Event-chain Monte Carlo algorithm for continuous spin systems and its application

Yoshihiko Nishikawa
Department of Basic Science, The University of Tokyo 3-8-1 Komaba, Meguro, Tokyo 153-8902, Japan
E-mail: nishikawa@huku.c.u-tokyo.ac.jp

Koji Hukushima
Department of Basic Science, The University of Tokyo 3-8-1 Komaba, Meguro, Tokyo 153-8902, Japan
Center for Materials Research by Information Integration, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan
E-mail: hukusima@phys.c.u-tokyo.ac.jp

Abstract. The event-chain Monte Carlo (ECMC) algorithm is described for hard-sphere systems and general potential systems including interacting particle system and continuous spin systems. Using the ECMC algorithm, large-scale equilibrium Monte Carlo simulations are performed for a three-dimensional chiral helimagnetic model under a magnetic field. It is found that critical behavior of a phase transition changes with increasing the magnetic field.

1. Introduction
Since the proposal by Metropolis et al. [1], Markov-chain Monte Carlo (MCMC) algorithms have been used in a wide range of research fields such as statistics, chemistry, and physics. Particularly, in statistical physics, MCMC algorithms are powerful methods to study finite-dimensional effects of many-body systems. However, some simple algorithms with local updates including the original Metropolis algorithm frequently suffer from difficulties of slow relaxation such as critical slowing down associated with continuous phase transitions, nucleation process in first-order phase transitions, and glassy dynamics in complex systems. These slowing-down problems make Monte Carlo simulations take very long time and the precision of physical quantities be decreased. In order to overcome the slowing down, roughly two types of algorithms have been proposed: the first type is the cluster algorithms [2, 3] and the other one is the extended ensemble algorithm [4–9].

Recently, another type of algorithms has attracted a great interest: that is the Monte Carlo algorithms which break the detailed balance condition, but satisfy the global balance condition [10–12]. The event-chain Monte Carlo (ECMC) algorithm, originally proposed for hard-sphere systems [13], is one of such algorithms breaking the detailed balance condition. This efficient algorithm enables us to simulate about $10^6$ particles in equilibrium [14]. Furthermore, it can be generalized for more general particle systems such as soft-sphere and Lennard–Jones particles.
[15, 16], and continuous spin systems such as $XY$ and Heisenberg spin models [17, 18]. In the next section, we describe the ECMC algorithm for particle systems and continuous spin systems.

2. The event-chain Monte Carlo algorithm

Algorithm 1 describes the ECMC algorithm for hard-sphere systems in $d$ dimensions. We denote the radius of particles as $\sigma$, the total number of particles as $N$, the locations of particles as $\{x_k\}_{k=0, \cdots, N}$, and the standard basis of $\mathbb{R}^d$ as $\{e_k\}_{k=0, \cdots, d-1}$. In the function DISPLACEMENT $(i, v)$, we compute how long $i$-th sphere can move along the vector $v$ until it collides with another particle, and the collided particle starts to move along the same vector $v$. Consequently, many particles are moved along the same vector $v$ until the total displacement of particles reaches $\ell$, which is a tuning parameter of this algorithm. The displacement until the collision is uniquely determined by the configuration and the vector $v$, and thus the dynamics of particles is deterministic for given $v$, the initial particle $i$, and $\ell$. This algorithm breaks detailed balance because particles move along the same direction $v$ and never go back to the former position [13].

For the hard-sphere systems we can define a collision as the time when the distance between the moving particle $i$ and another particle is $2\sigma$ because the pair potential is 0 for non-overlapping configurations and infinity for otherwise. 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 a collision cannot be defined in the same manner as the case of hard-sphere systems. In order to define a collision for more general systems and generalize the

---

Algorithm 1: ECMC for hard sphere systems in $d$ dimensions

1: Input $N$, $\ell$, $\{x_0, \cdots, x_{N-1}\}$, $\sigma$
2: for $t \geq 0$ do
3:   $(i, v) \leftarrow$ RANDOM$(N, d)$
4:   $s \leftarrow 0$
5:   while $s < \ell$ do
6:     $(\delta, j) \leftarrow$ DISPLACEMENT$(i, v)$
7:     if $s + \delta < \ell$ then
8:       $(x_i, s) \leftarrow (x_i + \delta v, s + \delta)$
9:       $i \leftarrow j$
10:   else
11:      $(x_i, s) \leftarrow (x_i + (\ell - s)v, \ell)$
12:   end if
13: end while
14: end for
15: function RANDOM$(N, d)$
16:   Sample $i$ uniformly from $\{0, \cdots, N-1\}$
17:   Sample $v$ uniformly from $\{e_0, \cdots, e_{d-1}\}$
18:   return $(i, v)$
19: end function
20: function DISPLACEMENT$(i, v)$
21:   for $k \in \{0, \cdots, N - 1\} \setminus \{i\}$ do
22:     Compute $\delta_k$ such that $|x_i + \delta_k v - x_k| = 2\sigma$
23:   end for
24:   $j \leftarrow \arg \min_k \delta_k$
25:   $\delta \leftarrow \delta_j$
26:   return $(\delta, j)$
27: end function
ECMC algorithm to them, three essential concepts are introduced [16]; the factorized Metropolis probability, infinitesimal moves, and an event-driven Monte Carlo scheme [19]. Thanks to 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 which is infinitesimally close to the former state continues to be proposed, then at most a particle interacting with the moving one can reject it; the probability that more than two pairs simultaneously reject the proposal with infinitesimal displacements is higher-order infinitesimal. We define a collision as the probabilistic rejection which is caused by up to one interacting pair. Furthermore, an event-driven Monte Carlo scheme [19] 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.

We present the ECMC algorithm for more general systems in Algorithm 2, where $\beta$ is the inverse temperature. The Hamiltonian of the system considered in the algorithm is given by

$$H(x_0, \cdots, x_{N-1}) = \sum_{i<j} E_{ij}(x_i, x_j).$$

Note that $x_i$ represents a location 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 $\{\psi\}_{i=0, \cdots, p-1}$ is a set of linearly independent vectors. The state $x_i$ is updated by an operator $T_v(s)$; for particle systems $T_v(s)x_i = x_i + sv$, and for continuous spin systems $T_v(s)x_i = R_v(s)x_i$ where $R_v(s)$ is a rotation matrix around the vector $v$ with an angle $s$.

It is revealed that the ECMC algorithm outperforms other conventional algorithms in various systems [13, 15, 17, 20], and we can simulate very large systems consisting of about $10^6$ particles or spins in equilibrium by using the algorithm [14, 21, 22]. One of successful examples of the algorithm is the three-dimensional ferromagnetic Heisenberg spin model, in which the algorithm reduces the value of the dynamical critical exponent $z$ from $z = 2$ to $z \simeq 1$ [18].

3. Application to a three-dimensional classical Heisenberg spin model

We consider a classical Heisenberg spin model of a chiral helimagnet in three dimensions defined by the Hamiltonian

$$H(\{S_i\}) = -J \sum_{\langle i,j \rangle} S_i \cdot S_j - D \cdot \sum_i (S_i \times S_{i+\hat{y}}) - h \cdot \sum_i S_i,$$

where $S_i$ is a Heisenberg spin with unit length, $J > 0$ is a ferromagnetic coupling constant of an ordinary exchange interaction, and $h = h\hat{z}$ is a magnetic field. The bracket $\langle \cdot, \cdot \rangle$ in the first term of the Hamiltonian represents the neighboring pairs of sites, and the other summations run over all the sites. The second term in the Hamiltonian is a uniaxial Dzyaloshinskii–Moriya (DM) interaction with a DM vector $D = D\hat{y}$, which induces a helical structure into the system. The ground state of the system with/without the magnetic field was studied by a variational analysis of the one-dimensional continuum model [23–25]. When $h = 0$, the ground state has a simple helical structure characterized by one wave vector $q_{\text{chiral}} = \arctan(D/J)\hat{y}$, and when $h > h_c$ all of spins are parallel to the magnetic field $h$. A nontrivial and interesting structure, the chiral magnetic soliton lattice (CSL) structure, emerges in the intermediate region $0 < h < h_c$. The CSL structure is periodic as the helical structure at $h = 0$, but multiple wave vectors are needed to characterize the CSL structure.

We study the model at finite temperature with $D/J = 1$ in a three-dimensional simple cubic lattice. The lattice is a cuboid where the linear size of $y$ direction is 8 times as long as $x$ and $z$
Algorithm 2 ECMC for more general potentials

1: Input $N$, $\ell$, $\{x_0, \cdots, x_{N-1}\}$, $\{E_{ij}(x_i, x_j)\}_{i,j=0,\cdots,N-1}$, $\beta$
2: for $t \geq 0$ do
3:     $(i, v) \leftarrow \text{RANDOM}(N, p)$
4:     $s \leftarrow 0$
5:     while $s < \ell$ do
6:         $(\delta, j) \leftarrow \text{DISPLACEMENT}(i, v)$
7:         if $s + \delta < \ell$ then
8:             $(x_i, s) \leftarrow (T_v(\delta) x_i, s + \delta)$
9:                 $i \leftarrow j$
10:         else
11:             $(x_i, s) \leftarrow (T_v(\ell - s) x_i, \ell)$
12:         end if
13:     end while
14: end for
15: function RANDOM($N, p$)
16:     Sample $i$ uniformly from $\{0, \cdots, N - 1\}$
17:     Sample $v$ uniformly from $\{v_0, \cdots, v_{p-1}\}$
18:     return $(i, v)$
19: end function
20: function DISPLACEMENT($i, v$)
21:     for $k \in \{0, \cdots, N - 1\} \setminus \{i\}$ do
22:         Sample $r$ uniformly from $(0, 1)$
23:         Compute $\delta_k$ that satisfies
24:         $$r = \exp \left( -\beta \int_0^{\delta_k} \max \left[ 0, \frac{\partial E_{ik}(T_v(s) x_i, x_k)}{\partial s} \right] ds \right)$$
25:     end for
26:     $j \leftarrow \arg \min_k \delta_k$
27:     $\delta \leftarrow \delta_j$
28:     return $(\delta, j)$
29: end function

directions. The linear size of $x$ and $z$ directions of the lattice is denoted by $L$ and the total number of sites is $N = 8L^3$. Periodic boundary conditions are imposed on $x$ and $z$ directions and free boundary condition on $y$ direction. We perform large-scale equilibrium Monte Carlo simulations using the ECMC algorithm combined with the heat-bath algorithm, the over-relaxation updates [26, 27], and the exchange Monte Carlo method [7]. The largest system size in our simulations is $L = 64$, where the total number of spins $N = 64 \times 512 \times 64 > 10^6$.

We present in Fig. 1 the wave-number dependence of the magnetic susceptibility $\chi^\parallel(q)$ for $h/J = 0.1, 0.2,$ and $0.3$ at low temperatures. Here, the wave-number-dependent magnetization and the magnetic susceptibility with a wave-vector $q = q\hat{y}$ parallel to the DM vector $D$ is defined as

$$m^\parallel(q) = \frac{1}{N} \sum_i S_i \exp (i q \cdot r_i),$$

$$\chi^\parallel(q) = N \beta \left( \left\langle |m^\parallel(q)|^2 \right\rangle - \left| \left\langle m^\parallel(q) \right\rangle \right|^2 \right).$$
Figure 1. Wave-number dependence of $\chi^\parallel(q)$ of the chiral helimagnetic model in three dimensions for various system sizes in the low-temperature region. The values of the magnetic fields perpendicular to the DM vector are (left) $h/J = 0.1$, (center) $h/J = 0.2$, and (right) $h/J = 0.3$.

One can see in the figure that there exist multiple peaks for larger system sizes which characterize the CSL structure. While the CSL structure emerges in the low-temperature region independent of the magnetic field $h/J$ in our simulations, other thermodynamic quantities show completely different behaviors depending on the value of $h/J$. In Fig. 2, we show the specific heat $c = N\beta^2(\langle e^2 \rangle - \langle e \rangle^2)$, the magnetization parallel to the magnetic field $m_z = \sum_i \hat{z} \cdot \mathbf{S}_i/N$, and the uniform magnetic susceptibility $\chi^\parallel(0)$ for $h/J = 0.1$, 0.2, and 0.3. The specific heat and the uniform magnetic susceptibility for $h/J = 0$ are also plotted. As shown in the figure, the specific heat of the system for $h/J = 0.3$ shows a strong tendency to diverge at its transition temperature while that for $h/J = 0$, 0.1, and 0.2 has a finite value at their transition temperatures. Note that the system without the magnetic field belongs to the same universality class of the three-dimensional $XY$ model [22], and thus the specific heat does not diverge at the critical temperature in the thermodynamic limit. More strikingly, the uniform magnetic susceptibility for $h/J = 0.3$ also has a strong tendency to diverge at the finite temperature although the uniform magnetization does not characterize the CSL structure in the low-temperature region, and the magnetization parallel to the magnetic field changes rapidly near the transition temperature. These suggest that there exists a critical point $(T_d, h_d)$ with $0.2 < h_d < 0.3$ in the magnetic phase diagram of the system although the precise location of the critical point is not determined in this work. Recently, the existence of a critical point in the magnetic phase diagram of a magnetic compound $\text{Cr}_1/3\text{NbS}_2$, which has been extensively studied as a possible candidate of chiral helimagnets in experiments, is also suggested experimentally [28]. This might be consistent with that found in this work. In Ref. [25], Dzyaloshinskii predicts by
analyzing a one-dimensional continuum model that the specific heat \( c \) diverges with a logarithmic correction as \( c \sim \left( (T_\ast - T) \log^2(T_\ast - T) \right)^{-1} \) from below the transition temperature \( T_\ast \) although it does not diverge from above the transition temperature. The specific heat of the system with \( h/J = 0.3 \) in our results seems to also have an antisymmetric singular behavior. Larger-scale simulations of the system is needed to determine the critical exponents and examine the validity of Dzyaloshinskii’s theory.

acknowledgement
The authors thank S. Hoshino and Y. Kato for very useful discussions. Numerical simulation in this work has mainly been performed by using the facility of the Supercomputer Center, Institute for Solid State Physics, the University of Tokyo. This research was supported by the Grants-in-Aid for Scientific Research from the JSPS, Japan (No. 25120010 and 25610102), and JSPS Core-to-Core program “Nonequilibrium dynamics of soft matter and information.” This work was also supported by “Materials research by Information Integration Initiative (MI²I)” project of the Support Program for Starting Up Innovation Hub from Japan Science and Technology Agency (JST).

References
[1] Metropolis N, Rosenbluth A W, Rosenbluth M N, Teller A H and Teller E 1953 J. Chem. Phys. 21 1087
[2] Swendsen R H and Wang J S 1987 Phys. Rev. Lett. 58 86
[3] Wolff U 1989 Phys. Rev. Lett. 62 361
[4] Berg B A and Neuhaus T 1992 Phys. Rev. Lett. 68 9
[5] Lyubartsev A P, Martsinovskii A A, Shevkunov S V and Vorontsov-Velyaminov P N 1992 J. Chem. Phys. 96 1776
[6] Marinari E and Parisi G 1992 Europhys. Lett. 19 451
[7] Hukushima K and Nemoto K 1996 J. Phys. Soc. Jpn. 65 1604
[8] Wang F and Landau D P 2001 Phys. Rev. Lett. 86 2050
[9] Iba Y 2001 Int. J. Mod. Phys. C 12 623
[10] Suwa H and Todo S 2010 Phys. Rev. Lett. 105 120603
[11] Turitsyn K S, Chertkov M and Vucelja M 2011 Physica D 240 410
[12] Fernandes H C M and Weigel M 2011 Comput. Phys. Commun. 182 1856
[13] Bernard E P, Krauth W and Wilson D B 2009 Phys. Rev. E 80 056704
[14] Bernard E P and Krauth W 2011 Phys. Rev. Lett. 107 155704
[15] Peters E A J F and de With G 2012 Phys. Rev. E 85 026703
[16] Michel M, Kapfer S C and Krauth W 2014 J. Chem. Phys. 140 054116
[17] Michel M, Mayer J and Krauth W 2015 Europhys. Lett. 112 20003
[18] Nishikawa Y, Michel M, Krauth W and Hukushima K 2015 Phys. Rev. E 92 063306
[19] Bortz A B, Kalos M H and Lebowitz J L 1975 J. Comput. Phys. 17 10
[20] Isobe M and Krauth W 2015 J. Chem. Phys. 143 084509
[21] Kapfer S C and Krauth W 2015 Phys. Rev. Lett. 114 035702
[22] Nishikawa Y and Hukushima K 2016 (Preprint arXiv:1603.04200)
[23] Dzyaloshinskii I E 1964 Sov. Phys. JETP 19 960
[24] Dzyaloshinskii I E 1964 Sov. Phys. JETP 20 223
[25] Dzyaloshinskii I E 1965 Sov. Phys. JETP 20 665
[26] Creutz M 1987 Phys. Rev. D 36 515
[27] Brown F R and Woch T J 1987 Phys. Rev. Lett. 58 2394
[28] Tsuruta K, Mito M, Deguchi H, Kishine J, Kousaka Y, Akimitsu J and Inoue K 2016 Phys. Rev. B 93 104402