Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2020-0168

Vol. **28**, No. 5, pp. 1907-1936
November 2020

Random Batch Algorithms for Quantum Monte Carlo Simulations

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Received 29 August 2020; Accepted 11 October 2020

Abstract. Random batch algorithms are constructed for quantum Monte Carlo simulations. The main objective is to alleviate the computational cost associated with the calculations of two-body interactions, including the pairwise interactions in the potential energy, and the two-body terms in the Jastrow factor. In the framework of variational Monte Carlo methods, the random batch algorithm is constructed based on the over-damped Langevin dynamics, so that updating the position of each particle in an N-particle system only requires $\mathcal{O}(1)$ operations, thus for each time step the computational cost for N particles is reduced from $\mathcal{O}(N^2)$ to $\mathcal{O}(N)$. For diffusion Monte Carlo methods, the random batch algorithm uses an energy decomposition to avoid the computation of the total energy in the branching step. The effectiveness of the random batch method is demonstrated using a system of liquid ^{4}He atoms interacting with a graphite surface.

AMS subject classifications: 65C05, 81Q05, 82C31

Key words: Quantum Monte Carlo method, random batch methods, Langevin equation.

1 Introduction

One of the fundamental problems in chemistry is the computation of the ground state energy of a many-body quantum system. Although this major difficulty has been circumvented to some extent by the density-functional theory [29], the quantum Monte Carlo (QMC) method [2, 3, 13, 39, 46] still remains an important approach to determine the ground state energy and electron correlations.

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This paper is concerned with the implementation of the QMC for many-body systems. More specifically, we consider the Hamiltonian,

$$\widehat{H}=\sum_{i=1}^{N}-\frac{\hbar^2}{2m}\triangle_{\boldsymbol{r}_i}+\sum_{i\neq j}W(\boldsymbol{r}_i-\boldsymbol{r}_j)+\sum_{i=1}^{N}V_{ext}(\boldsymbol{r}_i). \tag{1.1}$$

Here we use $\boldsymbol{r}=(\boldsymbol{r}_1,\boldsymbol{r}_2,\cdots,\boldsymbol{r}_N)$ to denote the particle coordinates with N being the total number of particles. and the Laplacian $(-\triangle)$ in the first term of the Hamiltonian indicates the kinetic energy. The second term in the Hamiltonian, which is a double sum, embodies the pairwise interactions, e.g., Coulomb, while the last term includes the external potential, namely,

$$V_{ext}(\boldsymbol{r}_i)=\sum_{\alpha=1}^{M}U(\boldsymbol{r}_i-R_\alpha), \tag{1.2}$$

where R_α, for instance, can be the position of an atom.

In principle, the ground state can be obtained by computing the smallest eigenvalue and the corresponding eigenfunction. It can be expressed in terms of a Rayleigh quotient,

$$E=\min_{\Phi}\frac{\displaystyle\int_{\mathbb{R}^{3N}}\Phi\widehat{H}\Phi d\boldsymbol{r}_1\cdots d\boldsymbol{r}_N}{\displaystyle\int_{\mathbb{R}^{3N}}|\Phi|^2 d\boldsymbol{r}_1\cdots d\boldsymbol{r}_N}, \tag{1.3}$$

and the minimizer Φ corresponds to the ground state wave function. However, due to the high dimensionality, a direct numerical approach, e.g., using finite difference or finite element methods together with numerical quadrature for the integrals suffers from the curse of dimensionality, thus is typically prohibitively expensive.

Within the variational Monte Carlo (VMC) framework, this issue is addressed by selecting an appropriate ansatz, denoted here by $\Phi\approx\Psi_0$, for the many-body wave function. Then the multi-dimensional integral is interpreted as a statistical average, which can be sampled using a Monte Carlo procedure. Traditionally, Ψ_0 is constructed using the one-body wave functions, with the effect of particle correlations described by Jastrow factors [13]. Recently, artificial neural networks from machine learning have also been used to represent the many-body wave function [7,17,18,37]. In fact, the recent surge of interest in applying machine-learning algorithms to scientific computing problems has been a strong motivation for the current work.

The first part of this paper is concerned with the numerical implementation of VMC. Since VMC formulates the energy calculation as a sampling problem, the most natural approach is the Metropolis-Hastings (MH) algorithm which, in general, falls into the category of Markov chain Monte Carlo (MCMC) algorithms in statistics. At each step, the chain is updated by calculating the energy change. As can be seen from (1.1) and (1.3), this requires visiting all particles in the system. A direct treatment would involve $\mathcal{O}\big(N(N+M)\big)$ operations in each time step. The presence of the Jastrow factor further