CPSFM Center for Predictive Simulation of Functional Materials

EXASCALE COMPUTING PROJECT

QMCPACK Users Workshop 2019

Oak Ridge National Laboratory

May 14-15, 2019

Auxiliary-Field quantum Monte Carlo

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This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

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Overview

- AFQMC Basics
  - Single particle basis sets, second quantization, etc.
  - Slater determinants, Hubbard-Stratonovich transformation, etc.
- Real vs Orbital Space
  - Advantages/Disadvantages of each approach.
- AFQMC in QMCPACK
  - Workflow, features, examples.
- Tools (Fionn D. Malone)

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Useful references

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AFQMC: Projection QMC in Orbital Space

Shares many features with DMC

- Discrete walker representation of imaginary-time evolving distribution

$$\boxed{|\Psi_0\rangle = \int f(\phi)|\phi\rangle d\phi} \longrightarrow \boxed{|\Psi_0\rangle = \sum_{\phi} w_\phi |\phi\rangle,}$$

- Short time approximation to imaginary-time propagator with Trotter-like factorization

$$\boxed{|\Psi_0\rangle \propto \lim_{\tau\to\infty} e^{-\tau\hat{H}}|\Psi_T\rangle;} \qquad \boxed{|\Psi^{(n+1)}\rangle = e^{-\Delta\tau\hat{H}}|\Psi^{(n)}\rangle,}$$

- Mixed estimator for the energy. Backward walking or mixed estimator for general observables.

$$\boxed{\langle\hat{O}\rangle = \lim_{n\to\infty}\frac{\langle\Psi^{(n)}|\hat{O}|\Psi^{(n)}\rangle}{\langle\Psi^{(n)}|\Psi^{(n)}\rangle}} \qquad \boxed{E_0 = \lim_{n\to\infty}\frac{\langle\Psi_T|\hat{H}|\Psi^{(n)}\rangle}{\langle\Psi_T|\Psi^{(n)}\rangle}}$$

Walker Representation

- (N, N_α, N_β): # of electrons (total, spin up, spin down)

- $|\xi_i\rangle$ $(i = 1, \dots, M)$: Single-particle basis set.
  - Lattice site on a model Hamiltonian, plane waves, LCAO, etc.
  - Molecular orbitals, localized orbitals, etc.

- $c_i, c_i^\dagger$: annihilation and creation operators for the basis set .

- $|\psi_n\rangle$: Single-particle orbital set.
  - $|\psi_n\rangle = \sum_{i=1}^{M} D_{i,n} |\xi_i\rangle$

- In AFQMC, walkers represent Slater determinants. A walker is defined by a weight and the (M, N) Slater matrix $(D_{i,n})$ defining its occupied orbitals.
  - $|D\rangle = \prod_{n=1}^{N} \psi_n^\dagger \, |0\rangle$ Slater Matrix= $\begin{bmatrix} D_{1,1} & \cdots & D_{1,N} \\ \vdots & \ddots & \vdots \\ D_{M,1} & \cdots & D_{M,N} \end{bmatrix}$

Second Quantization

- Real space electronic Hamiltonian:
  - $\widehat{H} = \widehat{H}_1 + \widehat{H}_2 = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \sum_i V_{ext}(\overrightarrow{r_i}) + \sum_{i<j} V_{e-e}(\,|\overrightarrow{r_i} - \overrightarrow{r_j}|\,)$

- Given a single particle basis set, the corresponding second quantized Hamiltonian becomes:
  - $\widehat{H} = \sum_{ij} T_{ij}\, c_i^\dagger c_j + \frac{1}{2}\sum_{ijkl}(ik|jl)\, c_i^\dagger c_j^\dagger c_l c_k$
  - $\widehat{H}_2 = \frac{1}{2}\hat{v}_0 + \frac{1}{2}\sum_n \hat{v}_n^2$

- The Hamiltonian is defined through its matrix elements in the basis:
  - $(ik|jl) = <\xi_i\ \xi_j|\widehat{H}_2|\xi_k\ \xi_l>$
    $= \int d\vec{r}_1\vec{r}_2\ \xi_i^*(\vec{r}_1)\,\xi_k(\vec{r}_1)\,V_{e-e}(\,|\overrightarrow{r_1} - \overrightarrow{r_2}|\,)\ \xi_j^*(\vec{r}_2)\xi_l(\vec{r}_2)$
  - $T_{ij} = <\xi_i\,|\widehat{H}_1|\,\xi_j>$
    $= \int d\vec{r}_1\ \xi_i^*(\vec{r}_1)\,[-\frac{\hbar^2}{2m}\nabla_i^2 + V_{ext}(\overrightarrow{r_1})]\xi_j(\vec{r}_1)$

Walker Propagation - I

- One body propagators are easy!
  - $|D'\rangle = e^{(\sum_{ij} c_i^\dagger B_{ij} c_j)}|D\rangle \;\rightarrow\; D' = e^B D$
  - Main idea of AFQMC: Represent many-body propagator only with 1-body operators!

- Hubbard-Stratonovich (HS) transformation:
  - $e^{-\left(\frac{\tau}{2}\right)\hat{v}^2} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} d\sigma\, e^{-\sigma^2/2} e^{\sigma\sqrt{-\tau}\,\hat{v}}$

- Standard Approximations
  - $e^{-\beta\hat{H}} = \prod_n e^{-\tau\hat{H}}, \quad \beta = n\tau$ Break-up in timesteps
  - $e^{-\tau\hat{H}} = e^{-\frac{\tau}{2}\hat{H}_1} e^{-\tau\hat{H}_2} e^{-\frac{\tau}{2}\hat{H}_1} + O[\tau^2]$ Trotter approximation

- AFQMC: Many-body propagator as an integral over 1-body propagators
  - $e^{-\beta\hat{H}} = \prod_n \int d\vec{\sigma} P(\vec{\sigma})\hat{B}(\vec{\sigma}) + O[\tau^2]$
  - $\hat{B}(\vec{\sigma}) = e^{-\frac{\tau}{2}\hat{H}_1} e^{i\sqrt{\tau}\,(\vec{\sigma}\cdot\hat{v})} e^{-\frac{\tau}{2}\hat{H}_1}$

Walker Propagation - II

- Efficiency improvements: Similar to DMC
  - Mean-field subtraction: $v_n^{MF} = \langle\Psi_T|\hat{v}_n|\Psi_T\rangle / \langle\Psi_T|\Psi_T\rangle$

$$\hat{H}_2 = \left(\frac{1}{2}\hat{v}_0 + \sum_n v_n^{MF}\,\hat{v}_n - \frac{1}{2}\sum_n (v_n^{MF})^2\right) + \frac{1}{2}\sum_n (\hat{v}_n - v_n^{MF})^2$$

  - Importance sampling and force bias : $v_b = -\langle\Psi_T|\hat{v}|\phi_n\rangle / \langle\Psi_T|\phi_n\rangle$

$$\int d\sigma\, e^{-\sigma^2/2} e^{\sigma\hat{v}} \rightarrow \int d\sigma\, \frac{\langle\Psi_T|\hat{B}(\sigma)|\phi\rangle}{\langle\Psi_T|\phi\rangle} e^{-\sigma^2/2} e^{v_b\sigma - v_b^2/2} e^{\,(\sigma - v_b)\hat{v}}$$

$$|\Phi_{AF}\rangle = \frac{1}{N_w}\sum_n w_n|\phi_n\rangle \rightarrow \frac{1}{N_w}\sum_n w_n \frac{|\phi_n\rangle}{\langle\Psi_T|\phi_n\rangle}$$

  - Propagation step:
    1. $|\phi_n\rangle \rightarrow \hat{B}(\vec{\sigma})|\phi_n\rangle$
    2. $w_n \rightarrow w_n * \frac{\langle\Psi_T|\hat{B}(\sigma)|\phi\rangle}{\langle\Psi_T|\phi\rangle} e^{v_b\sigma - v_b^2/2} \approx e^{-[E_L(\phi)+E_L(\phi')]/2}$

"Local Energy Approximation"

"Hybrid Propagation"

Walker Propagation - III

- Sign problem: Phaseless approximation
  - $\hat{B}(\vec{\sigma}) = e^{-\frac{\tau}{2}\hat{H}_1} e^{i\sqrt{\tau}\,(\vec{\sigma}\cdot\hat{v})} e^{-\frac{\tau}{2}\hat{H}_1}$
  - Complex HS transformation leads to sign problem. Same origin as DMC sign problem. Same solution, but in Slater determinant space.

$$E = \frac{\langle \Psi_T | \hat{H} | \Phi_{AF} \rangle}{\langle \Psi_T | \Phi_{AF} \rangle} = \frac{\sum_n |w_n \langle \Psi_T | \phi \rangle|\ e^{i\theta(\phi)}\ E_L(\phi_n)}{\sum_n |w_n \langle \Psi_T | \phi \rangle|\ e^{i\theta(\phi)}}$$

  - Project random walk to real axis. Leads to real weights.

$$w_n \rightarrow w_n * \left| \frac{\langle \Psi_T | \hat{B}(\sigma) | \phi \rangle}{\langle \Psi_T | \phi \rangle}\ e^{v_b \sigma - \frac{v_b^2}{2}} \right| * \max(0, \cos(\Delta\theta))$$

$$\Delta\theta = \text{phase of } \frac{\langle \Psi_T | \hat{B}(\sigma) | \phi \rangle}{\langle \Psi_T | \phi \rangle}$$

  - Importance sampling leads to a seamless application of the approximation.

Observables

- Mixed distribution
  - $\left\langle \hat{O} \right\rangle_M = \frac{\left\langle \Psi_T \middle| \hat{O} \middle| \Phi_{AF} \right\rangle}{\langle \Psi_T | \Phi_{AF} \rangle} = \frac{\sum_n w_n O_M(\phi_n)}{\sum_n w_n}$, $O_M(\phi_n) = \frac{\left\langle \Psi_T \middle| \hat{O} \middle| \phi_n \right\rangle}{\langle \Psi_T | \phi_n \rangle}$
  - $\left\langle \hat{O} \right\rangle_M$: quadratic in $|\Psi_T - \Psi_{Exact}|$ for operators that commute with Hamiltonian. Linear for all others.
  - Small overhead, but can depend significantly on quality of Ψ_T.

- Back propagation:
  - $\left\langle \hat{O} \right\rangle_{BP} = \frac{\left\langle \Phi'_{AF} \middle| \hat{O} \middle| \Phi_{AF} \right\rangle}{\left\langle \Phi'_{AF} \middle| \Phi_{AF} \right\rangle} = \frac{\sum_n w_n O(\phi_m, \phi_n)}{\sum_n w_n}$, $O(\phi_m, \phi_n) = \frac{\left\langle \phi_m \middle| \hat{O} \middle| \phi_n \right\rangle}{\langle \phi_m | \phi_n \rangle}$
  - $\left\langle \hat{O} \right\rangle_{BP}$: quadratic in $|\Psi_T - \Psi_{Exact}|$.
  - Typically requires an overhead of 50-75%.

Real vs Orbital Space

AFQMC

- Direct connection between ab-initio and model Hamiltonians
- Flexible treatment of core electrons:
  - All-e, frozen-core, ECP, NCPP, LAPW, etc.
- Spin-orbit coupling easy to incorporate.
- Typically, smaller bias from phaseless approximation.
- Efficient/simple code.
  - GEMM, QR, Inverse

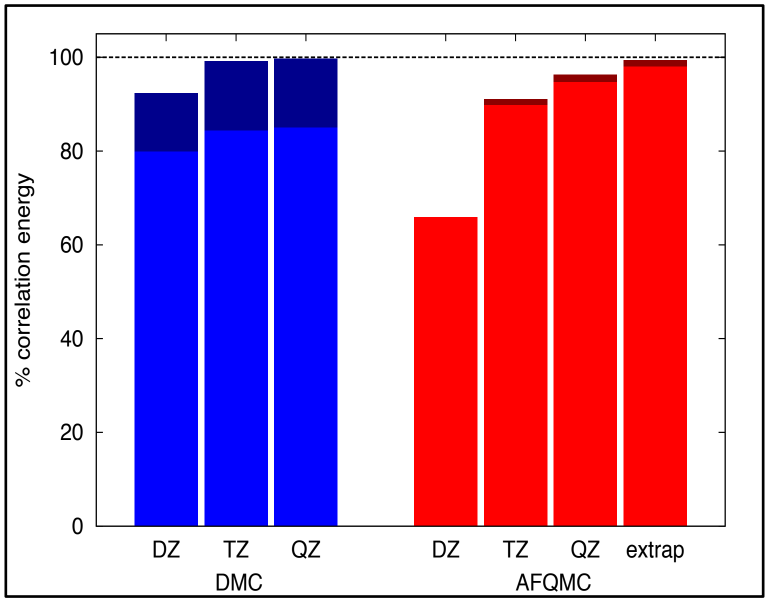
- Small ab-initio community.
- Basis set error.
  - Error cancellation is “transferred” to the basis.
- Requires 2-electron integrals.
  - ~~M^3 memory cost for propagation~~
  - ~~M^4 memory cost for energy~~
  - M^{2-3} memory cost
  - No “direct” algorithm.
  - Forces require xN_{atoms} more memory.

DMC

- Trivial explicit correlation.
  - Jastrow is almost free!
- No basis set extrapolation. Works at CBS limit.
- Memory friendly.
- Intuitive.

- Hard to simplify.
- Uncontrolled approximation needed for non-local ECP channels.
- Fixed-node error is large.
  - Error cancellation is needed for accurate results.
- Spin-orbit is not trivial (to me!!!).
- Divergent potentials.
  - Forces are noisy!

Real vs Orbital Space



Illustrative DMC – AFQMC comparison

- Cohesive energy of 2-atom unit cell of Carbon in diamond structure
- Bright (dark) region corresponds to a calculation with a single determinant (converged MSD).
    - SD DMC consistently recovers ~80% of the total correlation energy.
    - Fixed node error of ~20%.
    - Converged DMC-MSD almost reaches CBS at TZ.
    - Large basis set error for AFQMC.
        - Requires basis set extrapolation.
    - SD-AFQMC shows small phaseless error.
        - Short determinant expansion recovers remaining error.

Disclaimer: For illustration purposes only!

AFQMC in QMCPACK: Design Principles

- Code still under active development.
  - Always check developers version for latest functionality.
  - Significant extensions every 3-6 months.
- Core AFQMC algorithms within QMCPACK.
  - Mean-field calculations performed by external codes.
    - PySCF, Molpro, GAMESS, VASP, etc.
  - Basic input: 1-2 electron integrals and trial wave functions.
  - AFQMC code doesn’t ”know” about atoms, positions, basis sets, pseudopotentials, etc.
- Focus on efficient, large scale calculations.
  - Multiple levels of parallelization and data distribution.
    - Distribution of integrals over nodes.
  - xml input, hdf5 data, python analysis.

Sample Workflow

- Simple workflow. Relies on converter tools and post-processing scripts.
  - Many still under development.
  - Contributions are welcome.
  - Properties require custom (simple) post-processing scripts. Examples are offered for charge and spin densities.
- Sample workflow:
  1. python scf.py
  2. python pyscf_to_afqmc.py   [options]
  3. qmcpack afqmc.xml
  4. qmca [options] sample.scalar.dat
  5. python [options] –i sample.scalar.h5 analysis.py

Input Files - I

- Request AFQMC calculation with:
  - <simulation method="afqmc">
- Non-execute blocks must be “named” and are parsed first.
- “Execute” blocks are executed sequentially afterwards.
- Most decisions are made when pyscf_to_afqmc.py is executed.

```xml
<AFQMCInfo name="info0">
  <parameter name="NMO">2048</parameter>
  <parameter name="NAEA">256</parameter>
  <parameter name="NAEB">256</parameter>
</AFQMCInfo>

<Hamiltonian name="ham0" info="info0">
  <parameter name="filename">integrals.h5</parameter>
</Hamiltonian>

<Wavefunction name="wfn0" type="MSD" info="info0">
  <parameter name="filetype">ascii</parameter>
  <parameter name="filename">wfn.dat</parameter>
</Wavefunction>

<WalkerSet name="wset0">
  <parameter name="walker_type">closed</parameter>
</WalkerSet>

<Propagator name="prop0" info="info0">
</Propagator>
```

Input Files - II

- Execute blocks typically require some minimal customization.
- Observables are defined locally in these blocks.
- Wavefunctions used in observables can be independent from the one used for propagation (phaseless constraint and importance sampling).
- Triple loop structure:
  - blocks: Observables are calculated and data is written to disk. Checkpoint occurs if requested.
  - steps: Branching and load balancing at every step. Orthogonalization occurs with given frequency.
  - substeps: Only propagation.

```xml
<execute wset="wset0" ham="ham0" wfn="wfn0" prop="prop0" info="info0">
  <parameter name="timestep">0.005</parameter>
  <parameter name="blocks">1000</parameter>
  <parameter name="steps">10</parameter>
  <parameter name="substeps">4</parameter>
  <parameter name="nWalkers">100</parameter>
  <Estimator name="energy" wfn="wfn_estimator">
    <parameter name="print_components">yes</parameter>
  </Estimator>
</execute>
```

Hamiltonians

Cholesky Factorization

$$(ik|jl) = M_{\mathrm{ik},jl} = \sum \mathrm{L}_{ik}^{n} \mathrm{L}_{lj}^{n*} .$$

Sparse Representation: (Only option for molecular problems)

- Storage of L_{ik}^{n} and $M_{ik,jl}$ as a sparse matrices. Elements below a certain cutoff are set to zero.
- Automatically incorporates any symmetries present in the system.
- Relies on less efficient sparse linear algebra (compared to dense storage).
- Very large setup cost! Must generate M from L, $O[N^2 M^2 n_{chol}]$.

K-Point Representation: (Only for periodic systems with k-points)

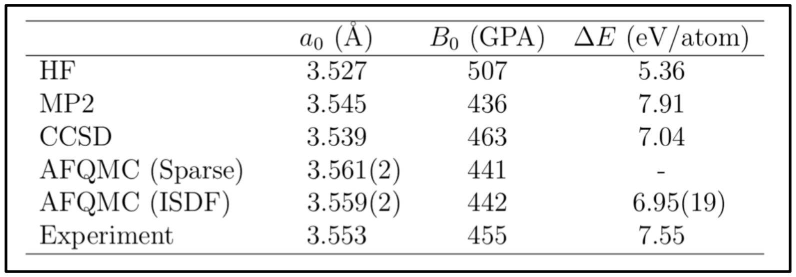
- Explicit use momentum conservation. Ideal for small unit cells with lots of k-points.
- Reduction of $1/N_k$ in memory and computation cost compared to direct algorithm.
- Based on highly efficient batched linear algebra operations.
- Scales poorly with size of the primitive cell. Not practical for large supercells.

Tensor Hyper-Contraction

$$(ik|jl)= \sum \phi_{i,\mu}^{*} \phi_{k,\mu} M_{\mu,\nu} \phi_{j,\nu}^{*} \phi_{l,\nu}$$

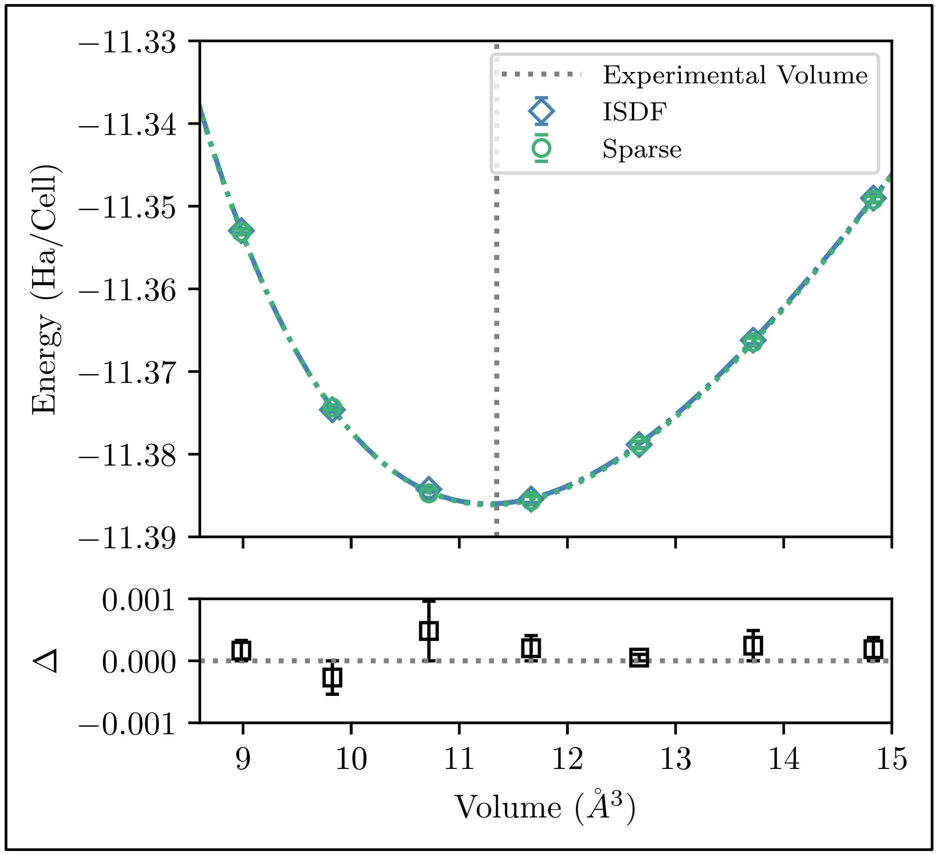
- Factorize integral tensor as a contraction of 2nd-order tensors. Quadratic memory requirements. Cubic computational cost.
- Popularized in QC by Todd Martinez. Made practical in PBC by Lin Lin.
- Ideal for large supercells at the Gamma point or large molecular problems with no symmetry.
- Does not currently benefit from symmetries in the system.
- Large prefactor, specially for small system sizes. Currently problematic for heavier atoms.

Cholesky vs THC



	a_0 (Å)	B_0 (GPA)	ΔE (eV/atom)
HF	3.527	507	5.36
MP2	3.545	436	7.91
CCSD	3.539	463	7.04
AFQMC (Sparse)	3.561(2)	441	-
AFQMC (ISDF)	3.559(2)	442	6.95(19)
Experiment	3.553	455	7.55

- THC (ISDF) is only moderately slower even though it does not make use of any symmetries.
- Only practical choice for large unit cells.
  - Actual calculations are done in a supercell representation.
- Same accurate answer regardless of approach.



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Hamiltonians

Systems without K-Point Symmetry

Representation	Memory		Computation	
	HS Potential	Energy	HS Potential	Energy
Sparse Cholesky	$s\ x_c\ M^3$	$s'\ N^2M^2$	$s\ x_c\ M^3$	$s' N^2M^2$
Dense Cholesky	$x_c\ M^3$	$x_c\ NM^2$	$x_c\ M^3$	$x_c\ N^2M^2$
THC	$x_\mu^2\ M^2$	$x_\mu^2\ M^2$	$x_\mu\ M^2$	$x_\mu^2\ M^2$

Systems with K-Point Symmetry (N_k: # kpoints)

Representation	Memory		Computation	
	HS Potential	Energy	HS Potential	Energy
Sparse Cholesky	$s\ x_c\ M^3$	$s'\ N^2M^2$	$s\ x_c\ M^3$	$s' N^2M^2$
Dense Cholesky	$x_c\ N_k^2\ m^3$	$x_c\ N_k^2\ nm^2$	$x_c\ N_k^2\ m^3$	$x_c\ N_k^3\ n^2\ m^2$

- Always useful to use K-Point representation.
- Dense representation is generally more efficient.

s, s': Sparsity of corresponding structures
x_μ: THC prefactor, typically 5-20.
x_c: Cholesky prefactor, typically 5-20.

Orthogonal vs Non-Orthogonal Determinants

$$|\Phi_T\rangle = \sum_i c_i |D_i\rangle$$

Orthogonal (PHMSD)

$$\langle D_i | D_j \rangle = \delta_{ij}$$

- Robust and well-controlled.
- Some form of CI typically involved in construction.
  - Truncated-CI, CASCI, selected CI, etc.
- Size consistency problems.
  - Possibly fatal for bulk.
- Fast evaluation algorithms:
  - Cost proportional to rank of the update
- Lower memory overhead for large expansions.

Non-Orthogonal (NOMSD)

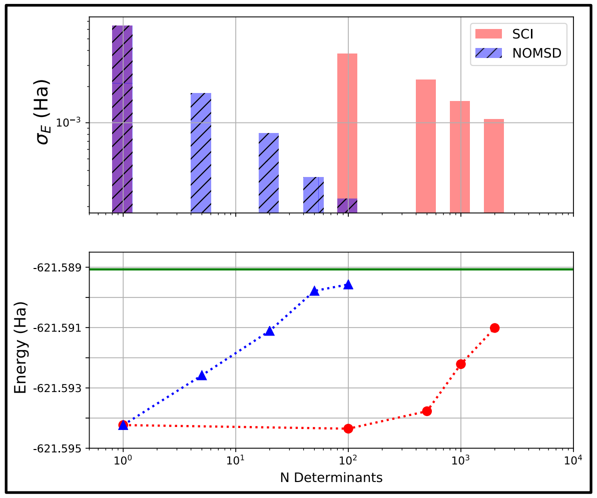
$$\langle D_i | D_j \rangle \neq \delta_{ij}$$

- Not common/routine in QC community.
- Several algorithms:
  - Iterative HF: 1-det at a time
  - Resonating HF: N-dets simult.
  - Complicated optimization problem.
- Size consistency problem less severe.
- Fastest convergence in MSD ansatz.
- Linear cost with #dets.
  - Both computation and memory.
  - Large memory overhead ultimately makes the approach impractical for large systems.

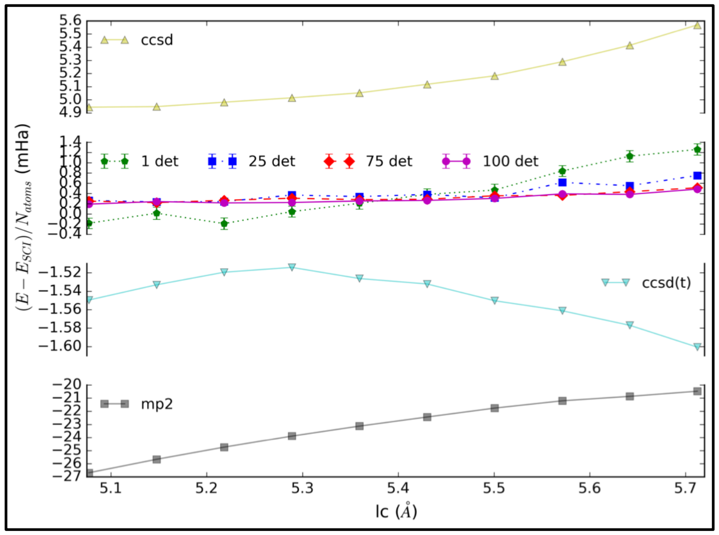
- Different wavefunctions can be combined in a single execution.
  - NOMSD for propagation, PHMSD for energy evaluation.

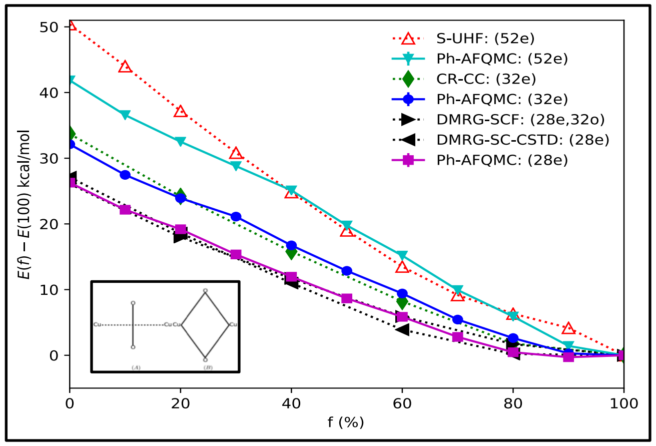
Systematic Improvable Wavefunctions

NOMSD vs PHMSD



Si (diamond) with NOMSD





Cu_2O_2 with NOMSD

- NOMSD offer great promise for compact and accurate trial wavefunctions.
- Mostly unexplored territory.
    - Great opportunity!

Observables

- Slowly expanding list of observables.
  - Currently: energy, static 1-RDM
    - 1-RDM can be used to calculate many properties: spin and charge densities, occupancies, momentum distribution, magnetic moments, etc.
  - In development: dynamic 1-RDM, 2-RDM, contractions of the 1-/2-RDM, forces.
- Back propagation (in principle) available for any observable.
  - Currently limited to 1-RDMs.

```
<Estimator name="back_propagation">
  <parameter name="nsteps">500</parameter>
  <parameter name="naverages">5</parameter>
  <parameter name="ortho">25</parameter>
  <parameter name="block_size">10</parameter>
</Estimator>
```

Data Distribution

- Large data structures can be distributed over multiple memory spaces (nodes, GPUs, etc).
  - *“**nnodes**”* parameter in wavefunction and propagator.
  - Distributed algorithms are automatically chosen if nnodes > 1.
  - Enables calculations on large systems.
    - Some communication overhead. Typically modest.
  - Does not change the number of walkers, only static data layout.
- Walker sets can be shared over multiple cores in a node.
  - Use “***ncores***” parameter in the execution block.
  - Operations on the walker set are distributed over all cores in the group.
    - nWalkers defines the number of walkers per “working” group.
  - Improved time to solution.
    - Allows 1 walker per node, useful for large systems.

Warning: Use with caution!

GPUs

- AFQMC code is actively being ported to GPU.
  - Currently: Production level GPU port for K-Point dense Hamiltonian.
    - 15-40x speed-up for DP, 10-25x speed-up for SP compared to good CPU.
    - Larger performance gains for large systems.
  - Mixed precision build recommended for GPUs.
    - Memory is the more important resource!
  - No real build on GPUs yet (no molecules or gamma point).
  - Summit/Sierra enable AFQMC calculations on systems with 250 atoms.
    - Bcc Fe with 6x6x6 k-point grid.
    - C (diamond) with 5x5x5 k-point grid.
    - AFM-NiO with 3x3x3 k-point grid including back propagation and magnetic moment.

Upcoming Features

- Full GPU coverage (3-6 months)
- Finite-T algorithm (3 months)
- Spin-Orbit coupling and non-collinear magnetism (6 months)
- Forces (6-12 months)
- VASP interface (3 months)
- K-Point THC (6-12 months)