Quantum Monte Carlo Simulation Tools: *qmcPlusPlus*

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Motivations and goals

Quantum Monte Carlo (QMC) methods can, in principle, calculate exact properties of many-body systems. With recent developments in QMC algorithms and ever-growing computing powers, QMC methods have become powerful and practical tools to study a wide range of problems with direct connections to high pressure physics, materials science, surface science, the theory of strongly correlated electrons and low-temperature physics.

We are developing comprehensive computational frameworks for QMC simulations built upon the innovative algorithms and numerical methods for the advanced computing environments of today and future. One of the components of the tools is **qmcPlusPlus**, an object-oriented QMC code, the focus of this presentation. **qmcPlusPlus** is the computational core of our tools and is the building block for future tool development.

Flexible computational frameworks for Quantum Monte Carlo simulations that accelerate developments of new algorithms.

- Easy-to-use user interfaces for a wide range of users
- Deployment as portal applications at NSF HPC centers
- Integration with data mining and visualization portals simulations.

Combine ever-better hardware with new software engineering technology

- **Use of standard, open-source software** for dynamic, maintainable and adaptable scientific code.
- **Use of standard IO** for communication between diverse applications.
- **Use of standard tools**
  - Compilers: C/C++, OpenMP
  - Documentation: deoxygen, docbook
  - Development environment: Cmake and GNU automake/libtool).

What is qmcPlusPlus?

- Open-source library and application package to perform Quantum Monte Carlo Simulations
- Developed at MCC and NCSA, at UIUC
- A new C++ code modeled after QMC codes developed by D. Ceperley and his collaborators
- Implements various QMC algorithms: Variational, Diffusion and Reptation Monte Carlo methods and optimizations
- Utilize standard open-source libraries and utilities for development and executions
- Collaborative developments
  - Contributing developers at UIUC: J. Kim, J. Vincent, Dyutiman Das, S. Chiesa, K. DeLaney, K. Esler
  - Interactions with external developers and external projects: NRLMOL (Peterson et al. at Naval Research Laborary), GEMSTONE (Baldridge et al. at San Diego Supercomputing Center) and other Density Funtional Theory and Quantum Chemistry developers
- Release at MCC Software Archive scheduled in November 2005

Toward open standards of quantum materials simulations

Our development promote open I/O standards for quantum simulations and provide tools to facilitate communications between the materials applications in general.
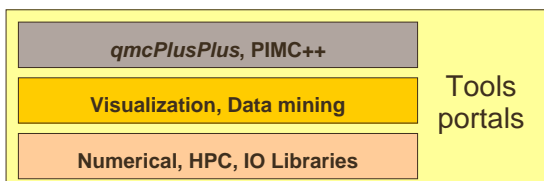
XML driven IO
- Job management and project descriptions
- Setting up complex simulations
- Human-readable and easily transformed to various formats.
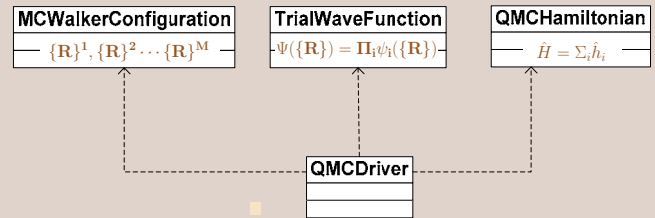- Solution for the complex problems of analyzing, mining, storing, and accessing vast stores of data

HDF5-driven IO
- HDF5, a general purpose library and file format for storing scientific data
  http://hdf.ncsa.uiuc.edu
- Efficient IO on serial and parallel computers.
- Facilitate scientific data exchange, access, analysis, archiving and discovery.

Vision for Quantum Monte Carlo Toolkits and beyond

| *qmcPlusPlus*, PIMC++ |
| Visualization, Data mining |
| Numerical, HPC, IO Libraries |

Tools portals

Generic design of *qmcPlusPlus*

MCWalkerConfiguration	TrialWaveFunction	QMCHamiltonian
$\{\mathbf{R}\}^1, \{\mathbf{R}\}^2 \cdots \{\mathbf{R}\}^M$	$\Psi(\{\mathbf{R}\}) = \Pi_i \psi_i(\{\mathbf{R}\})$	$\hat{H} = \Sigma_i \hat{h}_i$

QMCDriver

Many-body wave functions

- Evaluations of the trial wave function and local energies with

$$\ln \Psi(\{\mathbf{R}\}) = \sum_i \ln(\psi_i(\{\mathbf{R}\}))$$

  - A trial wave function is a collection of *many-body orbitals*
  - Each *Orbital* implements evaluation of

$$\ln|\psi_i|, \nabla \ln \psi_i \ \& \ \nabla^2 \ln \psi_i$$

  - The sign of each *Orbital* and their total sign is evaluated separately

- Typical Slater-Jastrow wave function for electrons takes

$$\Psi(\{\mathbf{R}\}) = \Pi_i e^{J_i} \underbrace{D_j^\uparrow D_j^\downarrow}_{Fermion} \Rightarrow \Pi_i e^{J_i} \sum_j C_j D_j^\uparrow D_j^\downarrow$$

multi determinants

Many-body Hamiltonian

- A many-body Hamiltonian consists of *operators* as

$$\hat{H} = \Sigma_i \hat{h}_i$$

- The *operators* which evaluate $\Psi^\dagger \hat{h}_i \Psi$ make up a total energy operator.

- A generic Hamiltonian for the electronic structure calculations

$$\hat{H} = -\sum_i \frac{1}{2m_e}\nabla^2 + \sum_i V_{ext}(\mathbf{r}_i) + \frac{1}{2}\sum_{i \neq j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$

Kinetic operator
Coulomb potentials: el-e, ion-el,ion-ion   Core-polarization potential
Pseudo-potentials   Valence/conduction band offsets

QMC algorithms and implementation details

- VMC and DMC moves
  - walker-by-walker : evaluate from scratch
  - particle-by-particle : update using ratio
- Optimization and RMC are based on walker-by-walker moves
- Optimizations of trial wave functions with energy, variation and $|E - E_{target}|^p$ minimizations

- Energy-difference methods
  - VMC and RMC
  - Correlated sampling over multiple wave functions and Hamiltonians
  - Examples: energy barrier of H2 dissociation, optical gaps

Applications of *qmcPlusPlus*

- Optical properties of Ge clusters (poster by J. Vincent)
- Electronic properties of coupled quantum dots (poster by D. Dyutiman)
- Energetic materials (S. Chiesa)
- Super-molecules based on H_2O (J Kim in collaborations with B. Militzer)

Works in progress

- Total energy calculations of periodic systems (K. Delaney*)
- Improvement of energy-difference methods (S. Chiesa*)
- Improvement of optimization methods
- Interfaces to various Quantum Chemistry and DFT programs
- GUI/Web interfaces
* Leading developers for the projects