Accelerating Full Configuration Interaction Quantum Monte Carlo

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Part I

Introduction: The Full Configuration Interaction Quantum Monte Carlo Algorithm
To estimate the ground state energy of a Molecule with \( N \) electrons solve:

\[
\hat{H} |\psi\rangle = E |\psi\rangle \tag{1}
\]

where \( |\psi\rangle \) is in some finite basis (at fixed geometry).

If we let \( |\psi\rangle \) be a single determinant of \( M \) Molecular Spin Orbitals (MSO), Hartree-Fock lets us compute the variations minimal single determinant wavefunction \( |D_0\rangle \).

Full Configuration Interaction (FCI) adds into \( |\psi\rangle \) all possible determinants \( |D_1\rangle \) with \( N \) MSO occupied and \( M - N \) unoccupied.
Want to solve the eigenvalue problem $H|\Psi\rangle = e|\Psi\rangle$ where $|\Psi\rangle = \sum_{i} C_{i}|D_{i}\rangle$

Cast in to a matrix problem diagonalise matrix of $\langle D_{i}|\hat{H}|D_{j}\rangle$

Unfortunately this turns out to be impossibly large: $\binom{M}{N}$ by $\binom{M}{N}$.

Can use Monte Carlo to sample this space.

Little communication overhead, can use massively parallel computers.

Only need to store a stochastic representation of the eigenvector.

Stochastic, quantifiable error (system and dynamics dependent) can be reduced to FCI accuracy by running for longer.

**How quickly does this error converge?**

**Can we find most efficient FCIQMC algorithm? i.e. how can we make the stochastic error converge quickest as a function of computer time?**
Denote the exact solutions (in a finite basis):

$$|\Psi_0\rangle, |\Psi_1\rangle, \ldots, |\Psi_N\rangle \quad (2)$$

with energies:

$$E_0, E_1, \ldots, E_N \quad (3)$$

We can expand our wavefunction in this basis:

$$|\psi\rangle = \sum_{i}^{N} a_i(\tau) |\Psi_i\rangle \quad (4)$$

If we apply the diffusion equation.

$$\frac{\partial |\psi\rangle}{\partial \tau} = -(\hat{H} - E_r \hat{1}) |\psi\rangle \quad (5)$$

and take $\langle \Psi_j |$:

$$\frac{\partial a_j(\tau)}{\partial \tau} = -(E_j - E_r) a_j(\tau) \quad (6)$$

Then:

$$a_j(\tau) = e^{-(E_j - E_r) \tau} a_j(\tau = 0) \quad (7)$$

Excited states die as $\tau \to \infty$ and if $E_r < E_0$ the $|\Psi_0\rangle$ contribution grows.
First discretise our determinant space:

- Positive coefficients are represented by a number of positive psips ($\psi$ particles).
- Negative coefficients are represented by a number of negative psips.

$$|\psi(\tau)\rangle = +0.25 \ |D_0\rangle + 0.5 \ |D_1\rangle - 0.25 \ |D_2\rangle$$

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- Negative coefficients are represented by a number of negative psips.

\[ |\Psi(\tau)\rangle = |D_0\rangle + |D_1\rangle + |D_2\rangle \]

Can move $\tau$ forwards by $\delta\tau$ by applying:

$$e^{-\left(\hat{H} - E_r\hat{1}\right)\delta\tau} \approx \left(\hat{1} - \left(\hat{H} - E_r\hat{1}\right)\delta\tau\right)$$ \hspace{1cm} (8)

FCIQMC stochastically applies Eq. 8 in 3 steps, on each iteration.

1. Spawn
2. Diagonal Death
3. Annihilation

These define the psip population dynamics of FCIQMC.

Thus the ground state wavefunction comes out if we start with a $\psi$ such that $\langle \psi | \hat{H} | \psi \rangle \neq 0$ and run for many steps.
FCIQMC Population Dynamics 1. Spawning

- Each psip attempts to spawn a child psip on a randomly selected determinant.

\[ |\psi(\tau)\rangle = \sum_{0}^{i} |D_i\rangle + \cdots + |D_j\rangle + \cdots \]
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- with probability \( \langle D_i | H | D_j \rangle \delta \tau \)
- if \( \langle D_i | H | D_j \rangle \delta \tau < 0 \) psip has same sign as parent and vice-versa.
Each parent psip attempts to die or is cloned.

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- Death occurs with probability \((\langle D_i|H|D_i \rangle - E_r)\delta\tau\)
- Cloning occurs (population becomes more negative or positive) if \((\langle D_i|H|D_i \rangle - E_r) > 0\)
- \(E_r\) is initially set to the energy of the Hartree-Fock until the psip population reaches the desired level.
- After which \(E_r\) is periodically updated to keep the population at the desired level.
Positive and negative psips residing on the same determinant annihilate:

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Essential so that the step-wise average of psip vector is the eigenvector with smallest eigenvalue of the FCI matrix.

If we use enough psips.

Projected energy:

$$E = \frac{\langle D_0 | \hat{H} e^{\hat{H} \tau} | D_0 \rangle}{\langle D_0 | e^{\hat{H} \tau} | D_0 \rangle} = \frac{\langle D_0 | \hat{H} | \Psi_0 \rangle}{\langle D_0 | \Psi_0 \rangle}$$  \hspace{1cm} (9)

$$\langle D_0 | \hat{H} e^{\hat{H} \tau} | D_0 \rangle$$ equals a factor of:

- $\langle D_0 | H | D_i \rangle$
- $-\langle D_0 | H | D_i \rangle$ sum over every psip, sum over every determinant.

$$\langle D_0 | \Psi_0 \rangle$$ equals the number of psips on the Hartree–Fock.

Average over every step after the simulation has equilibrated.

Need to estimate errors carefully due to serial correlation. As $\delta \tau$ is small the stochastic representation of the eigenvector changes only a small amount between iterations, correlating estimates close in iteration space.
The Initiator Approximation

- Allow only psips on determinants with a population above a threshold (initiator determinants) to spawn onto unoccupied determinants.

\[ |D_i\rangle + \cdots |D_j\rangle \]

- Error bars converge faster and we need fewer psips.

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Part II

How can we use current algorithms most effectively
In FCIQMC more psips equivalent to more steps in terms of computer time.

\(\mathcal{O}(l \log l)\) sorting of newly spawned psips before of annihilation is negligible (length of list to sort).

Fits to \(\frac{c}{N_p}\) shown (\(N_p\) number of psips).

What about the error bar?

Is it better to run for more steps or use more psips (which is a better use of resources)?
For any Monte Carlo algorithm the stochastic error (in some expectation value of the simulation) as a function of the number of steps $N$:

$$\sigma = \frac{a}{\sqrt{N}}$$  \hspace{1cm} (10)

So can use $a$ to quantify the efficiency of FCIQMC, provided no systematic error is introduced.

Small $a$ is good, errors converge fast.
\[ \sigma = \frac{a}{\sqrt{N_s}} \]  

(11)

- How does \( a \) depend on the number of psips \( N_p \) in the simulation (\( N_s \) number of iterations).

- One should fill the memory with psips if \( a \to 0 \) faster than \( O\left(\frac{1}{\sqrt{N_p}}\right) \).

- For FCIQMC, \( a \) decays faster than \( O\left(\frac{1}{\sqrt{N_p}}\right) \), for i-FCIQMC seems to decay as \( b\sqrt{N_p} \) meaning more psips equivalent to more iterations.
Empirical Results: Scaling with the number of psips 2

\[
\sigma = \frac{a}{\sqrt{N_s}}
\]  

(12)

Other systems show similar results.
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(13)

- Other systems show similar results.
Conclusions

- For calculations with the initiator approximation more psips is equivalent to more steps in terms of $\sigma(E)$.
- For other systems the error decreases faster as the number of psips increase getting closer to the initiator limit.
- At the limit of a large number of psips, trivial parallelism mode (running multiple independent simulations).
- We now have a way of comparing different Monte Carlo algorithms.
Part III

Novel Hardware
Field Programmable Gate Arrays (FPGA’s)

- A programmable grid of logic components.
- Components can be grouped and connected so that each group performs an operation and passes it too the next group each clock cycle.
- Sending data back up the chip can be tricky as we have to meet timings.
- Clock rate of $\sim 100$ MHz c.f. CPU $\sim 1000$ MHZ.

![Diagram of FPGA and DRAM connections](image-url)
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![FPGA DRAM Diagram](image)
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![Diagram showing data flow through FPGA components.](image_url)
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![Diagram of FPGA and DRAM with arithmetic operations and clock rates](image_url)
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The psip vector makes a good candidate for streaming through the FPGA.

- Diagonal death $O(L)$ and spawning $O(N_p)$. Where $L$ is the length of psip vector.
- Annihilation requires sorting the newly spawned psips $O(l \log l)$
- Efficient sorting tricky.
- Send to CPU for sort.
- Currently investigating the Hubbard model (can store the integrals on chip as they have a simple structure).
FCIQMC on FPGA's

- FPGA DRAM
  - Annihilate
    - Diagonal Death
    - Spawn
      - Quick Sort on CPU
Conclusions and Directions

- Move to multiple FPGAs and CPUs.
- Investigate the Hubbard Model and quantify speed up.
- Real chemical systems require access of the integrals to generate the matrix elements, this will be tricky.
- It may be more efficient for all psips on a determinant to spawn at once Diagonal Death and spawning both $O(L)$.
- Is this version more efficient for an FPGA? (Work in progress)
Acknowledgements

- Alex Thom, Michael Bearpark, James Spencer.
- EPSRC for a studentship.
- Stephen Girdlestone, Craig Davies, and Robin Bruce at Maxeler Technologies
- All calculations ran using HANDE (developed at Imperial College) and the Imperial College High Performance Computing Service.
As $\tau$ is small the vector of psips only changes a small amount between iterations.

Thus expectation values close in iteration space are correlated.

One has to remove this serial correlation by blocking:
Average into blocks and compute standard error of blocks.

We used the Iterative algorithms for optimal block size in: