Introduction to Diffusion Monte Carlo

David M. Ceperley, University of Illinois Urbana-Champaign

In the Projector Quantum Monte Carlo method, one uses a function of the hamiltonian to sample a distribution proportional to the exact ground state wavefunction, and thereby compute exact matrix elements of it. In this lecture we introduce the Diffusion Monte Carlo (DMC) method that involves drifting, branching random walks.

In DMC, a many-body projector $G(R, R') = \hat{G}$, is repeatedly applied to filter out the exact many-body ground state from an initial state. Let us denote the initial wavefunction by $\Psi^{(0)}(R)$. A sequence of many-body wavefunctions is defined by:

$$\Psi^{(n+1)}(R) = \int dR' G(R, R') \Psi^{(n)}(R'). \tag{1}$$

The projector is defined in terms of the many-body hamiltonian, $\hat{H}$ from which a zero of energy, the so-called trial energy E_T, has been subtracted; E_T is used to control the normalization.

$$\hat{G} = e^{-\Delta\tau(\hat{H}-E_T)} \tag{2}$$

As can be shown by expanding the effect of the projector on a basis of exact eigenfunctions, only the lowest energy state having a non-zero overlap with the initial trial function survives after many iterations.

$$\lim_{n\to\infty} \Psi^{(n)}(R) = e^{-n\Delta\tau(E_0-E_T)} \Phi_0(R) \langle 0|\Psi^{(0)}\rangle \tag{3}$$

Here $\Delta\tau$ is the (imaginary) "*time step*" and n is the number of iterations. Differentiating with respect to $\tau = n\Delta\tau$, we find the imaginary time Schroedinger Equation:

$$-\frac{d\Psi(R;\tau)}{d\tau} = (\hat{H}-E_T)\Psi(R;\tau) = -\frac{1}{2}\sum_{i=1}^{N} \nabla_i^2 \Psi(R;\tau) + (V(R)-E_T)\Psi(R;\tau). \tag{4}$$

To simulate this with Monte Carlo, an initial ensemble of $P^{(0)}$ configurations is constructed with a Metropolis sampling procedure for the initial state $\Psi^{(0)}$ (assuming it is real and non-negative). Configurations in the next "generation" are constructed by random diffusion of all the electrons with a mean squared step size of $\Delta\tau$. After all $3N$ electron coordinates have been moved, we make on the average $m = \exp[-\Delta\tau(V(R) - E_T)]$ copies of R'.

This simple implementation of the projection method becomes very inefficient as the number of electrons increases because the branching fluctuations are not controlled. An importance sampling transformation makes the algorithm much more efficient. After multiplying by a trial function $\Psi_T(R)$, the density $f(R;\tau) = \Psi_T(R)\Psi(R;\tau)$ satisfies the evolution equation:

$$-\frac{\partial f(R;\tau)}{\partial \tau} = -\frac{1}{2}\sum_i \nabla_i(\nabla_i f(R;\tau) - f(R;\tau) F_i(R)) + [E_L(R) - E_T] f(R;\tau) \quad (5)$$

where $E_L(R) = \Psi_T^{-1}\hat{H}\Psi_T(R)$ is the local-energy of the trial function and $F_i(R) = 2\nabla_i \ln \Psi_T(R)$ is its "quantum force".

For any state for a system with more than two electrons, one encounters the sign problem, limiting the direct application of these algorithms for most fermion systems. One can demonstrate that the signal-to-noise ratio for the simplest generalization of the DMC algorithm will decrease as $\exp(-\tau(E_F - E_B))$ where τ is the projection time and $E_F - E_B$ is the many-body energy difference between fermion and boson states. There is a simple way to avoid the fermion sign problem: forbid moves that change the sign of the trial function. This is the fixed-node (FN) approximation for a real trial function: one can achieve efficiency similar to variational Monte Carlo while achieving the best upper bound to the energy consistent with the constraints.

We will also discuss implementation of pseudopotentials within DMC and illustrate with recent calculations.

For further details and references see:

1. P. J. Reynolds, D. M. Ceperley, B. J. Alder and W. A. Lester Jr., *Fixed-node Quantum Monte Carlo for Molecules*, J. Chem. Phys. **77**, 5593 (1982).

2. L. K. Wagner and D. M. Ceperley, *Discovering correlated fermions using quantum Monte Carlo*, Rep. Prog. Phys. **79** 094501 (2016); arXiv cond-mat.str-el 1602.01344.

3. R. M. Martin, L. Reining and D. M. Ceperley, *Interacting Electrons, Theory and Computational Approaches*, Cambridge (2016).