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Lecture Note in Tutorial Sessions

Monte Carlo Methods

– Sampling from an Extended Ensemble –

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1 Introduction

Monte Carlo (MC) algorithm aims to generate samples from a given probability distribution $P(\boldsymbol{X})$ with unmanageably many degree of freedom by mimicking a random process in computers. The probability distribution $P(\boldsymbol{X})$ might be a Boltzmann-Gibbs distribution from statistical physics or a conditional distribution from statistical science. Since the Metropolis algorithm was introduced in 1953[1], the Monte Carlo methods have been used intensively in a wide area of physics[2] and statistical sciences[3, 4]. Most of the MC methods in statistical physics are based on the Metropolis strategy, in which a Markov chain is constructed in order for its invariant distribution to coincide with the desired distribution. According to a report[5], the MC method is chosen as one of the top 10 algorithms of the 20th century.

The conventional MC algorithm based on local updating processes in a canonical ensemble is, however, known to be inefficient for the so-called *hardly-relaxing* problems. An example is critical slowing down around a phase transition point which separates two phases in statistical physics. Another typical example occurs in systems with many conflicting constraints such as random magnets, protein problems in physics, and also optimization problems. In terms of physics, these systems commonly have numerous local free-energy minima which are separated to each other by energy barriers. The characteristic time for escaping from one of such local minima increases rapidly as temperature decreases, and equilibration of the system is hardly realized.

To overcome the difficulty in the conventional MC method mentioned above, various improvements have been and is being made on MC algorithms. There are mainly two categories in such algorithms, i.e., *non-local updating* (or *cluster*) *methods* and *extended ensemble methods*. As for the former improvement, Swendsen and Wang[6] have proposed how to construct a cluster which can be flipped with non-negligible probability. The SW method based on Fortuin-Kasteleyn's percolation representation[7] is known as the cluster MC method. Wolff has successfully developed the SW algorithm to a single cluster method and generalized to systems with continuous degrees of freedom[8]. The cluster MC algorithm eliminates the

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critical slowing down in many statistical-physics systems. It is, however, difficult to specify such clusters explicitly in more complex system such as protein problems.

An improvement has been developed on MC algorithm based on the idea of an extended ensemble[9, 3]. Namely, the ensemble or the weight to be simulated is modified or extended in such a way that the system visits more frequently to states which are less or hardly visited by the conventional MC algorithm. The multicanonical method[10], the simulated tempering (expanded ensemble)[11, 12], and the exchange MC method[13] belong to this category called the extended ensemble method. Particularly, the last method has been discovered independently in different areas[13, 14, 15, 16]. The idea of the extended ensemble gives us a general strategy for overcoming the hardly-relaxing problem. These methods have been applied to various hardly-relaxing systems and turned out to be quite useful.

The present paper is devoted mainly to a review of the exchange MC method. After describing briefly the two other improved MC algorithm, the multicanonical method and the simulated tempering, in the next section. We focus our attention to a Boltzmann-Gibbs distribution $P(\boldsymbol{X}) \propto \exp(-\beta E(\boldsymbol{X}))$ with $E(\boldsymbol{X})$ and β being a energy function and the inverse temperature, respectively, but an application for other distribution is straightforward. In Sec. 3, we explain the exchange MC method in detail. A way of preparing a parameter set before simulation and how to check equilibration of the system by the exchange MC method are also discussed. The last section is devoted to concluding remarks.

2 Extended Ensemble methods

The extended ensemble methods are based on the idea that an appropriate extension of the canonical ensemble may make MC sampling much more efficient at low temperatures. One of them is the multicanonical method[10]. For a given energy function $E(\boldsymbol{X})$, where $\boldsymbol{X}$ represents a state (or configurations) of the system, a weight factor different from the ordinary Boltzmann-Gibbs weight is introduced, namely the partition function or the normalization factor is expressed as

$$Z_{\mathrm{M}} = \sum_{\boldsymbol{X}} \exp(-E_M(\boldsymbol{X})) \tag{1}$$

with the effective energy function

$$E_M(\boldsymbol{X}) = \beta_M(E)E(\boldsymbol{X}) + \alpha_M(E) \tag{2}$$

where the parameter $\alpha_M(E)$ and $\beta_M(E)$ are to be chosen as a function of E such that the probability distribution $P_M(E)$ finding the system in states with the energy E is approximately flat in an energy range of interest;

$$P_M(E) = g(E)\exp(-E_M(\boldsymbol{X})) = g(E)\exp(-\beta_M(E)E + \alpha_M(E)) \simeq \text{constant}, \tag{3}$$

where $g(E)$ is the density of states.

The resultant MC simulation produces configurations with the multicanonical weight $\exp(-E_M)$ which is proportional to $g^{-1}(E)$. Therefore highly excited configurations between metastable states are much

frequently explored in the simulations and the system can easily visit various local minima, or the whole phase space. Since the multicanonical parameters α_M and β_M are prior unknown in general, they are estimated preliminary MC runs. Once setting the parameters, the canonical expectation value can be reconstructed for any temperature , in principle, by the re-weighting method[19] In applying random spin systems such as spin glasses, the multicanonical parameters should be estimated for each sample because it strongly depends on structure of local minima in each sample[20]. This is a time consuming part of the multicanonical method. This difficulty is recently resolved in a practical sense by using recursion scheme, called Wang-Landau algorithm[21].

In the simulated tempering[11, 12], on the other hand, the ensemble is extended such that temperature is also a state variable. A state is thus specified by $(\boldsymbol{X}, m)$, the configuration $\boldsymbol{X}$ and the inverse temperature $\beta = \beta_m$. Here β takes one of M values in $\{\beta_1, \beta_2, \cdots, \beta_M\}$. The partition function is then expressed as

$$Z_{ST} = \sum_{m}^{M} \sum_{\boldsymbol{X}} \exp\left(-E_{ST}(\boldsymbol{X}, m)\right) = \sum_{m}^{M} Z(\beta_m) \exp(g_m), \tag{4}$$

where $Z(\beta)$ is the partition function for the original system. The effective energy function for the simulated tempering is given by

$$E_{ST}(\boldsymbol{X}, m) = \beta_m E(\boldsymbol{X}) - g_m, \tag{5}$$

where the parameters $\{g_m\}$ are determined such that each β_m is equally realized in this ensemble. The best choice is given by equating the factor $Z(\beta_m)g_m$ to one, which means $g_m = -\log(Z(\beta_m))$. By applying the conventional MC dynamics to this extended ensemble, the state $(\boldsymbol{X}, m)$ traverses over the configuration space and also temperature, so that the system can escape from local minima by this self annealing and heating.

Although the simulated tempering works well for a random spin system[11], one may be faced to a difficulty in choosing appropriate g parameters, which should be determined before simulations. Since g_m is an extensive parameter, the probability for finding a given state m is very sensitive to the choice and temperature wandering would be broken down if the estimation of g_m is not suitable. For example, suppose the case that g_m is set to be a constant independent of m. Then, the state $(\boldsymbol{X}, m)$ is favorable to high temperature states by an entropic effect and never comes back to low temperatures of our interest. An appropriate choice of the parameter in the simulated tempering is crucial for efficiency of the simulation, which is similar to the multicanonical method,

3 Exchange Monte Carlo method

In this section we explain exchange Monte Carlo method (EMC), which is called also as parallel tempering[17, 18]. In EMC we treat a combined system which consists of non-interacting M replicas of the system described by a common energy function $E(\boldsymbol{X})$. The m-th replica is in contact with its own heat bath having inverse temperature β_m (for convenience we take $\beta_m < \beta_{m+1}$). A state of this extended ensemble

is specified by M configurations $\{\boldsymbol{X}\} = \{\boldsymbol{X}_1, \boldsymbol{X}_2, \cdots, \boldsymbol{X}_M\}$, and the partition function is given by

$$\mathcal{Z}_{\rm E} = \sum_{\{\boldsymbol{X}\}} \exp\left(-E_{EMC}(\{\boldsymbol{X}\};\{\beta\})\right) = \prod_{m=1}^{M} Z(\beta_m), \tag{6}$$

where the effective energy for EMC is defined as

$$E_{EMC}(\{\boldsymbol{X}\};\{\beta\}) = \sum_{m=1}^{M} \beta_m E(\boldsymbol{X}_m). \tag{7}$$

For a set of temperatures $\{\beta\}$ given, the simultaneous distribution for finding $\{\boldsymbol{X}\}$ is expressed as a simple product formula

$$\mathcal{P}_{EMC}(\{\boldsymbol{X}\};\{\beta\}) = \frac{e^{-E_{EMC}}}{\mathcal{Z}_E} = \prod_{m=1}^{M} P_{\rm eq}(\boldsymbol{X}_m, \beta_m), \tag{8}$$

where $P_{\rm eq}(\boldsymbol{X})$ is the canonical equilibrium distribution for the original system. It is noted that this extended ensemble is different from that of the simulated tempering. Namely, temperature is not a state variable in the present ensemble, and its phase space is a direct product of the original ones, while that of the simulated tempering is a direct sum of them. Because of this, the EMC method does not have any auxiliary parameter as in the simulated tempering.

We introduce two types of updating in constructing a Markov chain in EMC. One is conventional updates that satisfy the detailed balance condition for each canonical distribution $P_{\rm eq}(\boldsymbol{X}_m, \beta_m)$. In addition to the usual local updates, we define a replica exchange between two replicas, *i.e.,* $\{\boldsymbol{X}_m, \boldsymbol{X}_n\} \to \{\boldsymbol{X}_n, \boldsymbol{X}_m\}$. The replica exchange part of transition probability $W(\boldsymbol{X}, \boldsymbol{X}'; \beta_m, \beta_n)$ is determined by the detailed balance condition for the simultaneous distribution (8) and is obtained as

$$W(\boldsymbol{X}, \boldsymbol{X}'; \beta_m, \beta_n) = \begin{cases} \min\left(1, \exp(-\Delta)\right), & \text{for Metropolis type,} \\ \frac{1}{2}\left(1 + \tanh(-\frac{\Delta}{2})\right), & \text{for heat bath type,} \end{cases} \tag{9}$$

where

$$\Delta(\boldsymbol{X}, \boldsymbol{X}'; \beta_m, \beta_n) = (\beta_n - \beta_m)(E(\boldsymbol{X}) - E(\boldsymbol{X}')). \tag{10}$$

Note that the simultaneous distribution of Eq. (8) is invariant under these updates.

In the actual MC procedure, the following two steps are performed alternately:

(1) Each replica is simulated *simultaneously* and *independently* as canonical ensemble for a few MC steps by using a standard MC method.

(2) Exchange of two configurations $\boldsymbol{X}_m$ and $\boldsymbol{X}_{m+1}$, is tried and accepted with the probability (9).

Here we restrict the exchange processes to the case $n = m + 1$ because the acceptance ratio of the exchange trial decreases exponentially with the difference $|\beta_m - \beta_n|$ as shown in (9). By these processes each configuration can traverse along the temperature axis while it changes itself by the above process (1)(see Fig. 1). Consequently, slow relaxation at low temperatures is reduced by mixing of the fast

relaxation at higher temperatures. The canonical expectation value of a physical quantity A is measured in a usual way as

$$\langle A \rangle_{\beta_m} = \frac{1}{N_{\rm mcs}} \sum_{t=1}^{N_{\rm mcs}} A(\boldsymbol{X}_m(t)), \tag{11}$$

where $N_{\rm mcs}$ is the sampling number. The reweighting procedure is not needed as in the multicanonical method, because the Boltzmann weights are used as the ensemble for each m.

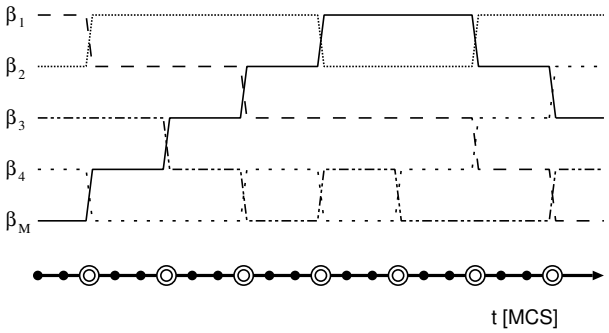

Figure 1: A schematic picture of the exchange MC method. Each line represents a configuration $\boldsymbol{X}_m(t)$ which is attached to the m-th heat-bath at $t = 0$. They are simulated by the standard MC method at times denoted by $\bullet$, and the exchange processes are tried at times denoted by $\circledcirc$.

3.1 Setting temperature points

The parameters we have to determine are only the set of (inverse) temperatures $\{\beta_m\}$. The highest temperature should be set sufficiently high so that there exists only one free energy minimum in the whole phase space and relaxation (correlation) time is enough short, otherwise the system would not completely forget where it was trapped before even if it visits to the highest temperature. On the other hand, the lowest temperature is somewhere in the low temperature phase whose properties we are interested in. An important point to be discussed is the number of temperatures required in the range thus specified. In order for each configuration to wander over the whole temperature range the acceptance probabilities of the exchange process for every pair of replicas at neighboring temperatures have to be of the order of unity and nearly constant. The logarithm of the exchange probability, eq. (9) with $\beta_{n+1} = \beta_n + \delta$ is, up to order δ^2,

$$\Delta = \delta(E(\boldsymbol{X}_{n+1}) - E(\boldsymbol{X}_n)) \sim \delta^2 \frac{\mathrm{d}}{\mathrm{d}\beta} E, \tag{12}$$

where the instantaneous value of the energy E is approximated by the thermal expectation value E. Since the energy E is an extensive variable and it is proportional to the system size N, δ should be of the order of $\frac{1}{\sqrt{N}}$ to satisfy the condition that $\Delta \sim O(1)$. In other words, the number of temperature points we have to simulate is of the order of $\sqrt{N}$.

In the case that a second-order phase transition occurs in the temperature range to be simulated, we have to take care of also a choice of the temperature points. Actually the exchange process is suppressed with increasing linear size L, when we choose equidistant $\{\beta_n\}$. An example is demonstrated for the simple $2d$ Ising ferromagnet in Fig. 2. Random walkers on the temperature axis in the EMC method become confined in high or low temperature phase as L increases.

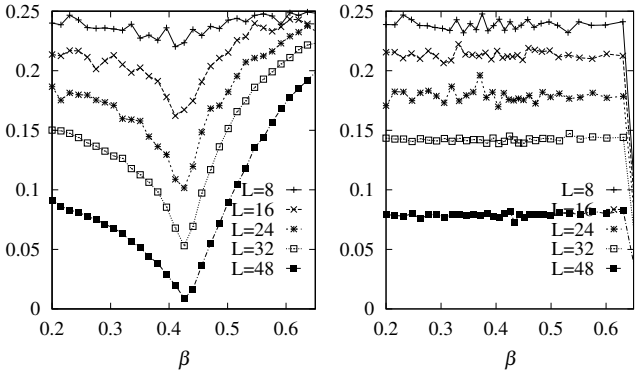

Figure 2: Acceptance probability for the exchange process as a function of the inverse temperature β in the two dimensional Ising ferromagnetic model. In the left panel, $\{\beta_n\}$ are chosen equidistant, while in the right panel they are determined by the iteration procedure in the text.

Here we propose a practical way to get rid of the difficulty mentioned just above. For simplicity, we consider a procedure for setting a temperature point β_n between two fixed ones, β_{n-1} and β_{n+1}. Our criterion is that acceptance probabilities for the exchange trial with both neighboring temperatures become equal:

$$\begin{aligned}(\beta_{n-1}-\beta_n)(E(\beta_{n-1})-E(\beta_n)) &= C,\\ (\beta_n-\beta_{n+1})(E(\beta_n)-E(\beta_{n+1})) &= C,\end{aligned} \tag{13}$$

where C and β_n are unknown constants. A formal solution for β_n is given by,

$$\begin{aligned}\beta_n = R(\beta_n) = \frac{1}{E(\beta_{n-1})-E(\beta_{n+1})} \times (\beta_{n-1}E(\beta_{n-1})\\ -\beta_{n+1}E(\beta_{n+1}) - E(\beta_n)(\beta_{n-1}-\beta_{n+1})).\end{aligned} \tag{14}$$

Regarding $\beta' = R(\beta)$ as a map of β to β', we find an fixed point of period 2 with $\beta_{n+1} = R(\beta_{n-1})$ and $\beta_{n-1} = R(\beta_{n+1})$. Therefore, we expect a repulsive fixed point between β_{n-1} and β_{n+1}. A new mapping to obtain the fixed point is given by[25],

$$\beta_n(t+1) = \frac{1}{2}(\beta_n(t) + R(\beta_n(t))), \tag{15}$$

where t is the iteration step. In actual iterations, the initial temperature points $\{\beta_n\}$ are set in a suitable way, for example, equidistant β. The convergence of the iteration is rapidly achieved in many systems we have investigated. By making use of the temperature points thus determined for the $2d$ Ising ferromagnet, the acceptance ratio almost independent of temperature is realized as shown in the right panel of Fig. 2.

From our experiences so far, efficiency of the EMC method is rather insensitive for the choice of temperature points, when it is applied to systems, such as spin glasses. This fact that it is not necessary to specify any parameters before main simulation is, in fact, one of big advantages of the EMC method against the other extended ensemble methods. Nevertheless we emphasize that a little effort on preparing the temperature points by pre-MC runs following the prescription described above ensures the acceptance ratio almost independent of temperature and so is quite useful.

3.2 Equilibration check

In MC simulations, one needs to check carefully whether the system really reaches equilibrium. A simplest check for equilibration is to see if measured quantities converge to a certain constant value. This is not sufficient for "hardly-relaxing" systems because the convergence apparently occurs even when system is got trapped into a metastable state. A strong criterion for equilibration has been proposed by Bhatt and Young[28] for the conventional MC simulation on spin glasses. In their procedure two estimates for one quantity are used. They are expected to come closer to an equilibrium value from the opposite sides as MC steps increase so that their coincidence is a criterion for equilibration. Explicitly, one of the estimates is the overlap of two sets of spins starting from configurations independent of each other, and the other is the overlap of one set of spins but at different MC times. For the EMC method, however, the two estimates exhibit common behavior after a short transient time because of the exchange process between (uncorrelated) replicas with different heat baths.

So far the following conditions have been proposed to check equilibration in the EMC method [13, 17].

(i) The exchange happens with a non-negligible probability for all adjacent pairs of replicas.

(ii) Each configuration moves around the whole temperature range in suitable MC steps.

(iii) In moving the temperature axis each configuration forgets where it was trapped before.

(iv) measured quantities of interest converge to a constant value.

Condition (i), with nearly equal acceptance ratios in the whole temperature range, is satisfied if we choose the temperature points as described in the previous subsection. A characteristic time scale in connection with condition (ii) is associated with a random walk of each configuration along the temperature axis. It is explicitly defined as the average MC step for each configuration to move from the lowest to the highest temperatures, and is called the ergodicity time (denoted by $\tau_{\rm erg}$) on the analogy of the multicanonical method[10]. The ergodicity time was observed in the mean-field Sherrington-Kirkpatrick(SK) spin-glass model with varying M[30]. It was found that $\tau_{\rm erg}$ increases almost linearly to the system size N when M is moderately increased with N. This $\tau_{\rm erg}$ is smaller by orders of magnitude than the time required to overcome free-energy barriers between the pure states (of the order of $N^{1/4}$) by the conventional MC process[29].

Even when one obtains a reasonable value of $\tau_{\rm erg}$, it may occur that the system does not forget where it was trapped before and has a long time memory. A possible reason for this is that the largest temperature used is not high enough. In order to examine condition (iii) explicitly, an autocorrelation function of each configuration $\boldsymbol{X}_m(t)$ (see Fig.1) ,

$$q(t,\beta_m) \equiv \langle \boldsymbol{X}_m(0) \cdot \boldsymbol{X}_m(t) \rangle, \tag{16}$$

was introduced and was examined in an Ising spin glass model[13]. The function was found to exhibit an exponential decay with a finite relaxation time $\tau_{\rm cor}$ (see Fig. 3). This indicates that each configuration

forgets about its history by a time scale of $\tau_{\rm cor}$ on average. At low temperatures $\tau_{\rm cor}$ is almost independent of temperature, and its value is comparable with $\tau_{\rm erg}$ and is largely reduced as compared with the correlation time measured by the conventional MC method (the latter grows to the order of 10^7 MC steps near the spin-glass transition temperature in a system with $L = 16$[27]).

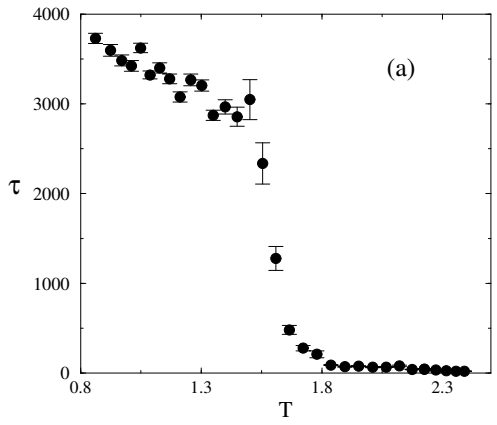

Figure 3: Temperature dependence of the relaxation time $\tau_{\rm cor}$ of the autocorrelation function of $\boldsymbol{X}_m(t)$, eq. (16), in a three-dimensional Ising spin-glass model, quoted from the reference [13].

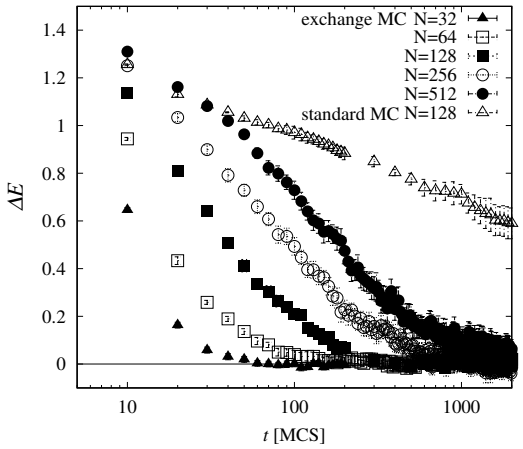

Figure 4: Relaxation dynamics of the difference between two kinds of energy as a function of the MC step for the N=32, 64, 128, 256, and 512. For comparison, the standard MC data for $N = 128$ are also shown by open triangles.

Given $\tau_{\rm erg}$ and $\tau_{\rm cor}$ ($\tau_{\rm erg} \sim \tau_{\rm cor}$), a time required for equilibration is estimated as at least $2N_{\rm l.m.}/M$ times $\tau_{\rm erg}$, where $N_{\rm l.m.}$ is the number of free-energy local minima which have non-negligible Boltzmann weight at the temperature of interest. Since $N_{\rm l.m.}$ is not known *a priori*, to see convergence of physical quantities revives as an equilibration check. It is, of course, desirable if there exist, even in the EMC method, certain quantities to which we apply the Bhatt-Young like procedure mentioned above.

For the SK model, for example, there is the rigorous relation between the equilibrium values,

$$E(T) = \frac{1}{2T}(1 - q^2(T)), \tag{17}$$

where E is energy evaluated in individual replicas and q^2 is the squared overlap function of a pair of replicas. Furthermore both sides of the above equation approach to an equilibrium value from opposite sides with each others as MC steps increase. It was found[30] in systems with $N \leq 512$ that difference between these estimates obeys almost an exponential law as a function of MC steps, instead of the power law usually observed in the conventional MC method (see Fig. 4). The characteristic time scale of the decay increases linearly to N and only weakly depends on temperature. This may imply that, at least in systems investigated with $N \leq 512$, $N_{\rm l.m.}$ is comparable to M (≤ 20 in the simulations) and/or M uncorrelated replicas are efficient for sampling configurations in the entire phase space.

4 Concluding remarks

We have presented the temperature exchange MC method in section 3.1, but an implementation for other exchange parameters other than temperature is straightforward. Namely, it is possible to construct the exchange MC algorithm for a parameter in the energy function of the system instead of temperature. Then, the parameter axis should include two important points at both ends. One is a target point in the ordered phase whose properties we are interested in and the other is a source point in a disordered phase. The EMC method lies on the expectation that configurations at the target point are refreshed through the exchange process from the source point where new configurations are produced within a limited number of MC steps. The multicanonical MC method and the simulated tempering share a similar idea.

One of the most important advantages of the extended ensemble MC over a conventional MC is to accelerate the slow relaxation. Another would be in the calculations of the density of states $g(E)$, the free energy or the normalization constant, which are hard to estimate directly by the conventional MC. In particular, the multicanonical method has frequently been used for obtaining $g(E)$ in various statistical-mechanical models[10]. The multicanonical method samples configurations with a weight of $1/g(E)$ which is approximately estimated in preliminary runs. As a result the marginal distribution of E becomes constant with a significant range of E, implying that a random walk along the energy axis is realized. The density of states $g(E)$ is efficiently calculated by a reweighting formula, because the random walk with the weight $1/g(E)$ covers a wide range of E. Recently, the Wang-Landau method has been proposed as a specialized version of multicanonical method for estimating the density of states with quite high accuracy [21]. EMC as well as the simulated tempering gives a set of the canonical distribution $g(E)e^{-\beta E}$ with a wide range of *temperature*. This is a counterpart of the multicanonical method which gives a relatively flat histogram with a wide range of *energy*. In EMC, a reweighing formula based on multiple-histogram method[19] would be suitable for calculating the density of states[22], while other attempts have been made[23, 24].

In conclusion, the idea of extended ensemble method in MC algorithms are reviewed. In particular, we discuss the exchange MC method which belong to the extended ensemble methods in detail. This method has been applied to various hardly-relaxing system and turned out to be quite useful in sampling from the distribution of the system. A prominent feature of the method is its simplicity and robustness. We expect that it provide us rich information on various hardly-relaxing problems, including optimization problems.

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