Irreversible Markov-Chain Monte Carlo methods

Koji HUKUSHIMA
Department of Basic Science, University of Tokyo
3-8-1 Komaba, Meguro-ku, Tokyo 153-8902

Abstract

We review irreversible Markov chain Monte Carlo (MCMC) methods, which violate detailed balance and yet still converge to a given target probability distribution. One way to construct an irreversible Markov chain is to enlarge the sampling space from the original space used in the reversible one. The idea is often referred to as "lifting". Two independent irreversible MCMC methods, belonging to the lifting MCMC, are discussed.

1 Introduction

Markov chain Monte Carlo (MCMC) methods have been intensively used as sampling tools from a high-dimensional probability distribution in a wide area of physics, biology and statistical sciences. In particular, MCMC methods are one of the non-peturbative analysis methods for many-body problems in the research field of statistical physics and condensed matter. Some advanced algorithms based on extended ensemble method [2] such as the multicanonical method [3], the simulated tempering [4, 5] and the exchange MC method [6] or parallel tempering, allows us to study more complex systems with rugged free-energy landscape, which are difficult to equilibriate by a simple MCMC algorithm with local update.

Since the seminal paper by Metropolis *et al.* in 1953 [1], most of the MCMC algorithms are on the basis of the Metropolis strategy, in which a Markov chain of the random variables to be sampled makes the target distribution an invariant distribution. Then, one may often impose the detailed balance condition (DBC) for Markov chain, called a reversible MCMC method. It is, however, not always necessary to construct the MCMC method using DBC. One of the pioneering works has been done by Suwa and Todo[7, 8], in which a systematic construction procedure is proposed for the MCMC algorithm without DBC, but with the global balance condition, called an irreversible MCMC method. They showed that the proposed method is able to bring about several times reduction in the correlation time of Potts model and a quantum spin model. Subsequently, Turitsyn *et al.* [9] and Fernandes and Weigel [10] have proposed another type of MCMC method without DBC separately and they also found a qualitative improvement in efficiency of the MCMC method in a mean-field Ising model. Furthermore, from a completely different context in statistical physics, another MCMC algorithm breaking DBC, called event-chain Monte Carlo algorithm, has been developed mainly for interacting particle systems.

These works have attracted a great deal of attention to the MCMC algorithms without DBC. The Markov chain dynamics with DBC exhibits diffusive behavior in sampling space, which yields slowing down close to phase transitions. We expect that it would be helpful to have some inertia effect by breaking DBC as if the sugar in a cup of coffee is spread faster using a spoon to stir the cup. In the framework of DBC, a useful guiding principle for constructing an efficient MCMC algo-

rithm is given by Peskun's theorem [11]. According to the theorem, it turns out that an MCMC algorithm is improved in quality by reducing a rejection probability in the sense that asymptotic variance of any observable becomes small. The strategy of Suwa-Todo algorithm follows this line. In general, however, no such a principle is satisfied in the case of the MCMC method without DBC. Therefore, it would be worth establishing an intrinsic principle of the MCMC method without DBC. In the mathematics literature[19], the idea of lifting is discussed as a promising way to introduce an irreversible MCMC method by enlarging sampling space from the original one. In fact, some of the above-mentioned MCMC algorithms without DBC belong to the lifting MCMC method[18].

In the present report, we make a review on irreversible MCMC methods, in which the basic idea and an implementation of the algorithm are discussed. In particular, we focus our attention to two different irreversible MCMC methods, one with a skew detailed balance condition (SDBC) [9] and the event-chain MCMC method.

2 Irreversible MCMC with skew detailed balance condition

2.1 Skew detailed balance conditions

In this section, we review an irreversible MCMC method with the skew detailed balance condition originally proposed by Turitsyn, Chertkov and Vucelja [9]. Here, an Ising spin system is used for the purpose of illustration. It is straightforward to extend the method to any discrete state models [12] such as the Potts model. A state of the Ising model with N spins is specified by a vector $\boldsymbol{\sigma} = (\sigma_1, \ldots, \sigma_N)$ with $\sigma_j \in \{-1, +1\}$ for $j = 1, \ldots, N$. The target distribution $\pi(\boldsymbol{\sigma})$ for finding the state $\boldsymbol{\sigma}$ in the statistical physics is often proportional to the Boltzmann factor $\exp(-\beta E(\boldsymbol{\sigma}))$ where β is an inverse temperature and E is the energy of the system to be studied. The main aims of the MCMC methods are to generate samples of the state from the target distribution $\pi(\boldsymbol{\sigma})$, and to calculate an expectation value of a function $\hat{f}$ under the target distribution, e.g. $\langle \hat{f} \rangle_\pi = \sum_{\boldsymbol{\sigma}} \pi(\boldsymbol{\sigma}) f(\boldsymbol{\sigma})$ where $f(\boldsymbol{\sigma})$ is the realization of $\hat{f}$ with the state $\boldsymbol{\sigma}$ and $\sum_{\boldsymbol{\sigma}}$ denotes the summation over 2^N states.

In the lifting technique, the state space is doubled by introducing an additional Ising variable $\epsilon \in \{-1, +1\}$, which is called a lifting parameter. The state in the enlarged state space is denoted by $X = (\boldsymbol{\sigma}, \epsilon) \in \{-1, +1\}^{N+1}$ and the corresponding probability distribution $\tilde{\pi}$ is assumed to be independent of the lifting parameter ϵ:

$$\tilde{\pi}(\boldsymbol{\sigma}, \epsilon) = \tilde{\pi}(\boldsymbol{\sigma}, -\epsilon) = \frac{\pi(\boldsymbol{\sigma})}{2}. \tag{1}$$

We consider a single spin-flip update for both the original spin $\boldsymbol{\sigma}$ and the lifting parameter ϵ as an elementary process in the Markov chain. Let F_j be a spin-flip operator on the j-th site: $F_j\boldsymbol{\sigma} = (\sigma_1, \ldots, -\sigma_j, \ldots, \sigma_N)$. A transition rate per unit time from state $(\boldsymbol{\sigma}, \epsilon)$ to $(F_j\boldsymbol{\sigma}, \epsilon)$ is denoted as $w_j(\boldsymbol{\sigma}, \epsilon)$ and that from state $(\boldsymbol{\sigma}, \epsilon)$ to $(\boldsymbol{\sigma}, -\epsilon)$ is $\lambda(\boldsymbol{\sigma}, \epsilon)$. Using these transition rates, the balance condition (BC) is expressed as

$$\sum_j w_j(F_j\boldsymbol{\sigma}, \epsilon)\tilde{\pi}(F_j\boldsymbol{\sigma}, \epsilon) - \sum_j w_j(\boldsymbol{\sigma}, \epsilon)\tilde{\pi}(\boldsymbol{\sigma}, \epsilon) + \lambda(\boldsymbol{\sigma}, -\epsilon)\tilde{\pi}(\boldsymbol{\sigma}, -\epsilon) - \lambda(\boldsymbol{\sigma}, \epsilon)\tilde{\pi}(\boldsymbol{\sigma}, \epsilon) = 0.$$

This ensures that $\tilde{\pi}$ is the unique invariant distribution of the Markov chain. For the determination of the transition rate $w_j(\boldsymbol{\sigma}, \epsilon)$, we impose SDBC given by

$$\tilde{\pi}(\boldsymbol{\sigma}, \epsilon) w_j(\boldsymbol{\sigma}, \epsilon) = \tilde{\pi}(F_j\boldsymbol{\sigma}, -\epsilon) w_j(F_j\boldsymbol{\sigma}, -\epsilon). \tag{2}$$

This requires that the stochastic flow from state $(\boldsymbol{\sigma}, +\epsilon)$ to $(F_j\boldsymbol{\sigma}, +\epsilon)$ is balanced out

by that from $(F_j\boldsymbol{\sigma}, -\epsilon)$ to $(\boldsymbol{\sigma}, -\epsilon)$. In general, this condition breaks the detailed balance conditions (DBC): $\tilde{\pi}(\boldsymbol{\sigma}, \epsilon) w_j(\boldsymbol{\sigma}, \epsilon) = \tilde{\pi}(F_j\boldsymbol{\sigma}, \epsilon) w_j(F_j\boldsymbol{\sigma}, \epsilon)$. As a specific solution of (2) , the transition rate $w_j(\boldsymbol{\sigma}, \epsilon)$ is given by

$$w_j(\boldsymbol{\sigma}, \epsilon) = \frac{1}{2}\alpha \left(1 - \sigma_j \tanh \beta h_j\right)\left(1 - \delta\epsilon\sigma_j\right), \tag{3}$$

where α is a time constant and h_j is a local field acting on the site j. The possible range of δ is -1 to 1 and DBC is recovered in (3) with $\delta = 0$. The transition rate is equivalent to the conventional heat-bath transition rate under a virtual external field ϵH with $H = \frac{1}{\beta} \operatorname{arctanh} \delta$. Thus, the lifting parameter ϵ represents the direction of the virtual field in this case. While ϵ is coupled to the local order parameter σ_j in this transition rate, one can replace it with any other linear function of σ_j such as a local energy $\sigma_j h_j$. The choice of the transition rate might affect the efficiency of the MCMC method, depending on the model system to be studied, but this has not been clarified yet at this moment.

By using SDBC, BC is rewritten as

$$\lambda(\boldsymbol{\sigma}, \epsilon) - \lambda(\boldsymbol{\sigma}, -\epsilon) = \sum_j \left(w_j(\boldsymbol{\sigma}, -\epsilon) - w_j(\boldsymbol{\sigma}, \epsilon)\right). \tag{4}$$

The explicit form of the transition rate for ϵ flip is not unique. Turitsyn *et al.* [9] have proposed the transition rate as

$$\lambda(\boldsymbol{\sigma}, \epsilon) = \max\left(0, \sum_j \left(w_j(\boldsymbol{\sigma}, -\epsilon) - w_j(\boldsymbol{\sigma}, \epsilon)\right)\right), \tag{5}$$

which is referred to as the Turitsyn-Chertkov-Vucelja (TCV) type. Another type of $\lambda(\boldsymbol{\sigma}, \epsilon)$ is also given as

$$\lambda(\boldsymbol{\sigma}, \epsilon) = \sum_j w_j(\boldsymbol{\sigma}, -\epsilon), \tag{6}$$

which is referred to as the Sakai-Hukushima 1 (SH_1) type [13]. These transition rates are available for a general class of the Ising models.

2.2 Irreversible Metropolis-Hastings algorithm

In this subsection, we explain an actual procedure in MCMC simulations which is based on Metropolis-Hastings algorithm [14]. Let $X^{(n)}$ be the state in the enlarged state space after n iterations. The irreversible MCMC method starts with an arbitrary initial state $X^{(0)}$ and iterates the following steps for $n = 1, 2, \ldots$:

(a) Suppose that the current state $X^{(n)} = (\boldsymbol{\sigma}, \epsilon)$ and choose a site j at random.

(b) Accept the new state as $X^{(n+1)} = (F_j\boldsymbol{\sigma}, \epsilon)$ with the probability $w_j(\boldsymbol{\sigma}, \epsilon)$.

(c) If it is rejected, accept the ϵ flipped state as $X^{(n+1)} = (\boldsymbol{\sigma}, -\epsilon)$ with an acceptance rate

$$A(\epsilon \to -\epsilon; \boldsymbol{\sigma}) = \frac{\frac{1}{N}\lambda(\boldsymbol{\sigma}, \epsilon)}{1 - \frac{1}{N}\sum_j w_j(\boldsymbol{\sigma}, \epsilon)}. \tag{7}$$

(d) If it is also rejected, set $X^{(n+1)} = X^{(n)}$. Return to (a) and repeat the steps (a)–(d).

It is proved that these steps satisfy BC [12]. One MC step is defined as N iterations of the steps (a)–(d). To evaluate the acceptance rate in step (c), the summation with respect to the site is necessary and its computational complexity is of the order of N. In practice, once the summation is evaluated at the initial condition, it is sufficient to update the value of the summation when the spin-flip process is accepted. The complexity for the update is of the order of one in statistical-mechanical models with short range interactions.

2.3 Some applications

We demonstrate that the irreversible MCMC method explained above works efficiently in a statistical-mechanical model. Fig. 1 presents time dependence of autocorrelation function of the magnetization in a one-dimensional Ising

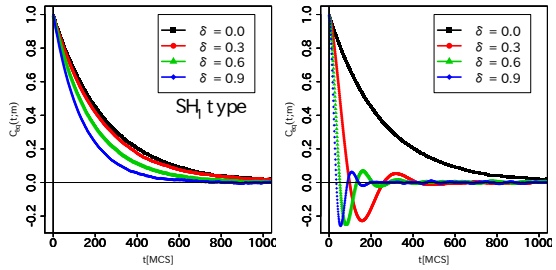

Figure 1: Time evolution of autocorrelation function of the magnetization density in the one-dimensional Ising model for different values of δ, which is a parameter representing the deviation from DBC. The chosen values of parameter in the simulations are $N = 2^7$, $\alpha = 10^{-2}$, $\gamma = 0.6$. The transition probability used is the SH_1(left) and TCV(right) types. Quoted from Ref. [13].

model using two different transition probabilities for SH_1 type (left) and TCV type (right). The autocorrelation decays fast with increasing the value of δ, indicating that breaking DBC makes the relaxation accelerate. Interestingly, oscillating behavior is clearly observed for TCV type. This is an intrinsic effect of the violation of DBC, never seen in the MCMC methods with DBC. The similar behavior is also found when the TCV type probability is applied to the mean-field Ising model[9]. These studies suggest that the dynamical exponent z could be reduced for the TCV type in the Ising models both in one dimension and the mean-field limit. However, such significant improvement of the efficiency is not confirmed in two- and three- dimensional Ising models[12].

On the other hand, the performance evaluation of the lifting MCMC methods has been extensively studied for an one-dimensional random walk problem. Several works showed that the diffusive dynamics in the problem is qualitatively changes by the lifting[19, 17]. While, no theoretical general criterion has not been established, it seems that an one-dimensional structure in the sampling space is necessary for the irreversible MCMC method with SDBC to work effectively.

2.4 Irreversible simulated tempering

Another interesting application is to combine the irreversible MCMC algorithm with the extended ensemble methods. In particular, the transition graph of the simulated tempering is exactly the same as that of the random walk problem. Thus, one may expect that SDBC makes the dynamics in the simulated tempering change qualitatively. Here we discuss the simulated tempering with SDBC[15, 16].

In the simulated tempering, the inverse temperature is treated as a random variable as well as the configuration $\boldsymbol{\sigma}$. More specifically, β takes R different values $\{\beta_r\}_{r=1}^R$ that should be determined before simulation. In addition, a lifting variable $\varepsilon \in \{+, -\}$ is also introduced to the system in the irreversible simulated tempering. Thus, a state in the irreversible simulated tempering is specified by $(\boldsymbol{\sigma}, \beta_r, \varepsilon)$. Accordingly, the target distribution is given as

$$P_{\mathrm{IST}}(\boldsymbol{\sigma}, \beta_r, \varepsilon) \propto \exp[-\beta_r E(\boldsymbol{\sigma}) + g_r], \qquad (8)$$

where g_r denotes a weight factor depending only on the inverse temperature.

An explicit update scheme of the irreversible simulated tempering algorithm consists of two steps. One is the update scheme of an original configuration $\boldsymbol{\sigma}$ for a fixed inverse temperature and the lifting variable with a conventional MCMC algorithm such as the Metropolis-Hastings algorithm and cluster algorithms. The other is the update scheme of the inverse temperature and the lifting variable for fixed $\boldsymbol{\sigma}$, described as follows:

(a) Let the current state be $(\boldsymbol{\sigma}, \beta_r, \varepsilon)$ and the candidate of the next inverse temperature β_l is determined with the probability $q_{r,l}^{(\varepsilon)}$ given as follows:

$$q_{1,2}^{(\varepsilon)} = q_{R,R-1}^{(\varepsilon)} = 1, \qquad (9)$$

$$q_{r,r\pm1}^{(\varepsilon)} = \frac{1 \pm \delta\varepsilon}{2}, \qquad (10)$$

for $1 < r < R$, and $q_{r,l}^{(\varepsilon)} = 0$ otherwise.

(b) Accept the next state $(\boldsymbol{\sigma}, \beta_l, \varepsilon)$ with the probability $W_{r,l}^{(\varepsilon)}$ given by

$$W_{r,l}^{(\varepsilon)} = \min\left[1,\ \frac{q_{l,r}^{(-\varepsilon)}}{q_{r,l}^{(\varepsilon)}} \frac{P_{\mathrm{IST}}(\boldsymbol{\sigma}, \beta_l, -\varepsilon)}{P_{\mathrm{IST}}(\boldsymbol{\sigma}, \beta_r, \varepsilon)}\right]. \tag{11}$$

(c) If the trial (b) is rejected, flip the lifting variable ε with the probability $\Lambda_r^{(\varepsilon)}$ given by

$$\Lambda_r^{(\varepsilon)} = \frac{\max\left[0,\ \varepsilon \sum_{\varepsilon'=\pm} \sum_{l\neq r} \varepsilon' q_{r,l}^{(-\varepsilon')} W_{r,l}^{(-\varepsilon')}\right]}{\left(1 - \sum_{l\neq r} q_{r,l}^{(\varepsilon)} W_{r,l}^{(\varepsilon)}\right)} \tag{12}$$

and set $(\boldsymbol{\sigma}, \beta_r, -\varepsilon)$ as the next state.

(d) If the trial (c) is also rejected, set the current state as the next state.

Note that the acceptance probability satisfies SDBC with respect to the target distribution $P_{\mathrm{IST}}(\boldsymbol{\sigma}, \beta_r, \varepsilon)$ and the global balance condition is fulfilled in the above procedure. The parameter δ in the proposal probability $q_{r,l}^{(\varepsilon)}$ controls the violation of DBC. When δ is set to zero, DBC is restored.

In Ref. [15], the irreversible simulated tempering algorithm has been applied to the two-dimensional ferromagnetic Ising model as a benchmark. It is numerically shown that the relaxation dynamics of the inverse temperature qualitatively changes from diffusive to ballistic behavior by violating DBC and consequently the autocorrelation time of the magnetization is reduced several times compared to the conventional simulated tempering for the case with an ideal choice of the weight factors. Thus, it is confirmed that the violation of DBC can improve the efficiency of simulated tempering algorithm. It is worth investigating whether the irreversible simulated tempering works effectively in a complex system such as spin glasses.

3 Event-chain Monte Carlo

The event-chain Monte Carlo (ECMC) algorithm is also one of the algorithms breaking DBC and is based on the idea of the lifting. The ECMC is proposed originally for hard-sphere systems[20] and is subsequently generalized for more general particle systems such as soft-sphere and LennardJones particles[22, 23], and continuous spin systems such as XY and Heisenberg spin models[24, 25]. This efficient algorithm enables us to simulate about 10^6 particles for the hard-sphere systems[21] and 10^6 spins for frustrated Heisenberg spin systems[26] in equilibrium. In this section, we describe the ECMC algorithm for particle systems and continuous spin systems.

3.1 Event-chain algorithm

We first explain the ECMC algorithm for hard-sphere systems in d dimensions. In the algorithm, the lifting parameter is defined as $U = (i, \vec{v})$ with i and $\vec{v}$ being the particle index and d dimensional vector, respectively. The particle i specified by the lifting parameter U moves along the direction $\vec{v}$ in U until it collides with another particle, and once the collision occurs the collided particle starts to move along the same direction $\vec{v}$. Consequently, many particles are moved along the same vector $\vec{v}$ until the total displacement of particles reaches ℓ, which is a tuning parameter of this algorithm. The displacement until the collision is uniquely determined by the configuration and the vector $\vec{v}$, and thus the dynamics of particles is deterministic for a given $\vec{v}$, the initial particle i, and ℓ. This algorithm breaks detailed balance because particles move along the same direction $\vec{v}$ and never go back to the former position [20].

For the hard-sphere systems, the pair potential is 0 for non-overlapping configurations and infinity for otherwise. Then, one can easily define a collision event as the time when the distance between the moving particle i and

another particle is twice of the particle radius. However, for general particle systems with an interaction potential such as Lennard–Jones systems, the pair potential for arbitrary distance always takes a finite value, and thus an event of collision cannot be defined in the same manner as the case of hard-sphere systems. The determination of a collision is essential for generalizing the ECMC method to more general interacting systems. This is possible by using three concepts[23]; the factorized Metropolis probability, infinitesimal moves, and an event-driven Monte Carlo scheme [27]. With the help of the factorization of the Metropolis transition probability, one can determine whether a proposal of a new state is accepted or not for each interacting pair independently, and the proposal is accepted only if all the interacting pairs accept it. If a new state is proposed by infinitesimally changing from the current state, then at most a particle interacting with the moving one reject the proposal; the probability that more than two pairs simultaneously reject the proposal with infinitesimal displacements is higher-order infinitesimal. Thus, we determine a collision as the probabilistic rejection which is caused by up to one interacting pair. Furthermore, an event-driven Monte Carlo scheme [27] allows us to compute the displacement until a collision efficiently. Consequently, a collision is defined in a probabilistic manner, and the ECMC algorithm is generalized for particle system with interaction potentials.

3.2 ECMC for general interacting systems

We present the ECMC algorithm for more general systems including some interacting particles system and also interacting spins systems in Algorithm 1. The Hamiltonian of the system considered in the algorithm is given by

$$H\left(\vec{x}_0, \cdots, \vec{x}_{N-1}\right) = \sum_{i<j} E_{ij}\left(\vec{x}_i, \vec{x}_j\right),$$

Algorithm 1 ECMC for more general potentials

Input N, ℓ, $\{\vec{x}_0, \cdots, \vec{x}_{N-1}\}$, $\{E_{ij}(\vec{x}_i, \vec{x}_j)\}_{i,j=0,\cdots,N-1}$, β
for $t \geq 0$ **do**
  $(i, \vec{v}) \leftarrow$ RANDOM(N, p)
  $s \leftarrow 0$
  while $s < \ell$ **do**
    $(\delta, j) \leftarrow$ DISPLACEMENT$(i, \vec{v})$
    if $s + \delta < \ell$ **then**
      $(\vec{x}_i, s) \leftarrow (T_{\vec{v}}(\delta)\,\vec{x}_i, s + \delta)$
      $i \leftarrow j$
    else
      $(\vec{x}_i, s) \leftarrow (T_{\vec{v}}(\ell - s)\,\vec{x}_i, \ell)$
    end if
  end while
end for
function RANDOM(N, p)
  Sample i uniformly from $\{0, \cdots, N-1\}$
  Sample $\vec{v}$ uniformly from $\{\vec{v}_0, \cdots, \vec{v}_{p-1}\}$ **return** $(i, \vec{v})$
end function
function DISPLACEMENT$(i, \vec{v})$
  for $k \in \{0, \cdots, N-1\} \setminus \{i\}$ **do**
    Sample r uniformly from $(0, 1]$
    Compute δ_k that satisfies

$$r = \exp\left(-\beta \int_0^{\delta_k} \max\left[0, \frac{\partial E_{ik}\left(T_{\vec{v}}(s)\,\vec{x}_i, \vec{x}_k\right)}{\partial s}\right] \mathrm{d}s\right)$$

  end for
  $j \leftarrow \arg\min_k \delta_k$
  $\delta \leftarrow \delta_j$ **return** (δ, j)
end function

where $\vec{x}_i$ represents a position vector of i-th particle for particle systems, or components of i-th spin for continuous spin systems. In the algorithm, p is the number of degrees of freedom per one particle or one spin, and $\{\vec{v}_i\}_{i=0,\cdots,p-1}$ is a set of linearly independent vectors. The state $\vec{x}_i$ is updated by an operator $T_{\vec{v}}(s)$; for particle systems $T_{\vec{v}}(s)\,\vec{x}_i = \vec{x}_i + s\vec{v}$, and for continuous spin systems $T_{\vec{v}}(s)\,\vec{x}_i = R_{\vec{v}}(s)\,x_i$ where $R_{\vec{v}}(s)$ is a rotation matrix around the vector $\vec{v}$ with an angle s. In this way, spin systems and particle systems are described by an ECMC algorithm on an equal footing.

It turns out that the ECMC algorithm out-

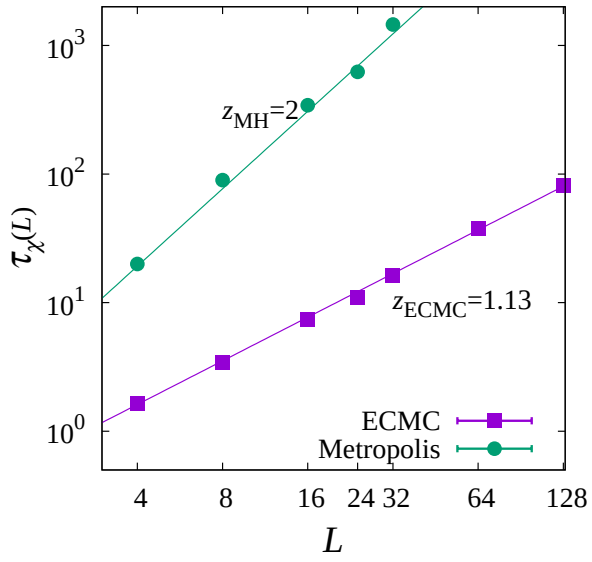

Figure 2: Linear-size dependence of characteristic time of susceptibility autocorrelation function in a three-dimensional Heisenberg ferromagnetic model obtained by ECMC and Metropolis-Hastings algorithm[25].

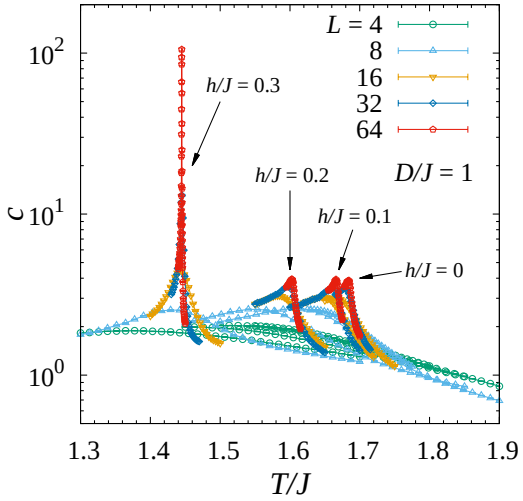

Figure 3: Temperature dependence of the specific heat of a three-dimensional chiral helimagnetic model under the external field h and the amplitude of DM interaction $D/J = 1$. The lattice is a cuboid and the total number of spins is $N = 8L^3$.

performs other conventional algorithms in various systems [20, 22, 28, 24], and one can simulate very large systems consisting of about 10^6 particles or spins in equilibrium by using the algorithm. We applied ECMC to a ferromagnetic Heisenberg ferromagnetic model in three dimensions, in which the algorithm reduces the value of the dynamical critical exponent z from $z = 2$ to $z \simeq 1$ [25], shown in Fig. 2. In contrast to cluster algorithms, the ECMC method works efficiently for frustrated spin systems. In fact, using a large scale simulation with ECMC, phase transitions in a Heisenberg spin model of a chiral helimagnet with the Dzyaloshinskii–Moriya (DM) interaction in three dimensions are studied[26]. In the presence of a magnetic field perpendicular to the axis of the helical structure, it is found that there exists a critical point on the temperature and magnetic-field phase diagram and that above the critical point the system exhibits a phase transition with strong divergence of the specific heat and the uniform magnetic susceptibility.

Quite recently, the ECMC algorithms have been developed for further generalization, which allows to simulate systems with three- and multi-body interactions. It is, however, still difficult to perform systems with anisotropic interactions. A naive implementation leads to multiple collisions yielding that the event chain splits into many chains, which is difficult to handle. In order to extend the ECMC algorithm for more complex systems such as polymers and protein problems, a certain key concept is required is required.

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