An overview of the HANDE QMC project

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http://www.hande.org.uk
Highly Accurate N-DEterminant QMC

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Stochastic diagonalisation

Stochastic coupled cluster

Software development

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Systems

Hubbard model
Systems

Hubbard model

Heisenberg model
Systems

Hubbard model

Heisenberg model

uniform electron gas
Systems

Hubbard model

Heisenberg model

uniform electron gas

benzene...
Outline

Stochastic diagonalisation

Stochastic coupled cluster

Software development
FCIQMC

Stochastically evolve $\frac{\partial \Psi}{\partial \tau} = -\hat{H}\Psi$.

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$^1$Booth, Thom, Alavi, JCP 131 054106 (2010); JSS, Blunt, Foulkes, JCP 136 054110 (2012)
Semi-stochastic Projection

Deterministically evolve core subspace.
Stochastically evolve remainder of Hilbert space.

\[ \text{Figure: Energy vs. } \tau \text{/hartrees}^{-1} \]

\[ E \text{/hartrees} \]

\[ \text{discrete, real, real + semi-stochastic} \]

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Hellmann–Feynman sampling

\[ \hat{H}(\lambda) = \hat{H} + \lambda \hat{O} \implies \langle \hat{O} \rangle = \frac{\partial E(\lambda)}{\partial \lambda} \bigg|_{\lambda=0}. \]

→ Sample \( \frac{\partial \Psi}{\partial \tau \partial \lambda} \bigg|_{\lambda=0}. \)
Density Matrix Quantum Monte Carlo\textsuperscript{4}

Stochastically evolve \( \frac{\partial \rho}{\partial \beta} = -\hat{H} \rho = -\frac{1}{2} \{ \hat{H}, \rho \} \).
Outline

Stochastic diagonalisation

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Coupled Cluster Monte Carlo\textsuperscript{5}

Stochastically evolve $\frac{\partial \Psi}{\partial \tau} = -\hat{H}\Psi$.

\[
\Psi = e^{\hat{T}} |\text{HF}\rangle ; \quad \hat{T} = \sum_{ia} t^a_i \hat{c}_a \hat{c}_i + \frac{1}{2} \sum_{ijab} t^{ab}_{ij} \hat{c}_a \hat{c}_b \hat{c}_j \hat{c}_i + \cdots.
\]

\textsuperscript{5}A.J.W. Thom, PRL 105 263004 (2010)
CCMC: full non-composite clusters algorithm\textsuperscript{6}

Problem—population on reference can grow slower than the rest of the space.

\textsuperscript{6}A.J.W. Thom, W.A. Vigor
CCMC: full non-composite clusters algorithm

Split cluster selection: select all occupied excitors and randomly select clusters of excitors.

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*A.J.W. Thom, W.A. Vigor*
Key difference from FCIQMC: cooperative spawning.

\[ t_i^a t_j^b \rightarrow t_{ij}^{ab} \]

Need to minimise communication to ensure good performance.
Parallel CCMC

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Solution—more Monte Carlo!

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A.J.W. Thom
Parallel CCMC\textsuperscript{7}

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**Solution**—more Monte Carlo!

“Randomly” rearrange excitors across processors.

FCIQMC: $$p(|D\rangle) = \text{hash}(|D\rangle) \mod N_p$$
Parallel CCMC

Key difference from FCIQMC: cooperative spawning.

\[ t^a_i t^b_j \rightarrow t^a_{ij} \]

Need to minimise communication to ensure good performance.

Solution—more Monte Carlo!

“Randomly” rearrange excitors across processors.

FCIQMC: \[ p(|D\rangle) = \text{hash}(|D\rangle) \mod N_p \]

CCMC: \[ p(|D\rangle) = \text{hash}(|D\rangle + o(|D\rangle)) \mod N_p \]

\[ o(|D\rangle) = (\text{hash}(|D\rangle) + N_{iter}) \gg x \]

\(^7\)A.J.W. Thom
Parallel CCMC: scaling
Outline

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Software development
A successful Git branching model, V.Driessen
Training

- new students
  - minimal ‘toy’ FCIQMC code
  - introductory(ish) projects
- ongoing
  - code review
  - encourage ownership
  - coding retreats
- scratch own itch
  - convert users \(\rightarrow\) developers
Swings and roundabouts

well documented
fast
flexible data structures
python scientific stack
lua-based input file (coming)
easy to extend
Swings and roundabouts

well documented
fast
flexible data structures
python scientific stack
lua-based input file (coming)
easy to extend

(some) global data
complex optimised code
legacy code
Outline

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Future work

Time for consolidation

- Systematic studies on ‘model’ quantum chemistry problems
- Coupled cluster Monte Carlo studies
  - Hilbert spaces
  - truncation levels
- Like-for-like comparison between methods on a range of systems
  - How does the sign problem vary?
  - Run with 1D Hubbard model datasets
- Fixed node approximations
  - implementation
  - N\textsubscript{2} dissociation
- Beyond the initiator approximation
  - ...

\footnotesize{DOI:10.6084/m9.figshare.1096136 and DOI:10.6084/m9.figshare.1106864, J.J. Shepherd and JSS
\footnotesize{9}Kolodrubetz, Clark, PRB 86 075109; Mukherjee, Alhassid, PRA 88, 053622; Roggero, Mukherjee, Pederiva, PRB 88, 115138
\footnotesize{10}}
Highly Accurate N-DEterminant QMC

\[ U \]

\[ t \]

\[ J \]

\[ k_f \]

\[ e | HF \rangle \]

\[ \Delta \tau \rightarrow \]

\[ e | HF \rangle \]

\[ \Delta \tau \rightarrow \]

\[ e | HF \rangle \]
HANDE team

Alex Thom  Nick Blunt  Will Vigor

Fionn Malone  Matthew Foulkes  James Shepherd

Past contributors: Will Handley, Tom Rogers, Joe Weston.
HANDE publications

▶ Understanding

▶ The sign problem and population dynamics in the FCIQMC method, JSS, N.S. Blunt, W.M.C. Foulkes, JCP 136 054110 (2012).

▶ Method and algorithm development

▶ Improved parallel algorithms for stochastic diagonalisation, F.D. Malone, W.M.C. Foulkes, JSS, in preparation.

▶ Approach to scientific software development