Quantum Monte Carlo Methods

Daniel Fisher, MSC 2005

Quantum Monte Carlo (QMC) methods for solving the Schrödinger equation for the electronic wavefunctions of molecules can in principle provide energies to within chemical accuracy (~2kcal/mol). The computational expense of QMC scales with system size as $O(N^3)$ or better, albeit with a large prefactor. This is much more favorable than other quantum mechanical methods capable of similar accuracy. Moreover, the stochastic nature of QMC methods makes it easy to parallelize over a large number of processors, which can allow calculations to finish in a reasonable amount of time despite the slow convergence of Monte Carlo.

As supercomputing resources improve and become more accessible to researchers, QMC will become a powerful tool for conducting simulations on large systems. Recent efforts in our group have focused on improving the efficiency of these calculations on heterogeneous and homogeneous computers. To this end, a finite all-electron QMC program, QMcBeaver, has been written and used to develop and demonstrate several new algorithms.

These new methods make QMC calculations easier to carry out by reducing the amount of data that has to be stored and communicated, performing automatic load balancing, and increasing the efficiency of parallel calculations. Together, they introduce the possibility of constructing an inexpensive, continuously upgradable, QMC specific supercomputer using commodity processors and inexpensive networking hardware.