Accelerating Full Configuration Interaction Quantum Monte Carlo

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Part I

Introduction: The Full Configuration Interaction Quantum Monte Carlo Algorithm

Solving the Schrödinger Equation in a Basis of Slater Determinants

- 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 $|D_{\mathbf{0}}\rangle$.
- Full Configuration Interaction (FCI) adds into $|\Psi\rangle$ all possible determinants $|D_{\mathbf{I}}\rangle$ with N MSO occupied and $M - N$ unoccupied .

Full Configuration Interaction

- Want to solve the eigenvalue problem $H|\Psi\rangle = e|\Psi\rangle$ where $|\Psi\rangle = \sum_I C_{\mathbf{I}}|D_{\mathbf{I}}\rangle$
- Cast in to a matrix problem diagonalise matrix of $\langle D_{\mathbf{I}}|\hat{H}|D_{\mathbf{J}}\rangle$
- Unfortunately this turns out to be impossibly large: $\binom{M}{N}$ by $\binom{M}{N}$.
- **Can use Monte Carlo to sample this space.**

G. H. Booth, A. J. W. Thom, A. Alavi, J. Chem. Phys. **131**, 054106 (2009)

Full Configuration Interaction Quantum Monte Carlo (FCIQMC) vs FCI

- 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?**

Full Configuration Interaction Quantum Monte Carlo: Projector

- Denote the exact solutions (in a finite basis):

$$|\Psi_0\rangle, |\Psi_1\rangle, \ldots |\Psi_N\rangle \tag{2}$$

with energies:

$$E_0, E_1, \ldots, E_N \tag{3}$$

We can expand our wavefunction in this basis:

$$|\psi\rangle = \sum_i^N a_i(\tau)|\Psi_i\rangle \tag{4}$$

If we apply the diffusion equation.

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

and take $\langle\Psi_j|$:

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

Then:

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

Excited states die as $\tau \to \infty$ and if $E_r < E_0$ the $|\Psi_0\rangle$ contribution grows.

Full Configuration Interaction Quantum Monte Carlo: Discretised Determinant Space

First discretise our determinant space:

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

$$|\Psi(\tau)\rangle = \quad +0.25 \quad |D_{\mathbf{0}}\rangle \quad +0.5 \quad |D_{\mathbf{1}}\rangle \quad -0.25 \quad |D_{\mathbf{2}}\rangle$$

J . B. Anderson J. Chem. Phys. **63**, 1499 (1975)

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

J . B. Anderson J. Chem. Phys. **63**, 1499 (1975)

Full Configuration Interaction Quantum Monte Carlo

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

$$e^{-(\hat{H}-E_r\hat{1})\delta\tau} \approx (\hat{1} - (\hat{H} - E_r\hat{1})\delta\tau) \tag{8}$$

- 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 ψ 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.

$$|\Psi(\tau)\rangle = \text{●} |D_0\rangle + \cdots \begin{matrix}\text{●}\\\text{●}\\\text{●}\end{matrix} |D_{\mathbf{i}}\rangle + \cdots \text{●} |D_{\mathbf{j}}\rangle + \cdots$$

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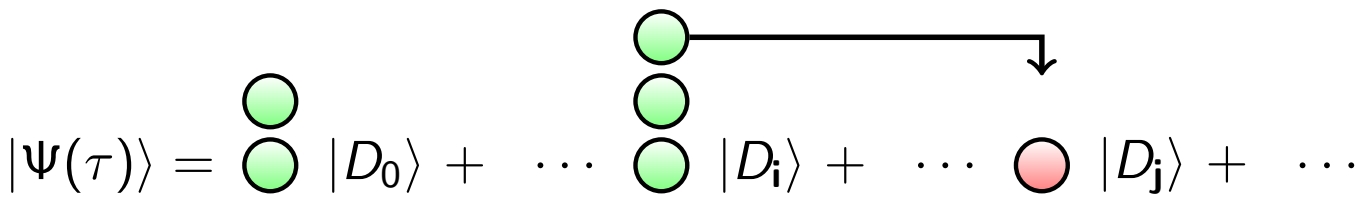

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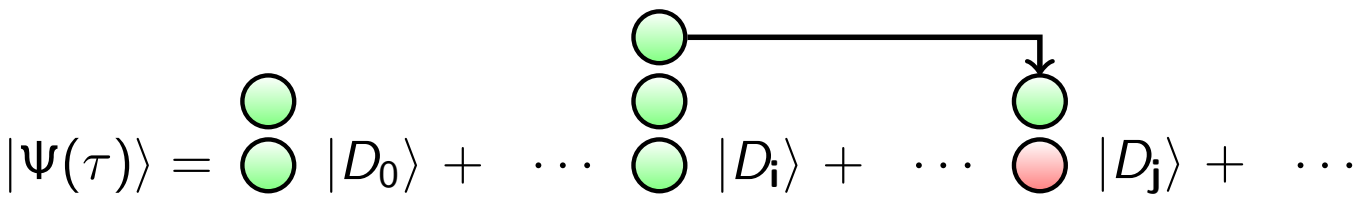
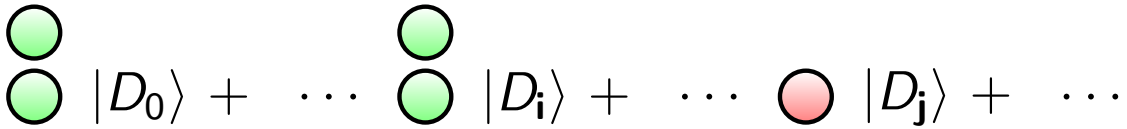


- with probability $(\langle D_\mathbf{i}|H|D_\mathbf{j}\rangle)\delta\tau$
- if $(\langle D_\mathbf{i}|H|D_\mathbf{j}\rangle)\delta\tau < 0$ psip has same sign as parent and vice-versa.

FCIQMC Population Dynamics 2. Diagonal Death

- Each parent psip attempts to die or is cloned.

$$|\Psi(\tau)\rangle = \quad |D_0\rangle + \quad \cdots \quad |D_{\mathbf{i}}\rangle + \quad \cdots \quad |D_{\mathbf{j}}\rangle + \quad \cdots$$



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- Death occurs with probability $(\langle D_{\mathbf{i}}|H|D_{\mathbf{i}}\rangle - E_r)\delta\tau$
- Cloning occurs (population becomes more negative or positive) if $(\langle D_{\mathbf{i}}|H|D_{\mathbf{i}}\rangle - E_r) > 0$
- 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.

FCIQMC Population Dynamics 3. Annihilation

- Positive and negative psips residing on the same determinant annihilate:

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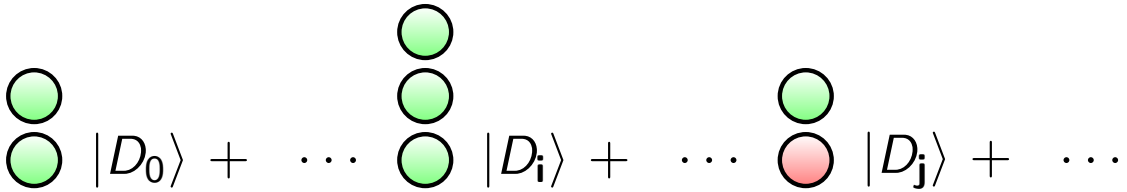

J. S. Spencer, N. S. Blunt, and W. M. C. Foulkes J. Chem. Phys. **136**, 054110 (2012)

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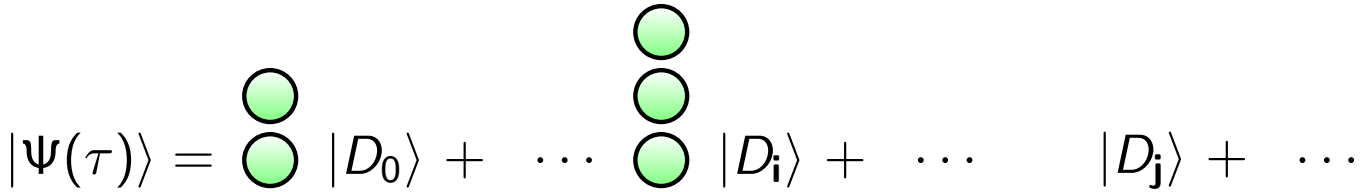

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- Essential so that the step-wise average of psip vector is the eigenvector with smallest eigenvalue of the FCI matrix.
- If we use enough psips.

J. S. Spencer, N. S. Blunt, and W. M. C. Foulkes J. Chem. Phys. **136**, 054110 (2012)

Accumulating Expectation Values

- Projected energy:

$$E = \frac{\langle D_0|\hat{H}e^{\hat{H}\tau}|D_0\rangle}{\langle D_0|e^{\hat{H}\tau}|D_0\rangle} = \frac{\langle D_0|\hat{H}|\Psi_0\rangle}{\langle D_0||\Psi_0\rangle} \tag{9}$$

- $\langle D_0|\hat{H}e^{\hat{H}\tau}|D_0\rangle$ equals a factor of:
  - $\langle D_\mathbf{0}|H|D_\mathbf{i}\rangle$
  - $-\langle D_\mathbf{0}|H|D_\mathbf{i}\rangle$

  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.

- Error bars converge faster and we need fewer psips.

D. Cleland, G. H. Booth, A. Alavi J. Chem. Phys. **132**, 041103 (2010)

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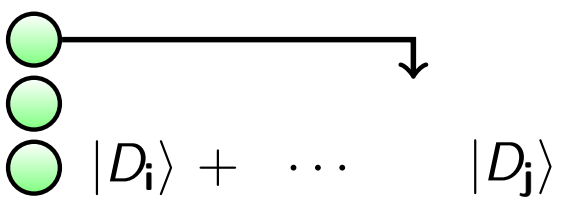

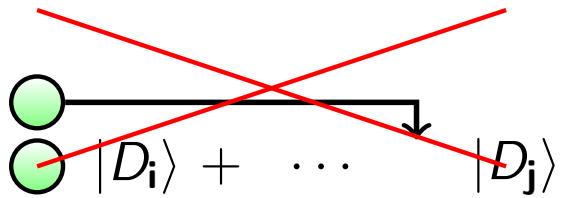

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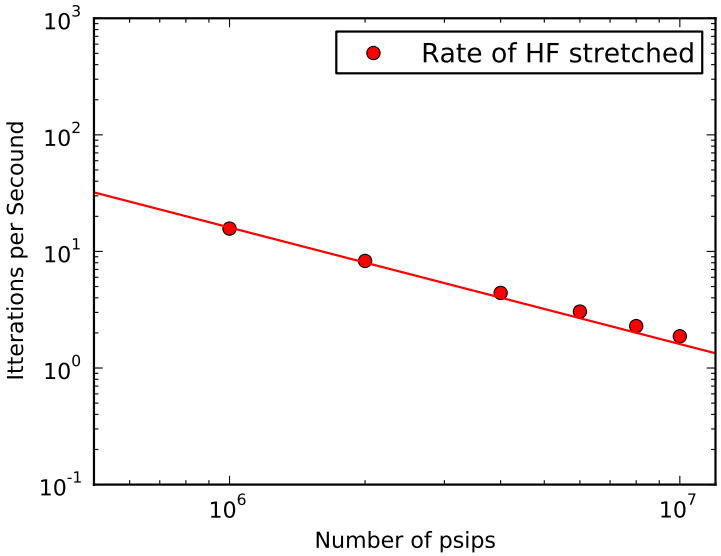
Part II

How can we use current algorithms most effectively

Computer time as a function of the number of psips

- 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 (l length of list to sort).
- Fits to $\frac{c}{N_p}$ shown (N_p number of psips).



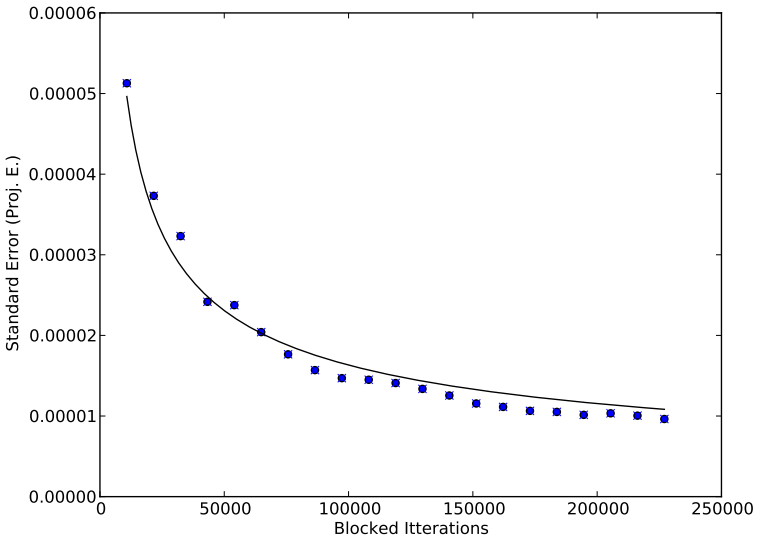
- What about the error bar?
- Is it better to run for more steps or use more psips (which is a better use of resources)?

Quantifying Efficiency Empirically 1

- For any Monte Carlo algorithm the stochastic error (in some expectation value of the simulation) as a function of the number of steps N :

$$\sigma = \frac{a}{\sqrt{N}} \qquad (10)$$

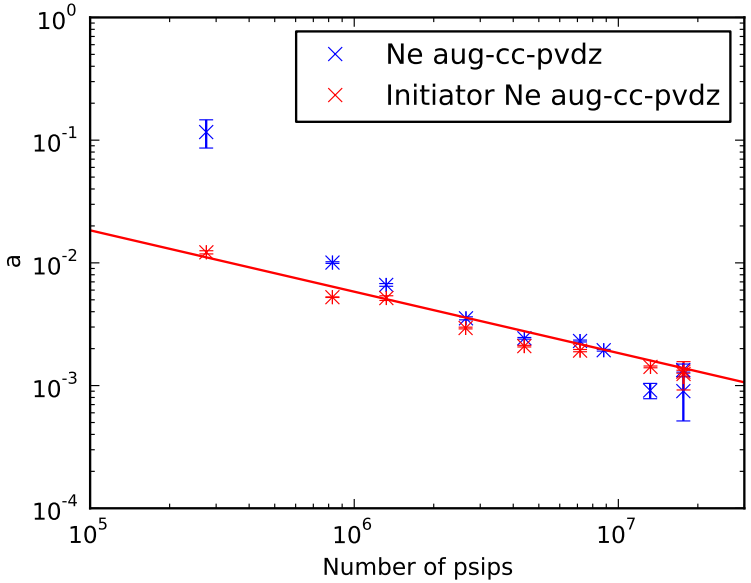
- So can use a to quantify the efficiency of FCIQMC, provided no systematic error is introduced.
- Small a is good, errors converge fast.



Empirical Results: Scaling with the number of psips 1

$$\sigma = \frac{a}{\sqrt{N_s}} \qquad (11)$$

- How does a depends 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 $\mathcal{O}(\frac{1}{\sqrt{N_p}})$.

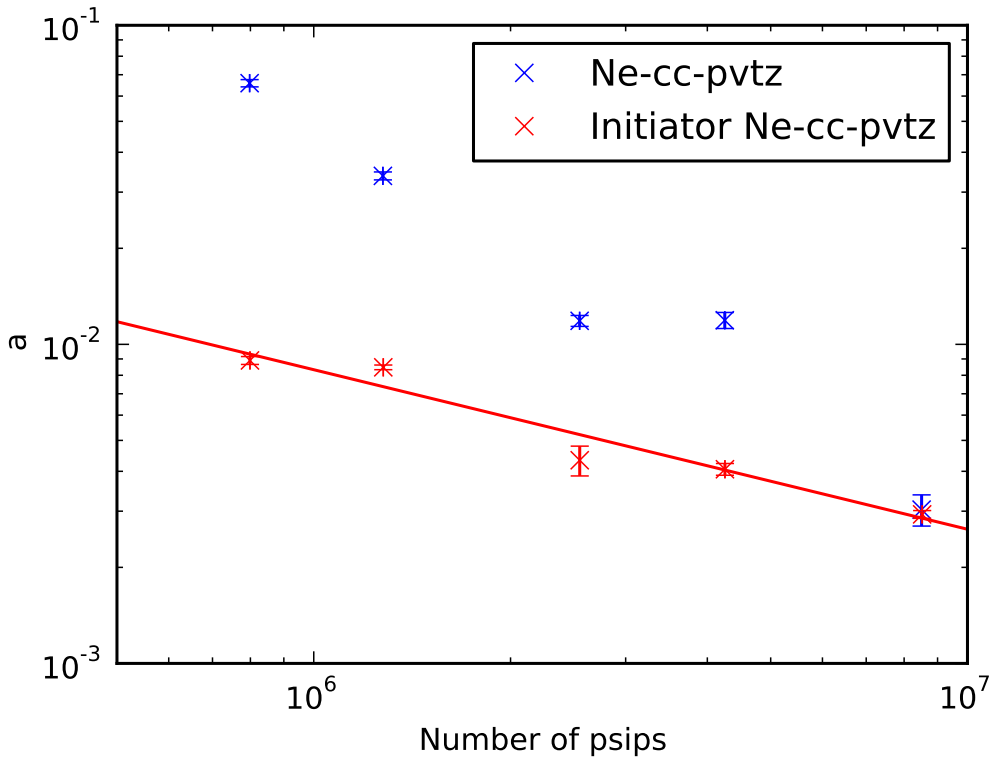


- For FCIQMC a decays faster than $\mathcal{O}(\frac{1}{\sqrt{N_p}})$, for i-FCIQMC seems to decay as $b\sqrt{N_p}$ meaning more psips equivalent to more iterations.

Empirical Results: Scaling with the number of psips 2

$$\sigma = \frac{a}{\sqrt{N_s}} \tag{12}$$

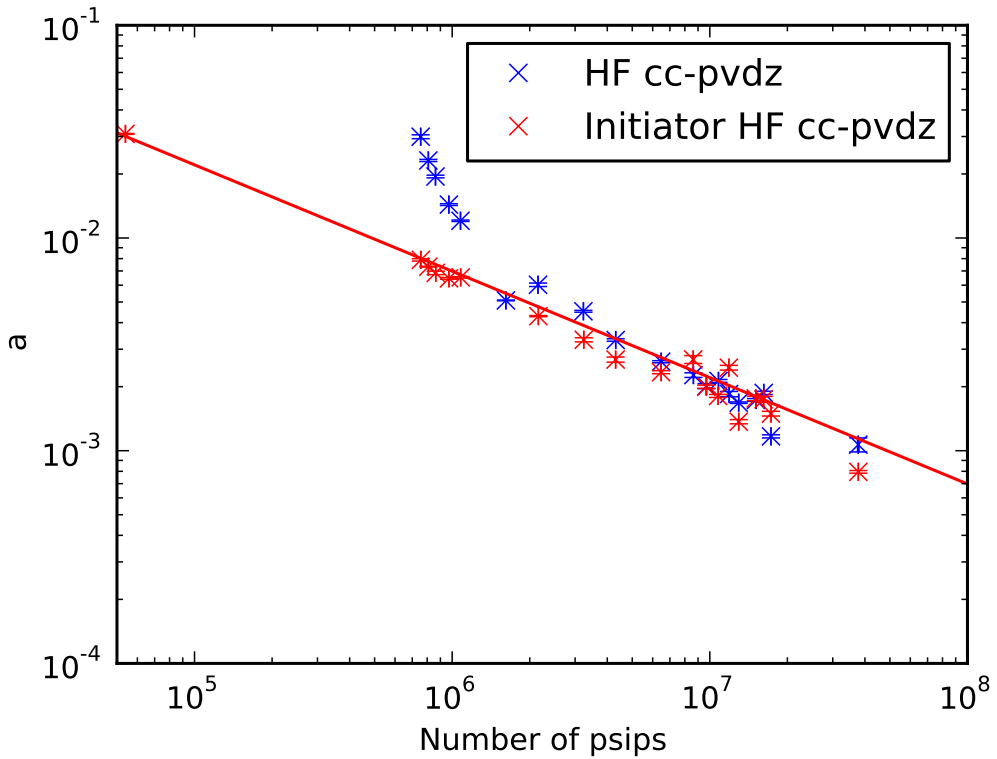
- Other systems show similar results.



Empirical Results: Scaling with the number of psips 3

$$\sigma = \frac{a}{\sqrt{N_s}} \tag{13}$$

- Other systems show similar results.



Conclusions

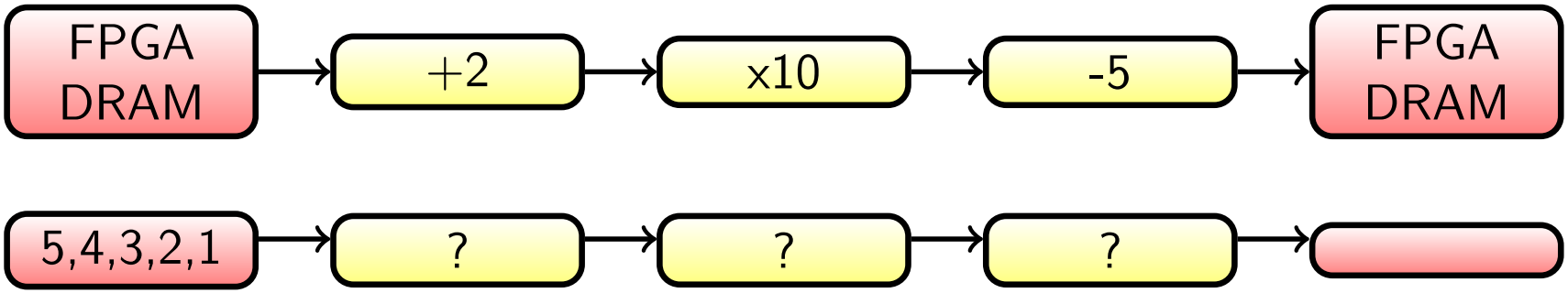
- For calculations with the initiator approximation more psips is equivalent to more steps in terms of $\sigma(E)$.
- For other systems the error decreases faster as the number of psips increase getting closer to the initiator limit.
- At the limit of a large number of psips, trivial parallelism mode (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 .



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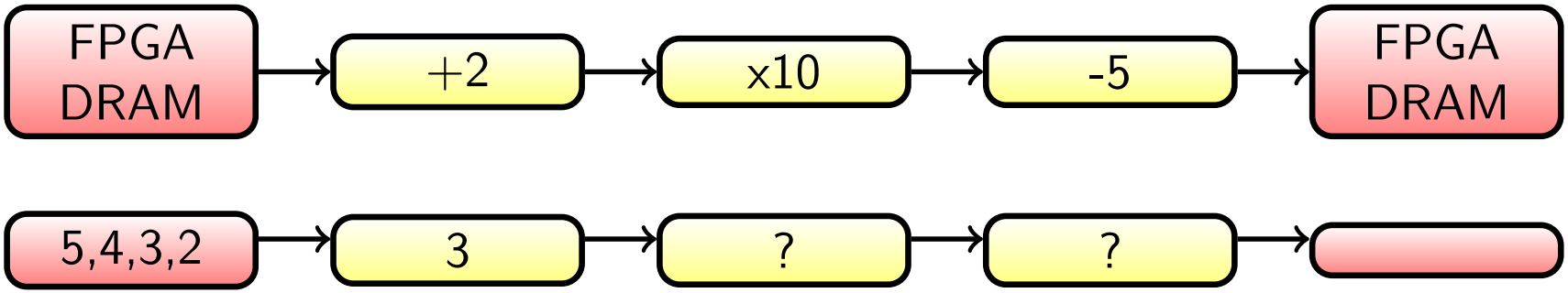

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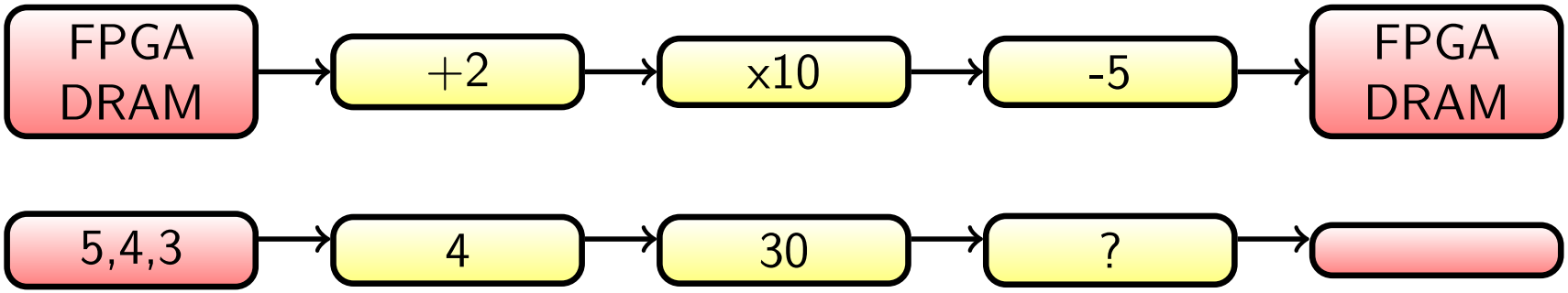

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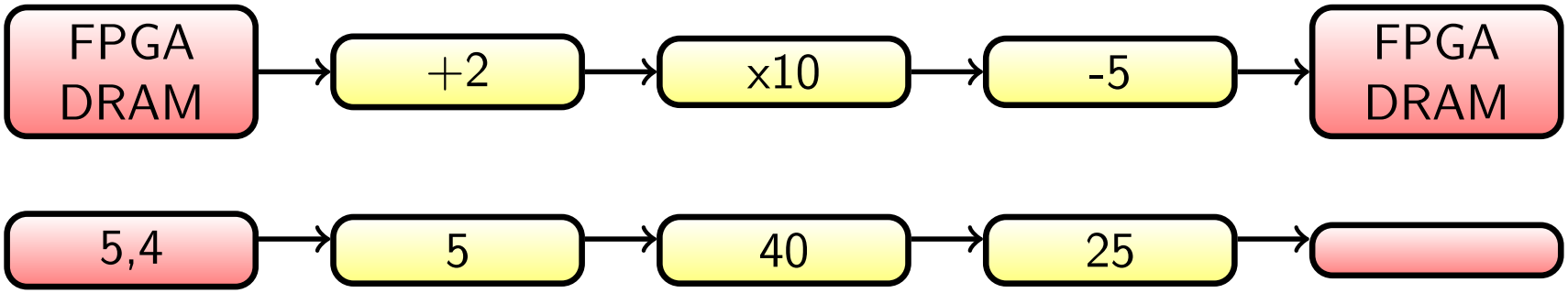

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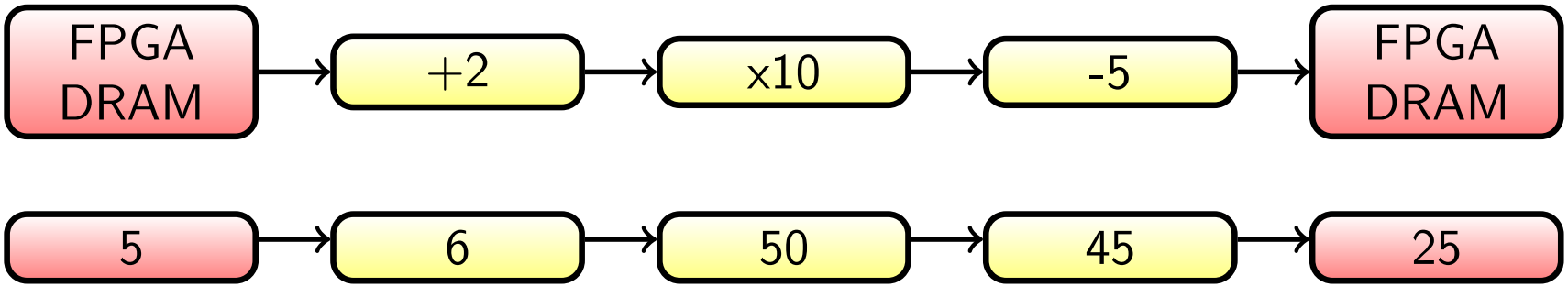

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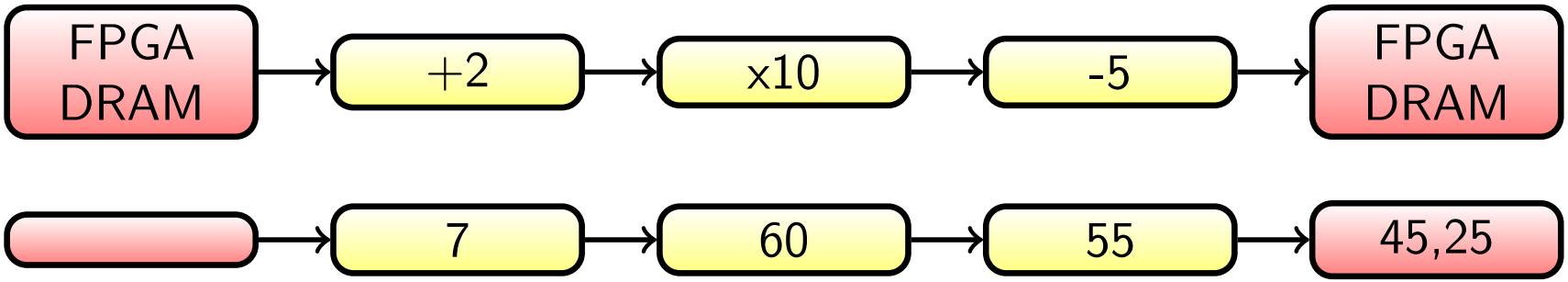

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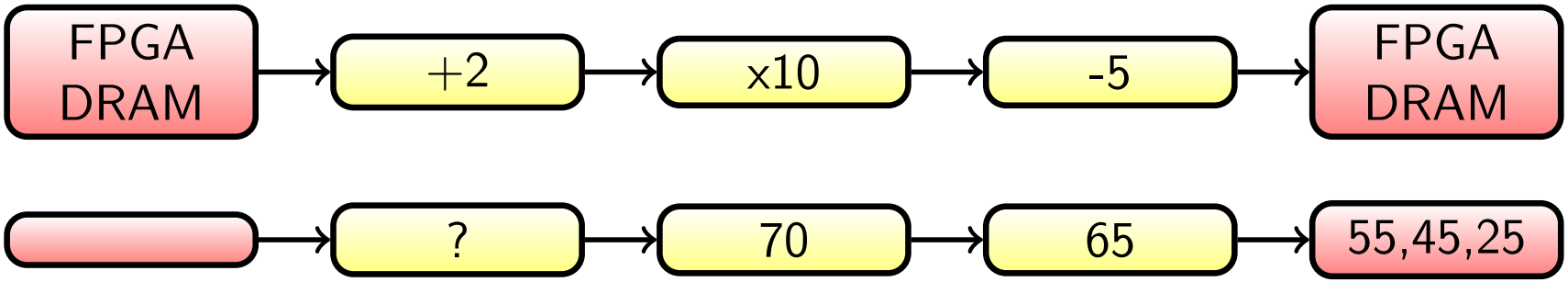

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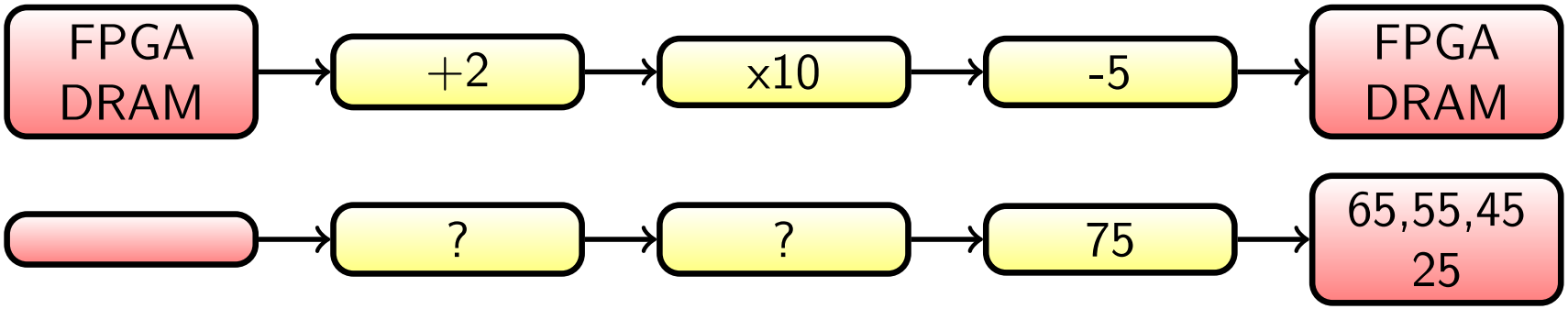

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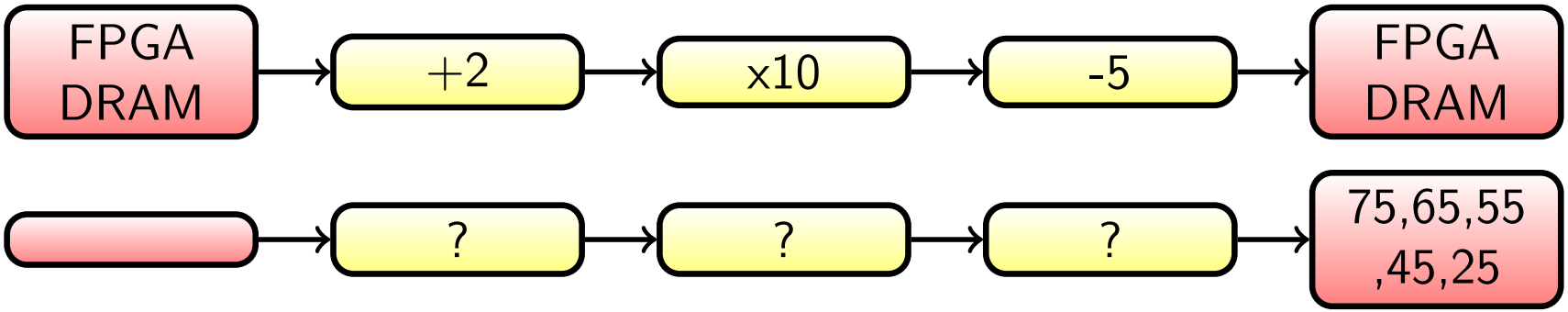
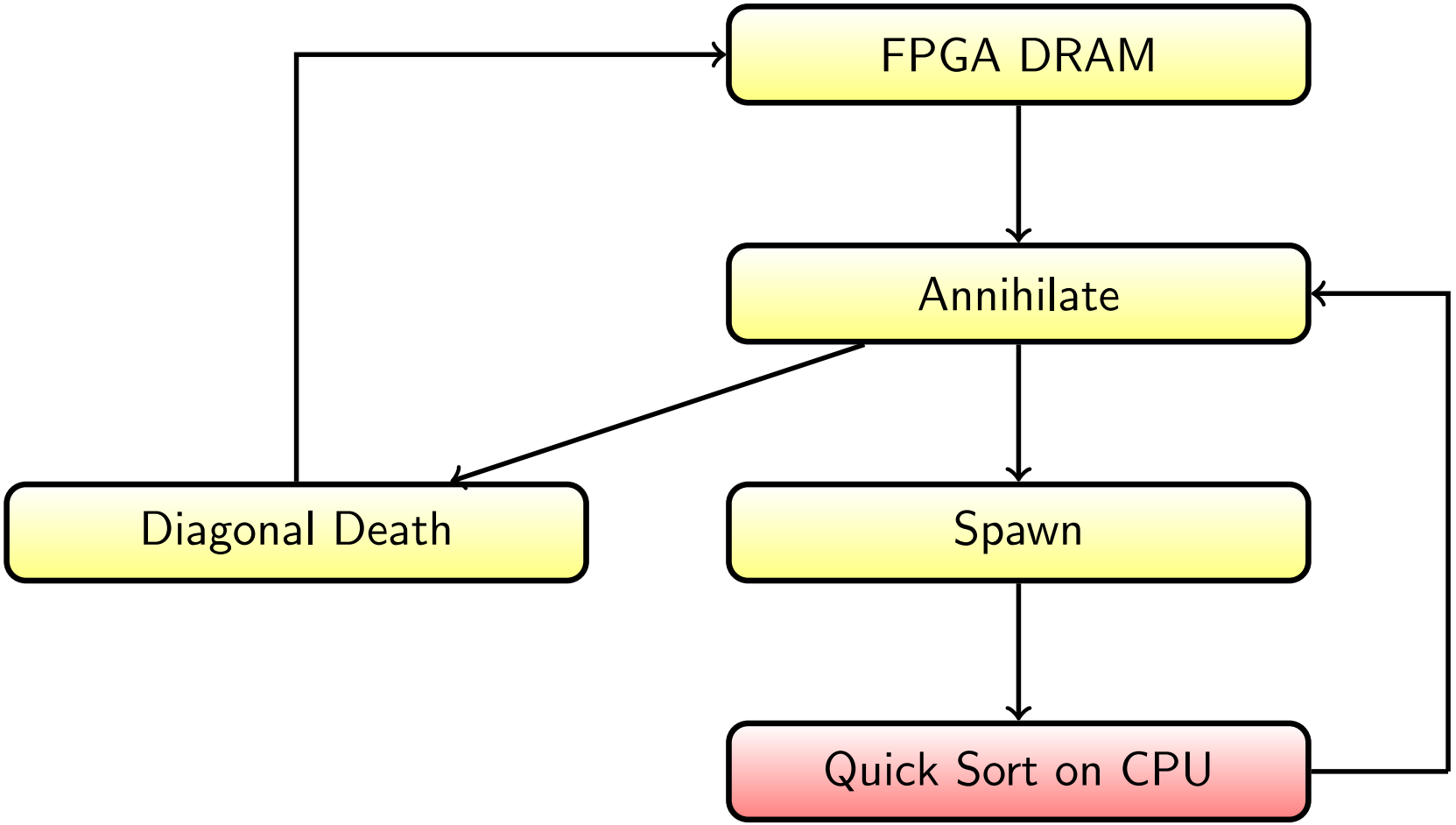


FCIQMC on FPGA's

- The psip vector makes a good candidate for streaming through the FPGA.
- Diagonal death $\mathcal{O}(L)$ and spawning $\mathcal{O}(N_p)$. Where L is the length of psip vector.
- Annihilation requires sorting the newly spawned psips $\mathcal{O}(l \log l)$
- 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



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 $\mathcal{O}(L)$.
- Is this version more efficient for an FPGA ? (Work in progress)

Acknowledgements

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Serial Correlation

- As τ 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:
  R. M. Lee, G. J. Conduit, N. Nemec, P. López Ríos, N. D. Drummond, Phys. Rev. E **83**, 066706 (2011)