ml`.

There are also a number of useful macros for measuring and manipulating spin values. `is_beta` and `is_alpha` test if orbitals have beta and alpha spin respectively, whilst `is_one_alpha_beta` test that two orbitals have differing spins. The `get_spin` macro gets the spin in the unusual format for 1 for alpha and 2 for beta as used in some other NECI routines, and `get_spin_pn` obtains the more standard values of ± 1. The `is_in_pair` macro tests if two orbitals belong to the same spatial orbital (including the case where they are the same orbital).

The macros `get_alpha` and `get_beta` obtain the alpha or beta orbital corresponding to the same spatial orbital as the current spin orbital (which may or may not be the same orbital). `ab_pair` obtains the spin paired orbital to the current one.

It is normally necessary to combine and manipulate symmetries, as for a double excitation $\Gamma_i \otimes \Gamma_j = \Gamma_a \otimes \Gamma_b$, but there is no reason for any of $Gamma_i, Gamma_j, Gamma_a, Gamma_b$ to be the same. The products of symmetry labels should be taken using `RandExcitSymLabelProd`, rather than directly using `ieor` commands (which will normally obtain the same result), to protect against the consequences of using different types of symmetry. When combining Ml values it is important to bear in mind the maximum permitted value of Ml, and abort the excitation if necessary.

The class count arrays, described above, are indexed by a a combined symmetry index, that combines spin, k-point, momentum and spatial symmetries. The index to this array is provided by the function `ClassCountInd`. Given a total spin, momentum and spatial symmetry, the paired class count index may be obtained using `get_paired_cc_ind`. The number of occupied, and unoccupied spin orbitals are stored in the data store as decribed above. The total number of orbitals corresponding with a given class count is found at the corresponding location in the array `OrbClassCount`.

The array `SymLabelList2` contains all orbitals sorted by symmetry class, with offsets given in `SymLabelCounts2`, such that all of the orbitals with the same symmetry as a given orbital, `orb`, may be found as follows

```
integer :: sym, spn, ml, norb, cc_ind, offset

! Obtain the symmetry labels associated with this orbital
sym = G1(orb)%Sym%s
spn = get_spin(orb)
Ml = G1(orb)%Ml

! Obtain the combined symmetry index
! cc_ind = ClassCountInd(orb) ! ... alternatively
cc_ind = ClassCountInd(spn, sym, ml)

! Get position and count of orbitals
norb = OrbClassCount(cc_ind)
offset = SymLabelCounts2(1, cc_ind)

! And this slice contains the appropriate orbitals (including orb)
SymLabelList2(offset:offset+norb-1)
```

3.6.3 Manipulating determinants, and bit representations

The primary output of the excitation generator is the newly generated determinant. It is much more computationally efficient to copy and modify the source determinant and bit representation than to start from scratch. As such there are two processes to consider.

Manipulating bit representations

Orbitals can be cleared from the bit representation using the macro `clr_orb`, and set using the macro `set_orb`. For an excitation from orbital `a` to orbital `i` this would look like

```
clr_orb(ilut, a)
set_orb(ilut, i)
```

make_single and make_double

> Manipulating the natural integer representation of determinants is substantially more complicated, as there is a *requirement* that they remain sorted by spin-orbital number. Although it would be straightforward to, essentially, replace the excited orbital with a new one, and sort it, this is inefficient as the parity of the excitation is going to be required. If the manipulation can be carried out in such a way that the parity is naturally returned this will substantially improve the efficiency.

> The routines `make_single` are passed the source determinant and respectively one or two source electron positions and target orbitals. They perform the substitution and measure how much the newly placed orbitals must be moved by to restore sorting (accounting for edge cases).

> These functions return the sorted determinant, the excitation matrix and the parity of the excitation. They should be used by all determinental excitation generators.

3.6.4 Data storage

Each site in the main particle list may be occupied by multiple particles. There is a reasonable amount of information which the excitation generator must generate for each site it excites from — it makes sense to store this information and reuse it for each of the particles on the site. A data structure of type `excit_gen_store_type` is passed to the excitation generator that it can use for this purpose:

```
type excit_gen_store_type
    integer, pointer :: ClassCountOcc(:) => null()
    integer, pointer :: ClassCountUnocc(:) => null()
    integer, pointer :: scratch3(:) => null()
    integer, pointer :: occ_list(:,:) => null()
    integer, pointer :: virt_list(:,:) => null()
    logical :: tFilled
    integer, pointer :: dorder_i (:) => null()
    integer, pointer :: dorder_j (:) => null()
    integer :: nopen
end type
```

The arrays that are required for the current excitation generator are allocated during calculation initialisation by the routine `init_excit_gen_store`.

When the excitation generator is being called on a new determinant, the `tFilled` variable will be set to `.false.` by the main loop code. Once the generator has filled in the required information this should be set to `.true.` to indicate that the data may be reused.

The arrays `ClassCountOcc` and `ClassCountUnocc` are initialised by calling `construct_class_counts` at the start of the excitation generator. They contain a count of the number of occupied, and the number of unoccupied, orbitals associated with each spin-symmetry combination. These are used for calculating the probabilities in essentially all excitation generators.

The `occ_list` and `virt_list` variables store only information relevant to the excitation generator in `symrandexcit3.F90`.

The `dorder_*`, `nopen` and `scratch3` variables are used in the CSF excitation generation code.

As there is only one instantiation of this data structure, in the main loop, adding additional elements adds only negligible overhead. If future excitation generators need a place to store information between calls, it should be added here.

The excitation generation routines should be as tightly coupled to the Hamiltonian matrix element generation routines as possible. In particular, information such as the excitation level and the excitation matrix are trivially available in the excitation generator and expensive to calculate otherwise. As it stands, the interface for the excitation generator permits passing the excitation level, parity and excitation matrix to the matrix element generation routines — this is sufficient for determinental systems.

If NECI is to be extended to efficiently consider other basis functions, then other data will be required. A structure should be created to pass this information around, so that each element which is added does not require adjusting the interface of each and every excitation generator. This has been done in the SPINS branch, with a type named `spawned_info_t`, which is unlikely to be merged into master for independent reasons, but may provide a template for doing this if required in the future.

3.6.5 Re-use and rescaling of random numbers

In determinental calculations, even with large basis sets, each site is connected to at most a few thousand others. A single 64-bit random number contains vastly more random information than is required to make a good choice between all of these options.

However, most of the potential algorithms for excitation generation involve a hierarchy of choices. The natural implementation of these choices is to generate a new random number for each new choice that is required. This is highly wasteful, especially as random number generation is relatively expensive.

More bang-for-your-buck can be extracted from random numbers by partitioning them, and rescaling them as you move through the hierarchy of choices. A simple example demonstrates this, considering the macroscopic choice between single excitations and double excitations:

```fortran
real(dp) :: r
r = genrand_real2_dSFMT()
if (r < pDoubles) then
    ! Double excitation selected. Now rescale r
    r = r / pDoubles
    ...
else
    ! Single excitation selected. Now rescale r
    r = (r - pDoubles) / (1.0_dp - pDoubles)
    ...
end if
```

This is not always done in the current implementations of excitation generators, but should always be considered for efficiency.

> ☞ This technique should not be used where selections may need to be redrawn. Repeated repartitioning and scaling of the random number will rapidly deplete the available randomness if it is repeated a number of times due to redrawing.

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3.6.6 Timestep selection and other control parameters

The spawning process is normally the limiting factor for the selection of the imaginary timestep. The magnitude of the spawn, n_s, is given by

$$n_s = \delta\tau \left| \frac{H_{ij}}{p_{\text{gen}}(j|i)} \right|.$$

As such, a limit on the value of $\delta\tau$ may be obtained from the maximum value of that ratio, combined with a (chosen) maximum size of spawn;

$$\delta\tau_{max} = n_{s,max} \times \left(\max \left| \frac{H_{ij}}{p_{\text{gen}}(j|i)} \right| \right)^{-1}.$$

The ratio should be accumulated through a calculation, and can be used to determine the optimum time step on the fly.

This approach may be generalised to a larger number of parameters. Additional control parameters that influence decisions in the excitation generator may be introduces (such as the choice between single and double excitations, or the extent to which a bias is made towards or against double excitations which are spin aligned).

Considering the different choices that are made in the excitation generator, this splits the excitations into a number of different categories. For optimal timestep values the worst case for each of these categories should be optimised to give the maximum spawn size.

The impact of each of the parameters to be optimised must be removed from the generation probability values, so that an unaffected value can be maximised. For example considering a split between single and double excitations;

$$n_{s,max} = \delta\tau \frac{\delta\tau}{p_{single}} \left| \frac{H_{ij} p_{single,iter}}{p_{\text{gen}}(j|i)} \right|_{single} = \delta\tau \frac{\delta\tau}{1.0 - p_{single}} \left| \frac{H_{ij}(1.0 - p_{single,iter})}{p_{\text{gen}}(j|i)} \right|_{double}.$$

In this case the current value of $p_{single,iter}$ (i.e. the value on the particular iteration the generation occurred) is removed from the ration which can then be maximised. Closed form expressions for the optimal values of $\delta\tau$ and p_{single} can then be found straightforwardly.

This approach can be extended, although the means to isolate the impact of parameters on the generation probability, and the structure of the final closed form expressions will depend on the form of the excitation generator.

3.6.7 Testing excitation generators

It is critical that excitation generators are *correct*. That is that all of the connected determinants are generated, and that the generated probability is correct.

There are a number of metrics that can be used to test this. A testing function should be written that takes a given source determinant as a parameter, and runs the excitation generator a very large number of times on this determinant (for example, 10 million times). This test function should contain a number of tests:

Are the correct determinants generated

A list of all single and double excitations of the correct symmetry should be enumerated in a brute force manner (see `GenExcitations3`). It should then be checked that *all* of the determinants in this list are generated by the excitation generator, and no determinants outside this list are generated.

Normalisation of generation probabilities

An accumulator value should be kept for each possible determinant that can be generated. Each time the determinant is generated, the value p_{gen}^{-1} should be added to that determinants accumulator.

On average this will add a value of 1.0 to the accumulator for every excitation generation attempt. Thus, when all of the accumulated values are divided by the number of generation attempts made by the test function, all of the values should give roughly 1.0.

There may be a reasonable amount of variation, but repeated across a few different runs with different random number seeds it should be clear that all of these values give roughly 1.0.

Note that if some connections are *extremely* strongly weighted against (as can happen with the weighted excitation generator) they will sum in a very large term very rarely, and so their averaged value can jump around quite dramatically.

Overall probability normalisation

As an extension to the above, the sum of all of the accumulators should stocastically tend towards the number of connections multiplied by the number of spawning attempts.

If this total accumulated value is divided by the number of connections multiplied by the number of spawning attempts it should average very strongly to 1.0, normally to four or five decimal places.

For an example test function, see `test_excit_gen_4ind` in `symrandexcit4.F90`. An excitation generator that passes these tests is not guaranteed to be correct, but it is quite likely.

3.6.8 How this interacts with HPHF functions

HPHF functions present a complexity for excitation generation. Excitation generation occurs on determinants, but the HPHF function includes the spin flipped pair. When there are only a small number of unpaired electrons, the possibility of the excitation generator having generated the spin flipped version also needs to be available, although this is not readily accessible in the excitation generator.

As a result, a routine must be provided to calculate the probability of generating $|D_j\rangle$ from $|D_i\rangle$ without actually generating an excitation.

☞ Once the excitation generator has been planned out, it makes sense to write this calculation function first (it tends to be simpler than the excitation generator). A call to it can then be included at the end of the excitation generator inside `#ifdef __DEBUG` flags, which provides a powerful correctness check, and catches any cases where these functions diverge.

3.6.9 The uniform selection excitation generator

A full discussion of this excitation generator is found in the paper (...). The operation of this excitation generator is also the basis for a number of other more specialised excitation generators (such as the CSF excitation generator). This excitation generator is implemented in `symrandexcit2.F90`.

Although the generation probabilities associated with this excitation generator are highly non-uniform, it fundamentally makes choices at each *stage* of the excitation generator uniformly between the options presented at this point.

For single excitations, an electron is chosen uniformly at random. This fully specifies a symmetry index, and from the appropriate list a vacant orbital is chosen at random. This selection is generally made by picking an orbital with the appropriate symmetry at random, and re-drawing if it is already occupied (unless there are very few available choices, in which case the n-th available orbital is chosen from an enumeration of available orbitals).

For double excitations, a pair of electrons are chosen at uniform (using a triangular mapping). This specifies the total symmetry of the excitation. A vacant orbital, a, is then chosen at random from the entire array of orbitals (in the same way as above, redrawing if an occupied one is chosen, or if an orbital is selected that has no available orbital b that could produce the correct total symmetry). This in turn specifies the symmetry of orbital b, which is chosen in the same way as the orbital for a single excitation.

The possibility of having picked the orbital b first, and then a must be accounted for in calculating the generation probabilities.

3.6.10 The weighted excitation generator

This excitation generation scheme is discussed in a great deal more detail in a paper which is currently pre-publication. This excitation generator is implemented in `symrandexcit4.F90` as `gen_excit_4ind_weighted`.

Fundamentally, a weighting value is used to bias the choice of orbitals towards those which are likely to correspond to large Hamiltonian matrix elements. This is done using a Cauchy–Schwarz decomposition of the Hamiltonian matrix elements. The specific elements used depend on the spin choices made, and are discussed in the referred paper.

For speed, the entire choice of orbitals of a given symmetry are considered, and the weightings corresponding to orbitals which are occupied in the source determinant are set to have a zero weighting.

For single excitations, an electron is chosen uniformly at random. This determines the target symmetry. A cumulative list of the weighted terms for each of the available orbitals is generated, and a random number on the range of the largest element in this list is generated. A specific index into this list is selected by binary searching for the first element in the cumulative list which is greater than or equal to this random number, and this index specifies which of the orbitals of the given symmetry are selected as the target orbital.

For double excitations, a choice is made of whether the two orbitals should have the same spin or different spin (the probability of either is optimised on the fly at run time). If the two electrons are to have the same spin, they are chosen uniformly using a triangular mapping, and otherwise uniformly using a rectangular mapping. This entirely determines the target combined symmetry index.

A list is constructed, with a length equal to the total number of available target symmetry indices. This is populated with a cumulative count of the product of the number of available orbitals of a given symmetry with the number of available orbitals of the paired combined symmetry required to result in the determined total symmetry. To prevent double counting, there are considered to be no combinations where the first index is larger than the second index. A pair of symmetries are chosen using binary searching as described before, weighted towards the symmetries with the most available choices.

Two orbitals, a, b, with the corresponding symmetries, are then picked in the same way as the orbital was selected for single excitations (although the weighting terms must now consider the effects of both source orbitals). When choosing orbital b, if it comes from the same symmetry category as orbital a the relevant elements must be adjusted in the cumulative list.

For calculating the probabilities, the only duplication of generating the same determinant is for the case when both orbitals have the same spin and symmetry. This must be accounted for in the generation probability.

3.7 Determinant data storage

There are two main locations where blocks of information concerning particles associated with determinants are stored.

3.7.1 Transmitted data

This concerns data that will be (or could be) transmitted between different processors. Essentially this includes persistent information that is generated by the excitation generator. Combined, this information forms the *bit representation* of a determinant.

All data access should be through the getter and setter functions in the `bit_reps` module (`BitReps.F90`), with the exception of the orbital representation which may be manipulated directly as it will always be first. There are general `encode_bit_rep` and `extract_bit_rep` routines which package and extract all of the relevant information, as well as specific accessors.

In most of the code the encoded values for specific determinants are referred to as `ilut`, standing for "Integer Look-Up Table" which relates to the orbital representation.

The packaging of this data varies substantially between different compiler and runtime configurations. For example, integer runs on 64-bit machines co-opt some of the additional bits in the storage of the signed particle counts to store the flags. It is essential that no attempt is made to access the data in this array direcly.

The representation of each determinant is of dimensions `0:nIfTot`, that is of length `nIfTot+1`. Unusually for an array in Fortran it is a 0-based index. The component

of the overall representation required to uniquely determine one site is `0:nIfDBO` (DBO stands for DetBitOps), which includes the orbital description and any CSF descriptiors.

Each of the components of the representation has a `nIf*` (Number of Integers For) and `nOff*` (offset of) value. These should not be used directly unless adding data to this representation.

Orbital description

Determinants are stored by a bit-representation of the choice of orbitals to construct their Slater Determinants from. This representation is of length $2M$, i.e. the same as the number of available spin-orbitals. An occupied orbital is represented with a 1, and a vacant orbital by a 0.

This representation can be accessed directly. To simplify things, various macros are available. The macros `IsOcc` and `IsNotOcc` test the occupancy of particular orbitals, and the macros `set_orb` and `clr_orb` modify it without requiring the developer to worry about the data representation.

To decode the bit representation of the orbitals into the natural orbital representation use the `decode_bit_det` routine. Equivalently, the `EncodeBitDet` generates the orbital bit representation from the natural integer version.

CSF descriptors

If CSF descriptor labels are required, they are stored here.

Signed particle count

The representation of the coefficient, or "sign" of the determinant is the primary value which is evolved during an FCIQMC simulation.

These values are represented by an array of `real`(dp) coefficients of length `lenof_sign`. In a standard simulation this length is unity, but for complex walkers two values are used and the double-run code uses extras.

These values can be used via the routines `extract_sign` and `encode_sign`. The specific elements of the sign array can be accessed by `extract_part_sign` and `encode_part_sign`. If all particles are to be removed the routines `nullify_ilut` and `nullify_ilut_part` can be used.

Flags

Any number of flags may be associated with a particular site. A current full list may be found in the file `bit_rep_data.F90`. The most commonly used flags are the `flag_is_initiator` and `flag_parent_initiator` flags — be aware that these are different names for the same thing (depends if considering particles in the main or spawned lists).

There is a pseudo-flag, `flag_negative_sign`, that only exists to help combining the representation of the coefficients and flags. It should never be used directly outside of the representation manipulation routines.0

These flags may be tested using the `test_flag` and `set_flag` routines referencing the specific flag desired from the above list.

Further, then entire set of flags may be extracted or stored using the `extract_flags` and `encode_flags` routines. Once they have been extracted, they may be examined and manipulated with the `btest`, `ibset` and `ibclr` in the same way as the set and

test functions above. A special routine `clear_all_flags` exists for resetting the flag status.

It is extremely important that the flags element of the bit representation is not accessed directly.

3.7.2 Locally stored data

This concerns information that will *never* be transmitted. All of this information is either used in tracking the status of an occupied determinant, or for values that could in principle be regenerated when required but are stored for optimisation.

All data access should be through the `get_*` and `set_*` routines found in the module `global_det_data`.

This data is stored in the global array `global_determinant_data`, but this array should not be accessed directly! The location of data within this array is determined by the initialisation routine in the module `global_det_data`, and depends on the calculation being performed.

The data currently stored in this array are

- The diagonal Hamiltonian matrix element for the determinant (`diagH`),
- The average signed occupancy of the determinant (`av_sgn`, only for RDMs).
- The iteration on which determinants became occupied, (`iter_occ`, only for RDMs) and
- The moment in imaginary time on which the (contiguous) occupation of this determinant began (`tm_occ`, only with experimental initiators).