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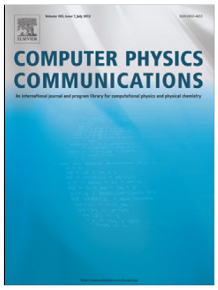

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Convergence estimation of flat-histogram algorithms based on simulation results

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The present work considers the question of convergence of Wang-Landau, multi-canonical and stochastic approximation Monte Carlo algorithms, which was previously investigated on very different level. In the case of the multi-canonical algorithms, a convergence behavior similar to either the original Wang-Landau or the stochastic approximation Monte Carlo algorithms is shown, depending on details of the algorithm. I suggest a method for error estimation based only on the results of simulations, not involving an information about the exact density of states, which is unknown for most practically interesting problems.

I. INTRODUCTION

The flat-histogram Monte Carlo algorithms [1–8] are widely used for estimation of the density of states (DOS) and related equilibrium properties of systems having complex energy landscapes (see for instance [9] and literature cited there). Suggested in [1, 2] and further developed later [3, 4], the multi-canonical Monte Carlo (MuCa) algorithm along with the Wang-Landau (WL) algorithm [5, 6] are the most common techniques for the numerical estimation of the density of states. In spite of the wide spread use of multi-canonical simulations, investigations of the convergence or accuracy of the method are very limited [10]. In contrast, the convergence of the Wang-Landau algorithm was investigated in many works [11–19] which stimulated further development of the technique. In the works [15–17] an empirical modification of the original WL algorithm which prevents saturation of the error, the $1/t$-WL, was introduced and analyzed. At the same time, Liang suggested a generalized simulation method: stochastic approximation Monte Carlo (SAMC) [7, 8] including the $1/t$-WL as a particular case. The theoretical background of the SAMC algorithm explains difficulties of the original WL method and guarantees decrease of the SAMC error under weak conditions (see below). However convergence investigations of flat-histogram algorithms are based typically on comparing with the exact DOS, whereas the relation of exactly calculated error and error estimated from the simulation results remains out of focus despite high practical interest.

II. GENERAL DESCRIPTION OF FLAT-HISTOGRAM METHODS

Despite the difference in the ways of the DOS estimation, the flat-histogram algorithms can be described by the following general scheme:

1. Choose the initial DOS estimation $g_0(E)$ (for instance $g_0(E) = 1$) , where E indicates an energy level of a discrete spectrum or an energy bin of a continuous one, and set the initial values of the visitation histogram $H(E) = h_0$, where h_0 can be 0 or any positive constant.

2. Perform a MC move from the current configuration x to a new one x' with the acceptance probability

$$p_{\text{acc}}(x, x') = \min\left[1, \frac{g(E(x))}{g(E(x'))}\right] \tag{1}$$

   where $g(E)$ is the current DOS estimation. If the move is accepted, modify the current configuration $x \to x'$ and update the visitation histogram $H(E(x')) \to H(E(x')) + 1$, else update the visitation histogram $H(E(x)) \to H(E(x)) + 1$.

3. If conditions of DOS modification are fulfilled, update current estimation of DOS and related parameters of the simulation.

4. Check the stop-condition of the algorithm, if it's not fulfilled go to 2.

The flat-histogram algorithms differ in details according to the last two items of the general scheme. The SAMC algorithm updates the DOS after every MC move [8, 20] as $\ln g(E) \to \ln g(E) + \gamma_t$, where E is an energy of the system at the end of the item 2 of the general scheme, and $\gamma_t = \gamma_0 t_0 / \max(t_0, t)$ is the modification factor depending on the MC time, t, and constants γ_0 and t_0. The typical stop-condition of the SAMC algorithm is either having performed a given number of MC moves or equivalently reaching a given value of the modification factor $\gamma_{\min}$. The stop-condition of the SAMC algorithm for all considered here examples will be performing 10^{10} MC moves.

The WL algorithm updates the DOS similar to the SAMC one, but the modification factor remains constant and changes only after fulfilling the flatness condition

$$|H(E) - \overline{H}(E)| < (1 - \alpha)\,\overline{H}(E) \quad \forall\, E \tag{2}$$

where $\overline{H}(E)$ is the arithmetical average of the visitation histogram values accumulated after the previous changing of the modification factor, and α is a flatness parameter. If the visitation histogram is flat enough, the

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