Optimization and Parallelization of Determinant Quantum Monte Carlo

- A. Traditional $o(N^3)$ Determinant Quantum Monte Carlo
- B. Status of Existing Code
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- D. Desired Interactions
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- F. Bai's Talk: $o(N)$ Hybrid Quantum Monte Carlo

A. Traditional $o(N^3)$ Determinant Quantum Monte Carlo

Goal: evaluate

$$
\begin{aligned}
\langle \hat{A} \rangle &= Z^{-1} \, \mathrm{Tr} \, [\hat{A} \, e^{-\beta \hat{H}}] \\
Z &= \mathrm{Tr} \, e^{-\beta \hat{H}}
\end{aligned}
$$

- $\hat{H}$ is the Hamiltonian expressed in terms of fermion creation and destruction operators $c^\dagger_{l\sigma}, c_{l\sigma}$.
- "Tr" is a trace over the 4^N dimensional Hilbert space.
- N is the number of sites.
- Each site $\quad |\cdot\rangle \quad |\uparrow\rangle \quad |\downarrow\rangle \quad |\uparrow\downarrow\rangle$.

Theorem for trace if $\hat{H}$ is *quadratic* in fermion operators:

$$
\hat{H} = \begin{pmatrix} c^\dagger_{1\sigma} & c^\dagger_{2\sigma} & . & . \end{pmatrix} \begin{pmatrix} h_{11} & h_{12} & . & . \\ h_{21} & h_{22} & . & . \\ . & . & . & . \\ . & . & . & . \end{pmatrix} \begin{pmatrix} c_{1\sigma} \\ c_{2\sigma} \\ . \\ . \end{pmatrix} .
$$

Here h is an NxN matrix of numbers.

The identity is:

$$Z = \mathrm{Tr}\, e^{-\beta \hat{H}} = \det[I + e^{-\beta h}].$$

- "Tr" over a quantum mechanical 4^N dim Hilbert space.
- "det" is a usual determinant of NxN matrices.
- "I" is the N dimensional identity matrix
- "h" is the matrix of *numbers* entering $\hat{H}$.

More general identity: *set* of quadratic $\hat{H}(l)$, $l = 1, 2, \ldots L$:

$$Z = \mathrm{Tr}\,[e^{-\hat{H}(1)} \ldots e^{-\hat{H}(L)}] = \det[\, I + e^{-h(1)} \ldots e^{-h(L)}].$$

In addition, "Green's function",

$$\begin{aligned} G_{ij} = \langle c_{i\sigma} c^{\dagger}_{j\sigma} \rangle &= Z^{-1}\, \mathrm{Tr}\,[c_{\,i\sigma} c^{\dagger}_{j\sigma}\; e^{-\hat{H}(1)} \ldots e^{-\hat{H}(L)}\,] \\ &= [\, I + e^{-h(1)} \ldots e^{-h(L)}\,]^{-1}_{ij} \quad . \end{aligned}$$

Electron-electron interactions $U n_{i\uparrow} n_{i\downarrow} = U c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$
(Discrete) Hubbard–Stratonovich transformation,

$$e^{-U\Delta\tau(n_\uparrow - \frac{1}{2})(n_\downarrow - \frac{1}{2})} = \frac{1}{2} e^{-\frac{U\Delta\tau}{4}} \sum_S e^{\lambda S(n_\uparrow - n_\downarrow)}$$

$\cosh\lambda = e^{U\Delta\tau/2}$, and $S = \pm 1$.
Isolate interactions: divide $\beta = L\Delta\tau$
$\hat{H} = \hat{K} + \hat{V}$ where $\hat{K}$ quadratic (kinetic), $\hat{V}$ interactions.
Trotter decomposition:

$$Z = \mathrm{Tr}\, e^{-\beta\hat{H}} \approx \mathrm{Tr}\left[e^{-\Delta\tau\hat{K}} e^{-\Delta\tau\hat{V}} \ldots e^{-\Delta\tau\hat{K}} e^{-\Delta\tau\hat{V}} \right] \,.$$

$e^{-\Delta\tau\hat{K}}$ quadratic
Each $e^{-\Delta\tau\hat{V}}$: N Hubbard–Stratonovich variables, S_{il}
- space i, imaginary–time l.

$e^{-\Delta\tau V_l}$ now quadratic.
V_l: different Hubbard–Stratonovich variables for each l.

Summary:

$$Z = \sum_{S_{il}} \det M_{\uparrow} \, \det M_{\downarrow}.$$

- Determinant for each of the two spin species.
- *Classical* monte carlo problem.
- Sum over real, classical, variables S_{il}.
- "Boltzmann weight": product of two determinants.

Explicit forms of matrices ($d = 1$ Hubbard model):

$$M_\sigma = I + e^{-k} e^{-v_{\sigma,1}} e^{-k} e^{-v_{\sigma,2}} \ldots e^{-k} e^{-v_{\sigma,L}}.$$

$$k = -\Delta\tau \begin{pmatrix} \mu & t & 0 & \cdots \\ t & \mu & t & \cdots \\ 0 & t & \mu & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \qquad v_{\sigma,l} = \lambda\sigma \begin{pmatrix} S_{1l} & 0 & 0 & \cdots \\ 0 & S_{2l} & 0 & \cdots \\ 0 & 0 & S_{3l} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Most primitive determinant QMC code:

- Initialize Hubbard-Stratonovich S_{il} (eg randomly).
- Compute matrices M_σ and determinants.
- Change S_{il}. Compute new M'_σ and determinants.
- Metropolis: Accept if $r < \det M' / \det M \qquad 0 < r < 1$.
- Repeat. Measure G_{ij} (M^{-1}_{ij}) and other observables.
- Scaling is $o(N^4 L)$. NL variables S_{il}. Each update $o(N^3)$.

Improvements/Subtleties:

- $\det M'/\det \mathrm{M} = \det(I + G\, dM)$.
  dM rank one update. CPU time independent of N and L!
  Need to recompute $G = M^{-1}$. Rank one update: $o(N^2)$.
  Scaling now $o(N^3 L)$.
- Round off errors/numerical instabilities (well understood).
  Product of matrices in constructing M.
  Repeated updates of G.
- Negative determinants/Sign problem.
- Dynamical measurements/observables generally.

B. Status of Existing Code

(Focussing on issues to address.)

- "Legacy code": 20 yrs, many authors, little documentation.
- f77; about 4000 lines
- Little (no?) work on optimization.
  WHY?!
  Bai/Schram "handwritten" linear algebra $\longrightarrow$ blas/lapack
- Serial.
- $N \approx 100 = 10 \times 10$ (Mostly $d = 2$); $\quad L \approx 100$.
- Number of Monte Carlo sweeps $\approx 10^4$.
  Number of determinant evaluations $\approx 10^8$.
- Important Note: Many versions.

C. Goals in Next Year

Address these issues!

[1.] Continued optimization (begun with blas/lapack)

[2.] New numerical tricks

"Delayed updating"

Improve measurements of τ dependent observables.

[3.] Parallelize.

$\longrightarrow$ Determinant QMC simulations at tera/petascale!

Simulations on $N = 32 \times 32$ lattices.

$o(N^3)$ scaling: cpu $o[(3.2)^6 \approx 10^3]$ increase (minimally).

Important Issues:

To what extent do we "start over"? (I think, not much).

How do we deal with multiple versions?

D. Desired Interactions

[1.] Continued optimization
   Scidac staff, D'Azevedo, Tomko, postdoc

[2.] New numerical tricks
   "Delayed updating"
   Jarrell, D'Azevedo, Maier, postdoc
   Improve measurements of τ dependent observables.
   Jarrell, Batrouni, D'Azevedo, postdoc
   Look for further ideas?
   Tomko, D'Azevedo

[3.] Parallelize: Library of equilibrated configurations?
   Postdoc, others?

Physics:

Jarrell, Maier, Savrasov, Varney, Macridin, Moritz,... ?

Magnetism/Mott behavior, esp. Triangular lattices

E. Hiring

UC Davis postdoc

Primary area of expertise?

Coding and applied mathematics

Second UCD postdoc (since no hiring in year one)?

ORNL postdoc: Pay through UCD.

Our administrative staff needs to be in loop.

How to get good people (nontrivial!)?