Parallel Strategies for FCIQMC

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- Can treat Hilbert spaces orders of magnitude larger than exact diagonalisation.
- Relatively straightforward to parallelise.
- It scales to 1000s of cores so we can use big computers.

Big Computers

Archer: 2014, cray XC30, 76000 cores, 1.5 petaflops, £43, 000, 000

www.archer.ac.uk

Big Computers

Fionn: 2014, 7600, 147 teraflops, € 3.7,000,000

www.ichec.ie

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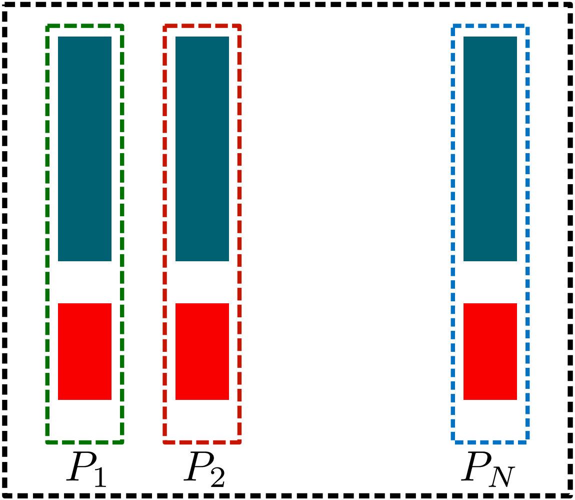
- Two of the biggest barriers to improved scaling are load imbalances and communication overhead.
- The use of non-blocking communications and improved load balancing was successful for CASINO (Gillan, Towler, Alfe) so can we use similar ideas here?

Parallel Strategies

Parallel Implementation (Booth, Smart, Alavi 2014)

- Distribute list of occupied determinants across all processors.

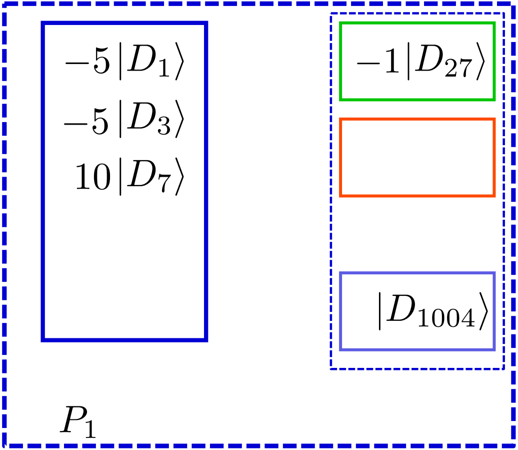


Parallel Implementation

- Each processor evolves main list and spawn into spawned walker list.

$$p_{\text{spawn}}(i|j) \propto \Delta\tau |H_{ij}|$$

$$p_{\text{die/clone}}(i|i) \propto \Delta\tau |H_{ii} - S|$$



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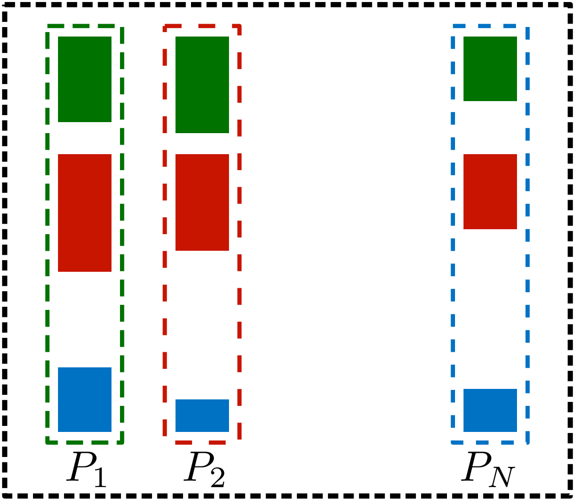
- Communicate spawned array using MPIAlltoAllv.



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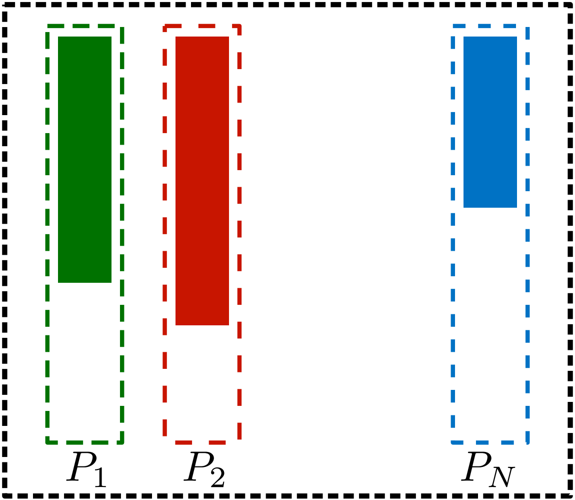

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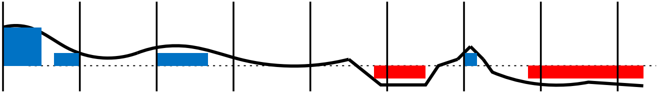

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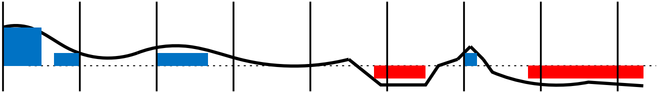

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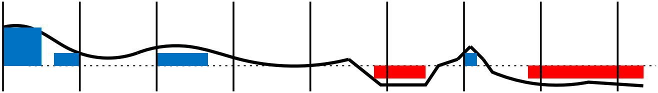
$|\Psi\rangle =$ 

- Use a hash function to randomise procedure somewhat.
- Assign determinant to processor as $p = \text{hash}(|D_i\rangle)\text{mod}N_p$, $\text{hash}(x) = a, a \in [0, N_{\max})$.

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- Can we do better?

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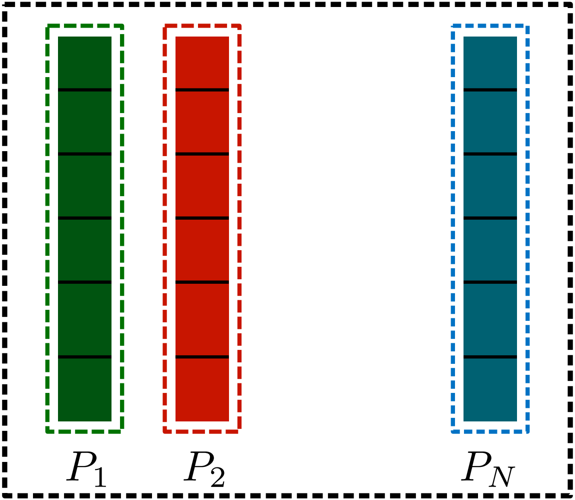


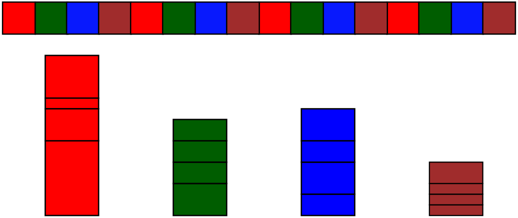
Load Balancing

Procedure:

1. Find processors with populations either above (P_i^d) or below (P_i^r) the ideal average walker population ($N_{\rm av} \pm \delta$).
2. Sort list of donor bins in increasing order of bin size.
3. Redistribute donor bins to receiver processors while $N_w(P_i^{\rm d}) \geq N_{\rm av} - \delta$ and $N_w(P_i^r) \leq N_{\rm av} + \delta$.

Picture

- Define array $p_{\text{map}}[i] = (0, 1, \dots, N_p, 0, \dots, N_p, \dots)$. So, $P(|D_i\rangle) = p_{\text{map}}[\text{hash}(|D_i\rangle)\text{mod}(N_p \times M)]$



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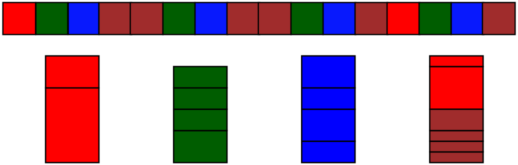
- Just modify entries in p_{map} so processors are mapped to new processor in the future.



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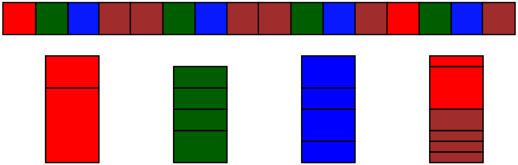

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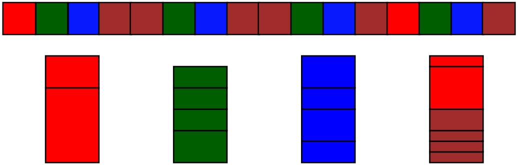

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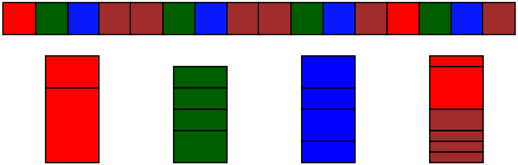

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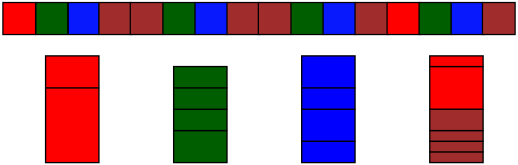

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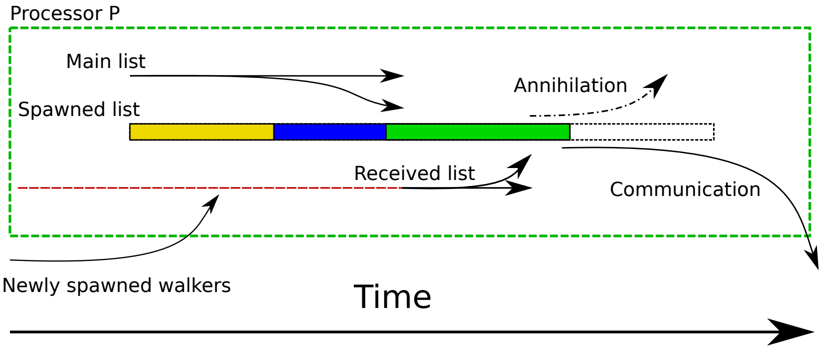
Non-Blocking algorithm

- Evolve main list to $\tau + \Delta\tau$ (receiving spawned walkers in background)
- Complete receive
- Evolve walkers spawned onto current processor to $\tau + \Delta\tau$
- Non-blocking send of walkers to their new processors.
- Annihilate walkers on current processor

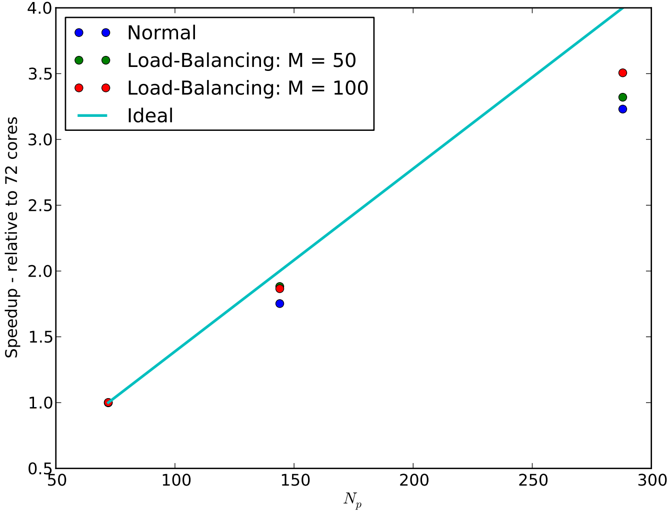
Picture


Processor P
Main list
Annihilation
Spawned list
Received list
Communication
Newly spawned walkers
Time

Test Case

- 18-site Hubbard model in momentum space basis.
- 86 million psips occupying 61.2 million determinants
- Run for 20000 iterations

Preliminary results: Load Balancing



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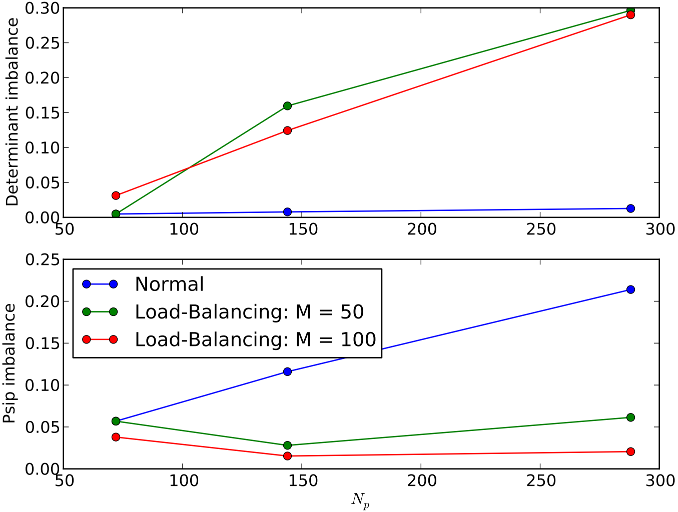
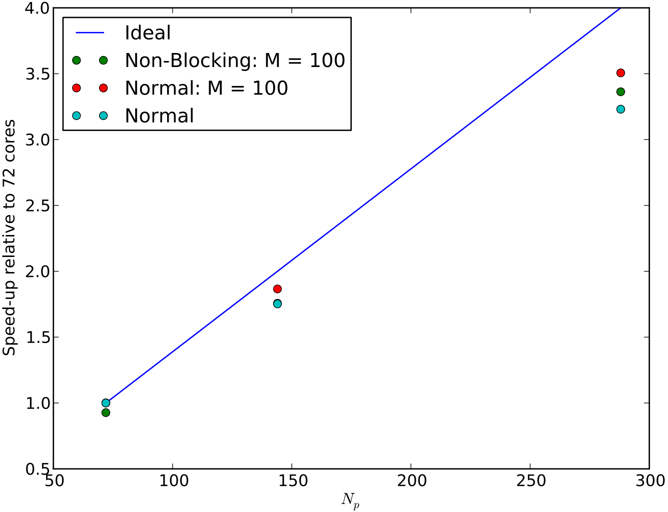


Preliminary results: Load Balancing + Non-Blocking



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- Next step run on larger computers - 1000s of cores.

Acknowledgemets

James Spencer & HANDE development team
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