Non-reversible Monte Carlo simulations of spin models

Heitor C.M. Fernandes, Martin Weigel *

Institut für Physik, KOMET 331, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55128 Mainz, Germany

ABSTRACT

Monte Carlo simulations are used to study simple systems where the underlying Markov chain satisfies the necessary condition of global balance but does not obey the more restrictive condition of detailed balance. Here, we show that non-reversible Markov chains can be set up that generate correct stationary distributions, but reduce or eliminate the diffusive motion in phase space typical of the usual Monte Carlo dynamics. Our approach is based on splitting the dynamics into a set of replicas with each replica representing a biased movement in reaction-coordinate space. This introduction of an additional bias in a given replica is compensated for by choosing an appropriate dynamics on the other replicas such as to ensure the validity of global balance. First, we apply this method to a mean-field Ising model, splitting the system into two replicas: one trying to increase magnetization and the other trying to decrease it. For this simple test system, our results show that the altered dynamics is able to reduce the dynamical critical exponent. Generalizations of this scheme to simulations of the Ising model in two dimensions are discussed.

© 2010 Elsevier B.V. All rights reserved.

1. Introduction

In the realm of Monte Carlo simulations, techniques based on Markov chains are by far the most common methods [1]. Based on the principle of detailed balance, the Metropolis–Hastings algorithm [2] is the workhorse of the Monte Carlo technique, unsurpassed in its most general applicability and technical simplicity. By construction, under its guidance the system performs a (biased) random walk in configuration space. While it samples states directly according to the equilibrium distribution, as desired, the diffusive motion in phase space makes convergence relatively slow. This is not much of a problem for the strongly localized distributions typical of, say, the canonical ensemble off criticality. The broadened distributions close to con-

1-dimensional configuration space {$k = 1, 2, \ldots$} by replicating the whole chain of states into + and − copies and performing two-step transitions as indicated in Fig. 1:
ues of the replica-change probability simulations of this type for the mean-field model for different values is small, the chain will continue moving in the same direction as long as the Metropolis steps are accepted.

2. Mean field Ising model

In the spirit of the above construction, we considered a ferromagnetic, mean-field Ising model with \( N \) spins and Hamiltonian

\[
H = -\frac{J}{2N} \sum_{i,j} s_i s_j = -\frac{J}{2N} M^2, \tag{3}
\]

which has the peculiarity that, due to the indistinguishability of aligned spins, its state is completely described by the total magnetization \( M \). Therefore, all microstates belonging to fixed magnetization \( M \) (or fixed energy \( E = -J M^2 / 2N \)) are completely equivalent. Under the usual single-spin flip dynamics with \( M \rightarrow M \pm 2 \) the system is, therefore, exactly described by the one-dimensional chain depicted in Fig. 1 with \( k = (M + N) / 2 \). The system undergoes a paramagnetic to ferromagnetic ordering transition at the critical coupling \( T_c = 1 \), and with a regular, reversible single-spin flip Metropolis dynamics, critical slowing down is observed. To update the configuration directly in terms of the magnetization \( M \) (and not in terms of the individual spins \( s_i \)), the degeneracy of microstates needs to be taken into account. The canonical distribution of magnetizations therefore is given by

\[
P(M) \propto \frac{N!}{N_+! N_-!} \exp\left(\frac{-\beta J M^2}{2N}\right), \tag{4}\]

where \( N_+ \) and \( N_- \) denote the number of up and down spins, respectively. Since \( M = N_+ - N_- \), this is equivalent to

\[
P(M) \propto \frac{N!}{(N_+ + N_-)! (N_+ - N_-)!} \exp\left(\frac{-\beta J M^2}{2N}\right). \tag{5}\]

Hence, the acceptance probabilities (2) for the moves \( M \rightarrow M \pm 2 \) become

\[
p_{acc} = \min\left[1, \frac{N \mp M}{N \pm M + 2} \exp\left(\frac{2 \beta J}{N} (\pm M + 1)\right)\right]. \tag{6}\]

The form of these probabilities as a function of \( M \) for \( T = T_c = 1 \) is illustrated in Fig. 2. Fig. 3 shows time series of non-reversible simulations of this type for the mean-field model for different values of the replica-change probability \( \theta \). For large values of \( \theta \), the algorithm behaves very similarly to the case of regular, reversible Metropolis simulations, and the temporal evolution of the magnetization \( M \) resembles a random walk. As \( \theta \) is gradually reduced, however, the system evolves for an increasing number of consecutive steps in the same direction before a change of replica and, therefore, a reversal of the direction of evolution of \( M \) occurs. Inspection of the acceptance probabilities in Fig. 2 reveals that, in fact, moves decreasing the magnetization \( M \rightarrow M - 2 \) are always accepted for \( M > 0 \) and, vice versa, moves increasing \( M \rightarrow M + 2 \) are always accepted if \( M < 0 \). Hence, the system must cross the symmetric point \( M = 0 \) before a reversal of the evolution direction can occur. This condition leads to the characteristic zig-zag pattern of the magnetization time series displayed in Fig. 3.

(a) a traditional, reversible Metropolis update between states \((k, \pm)\) and \((k \pm 1, \mp)\) according to the desired stationary distribution \( \pi(k, \pm) = \pi(k, -) = \pi(k, \pm) \), i.e., with acceptance rate

\[
p_{acc} = \min\left[1, \frac{\pi(k \pm 1)}{\pi(k)}\right] \tag{2}\]

and

(b) a transition \((k, \pm) \rightarrow (k, \mp)\) with a fixed probability \( 1 - \theta \).

Both transitions obviously leave \( \pi \) invariant, such that \( \pi \) is stationary, but the combination of the two steps is not reversible. Moreover, it is clear that if \( \theta \) is small, the chain will continue moving in the same direction as long as the Metropolis steps are accepted.

Fig. 1. Non-reversible dynamics on a one-dimensional chain of states with stationary distribution \( \pi \) and a fixed probability \( 1 - \theta \) of replica change.

Fig. 2. Acceptance probabilities according to Eq. (6) for non-reversible simulations of the mean-field Ising model (3) at the asymptotic critical temperature \( T_c = 1 \) for a system of \( N = 32 \) spins.

Fig. 3. Time series of the magnetization \( M \) in a non-reversible simulation of the mean-field Ising model at \( T = T_c \) for different choices of the replica-change probability \( \theta \).
The effect of this changeover from diffusive to quasi-ballistic evolution of the magnetization is corroborated by an analysis of the integrated autocorrelation times $\tau_{\text{int}}$. From a binning analysis [9], we determine $\tau_{\text{int}}(M)$ from the original time series data from the limit of large block lengths, where some care has to be taken due to the fact that the autocorrelation function does not simply decay exponentially, but features a superimposed oscillatory behavior resulting from the zig-zag pattern of the time series shown in Fig. 3. Estimating the autocorrelation times for a range of different system sizes results in the dynamical scaling data presented in Fig. 4. Fits of the expected functional form

$$\tau_{\text{int}} = AN^z$$

(7)

to the data for a range of successively smaller values of the replica-change parameter $\theta$ show a gradual reduction of the effective dynamical critical exponent $z$ from its value $z = 1.4390(33)$ for the reversible dynamics down to $z = 0.833(13)$ for the irreversible dynamics in the limit $\theta \to 0$. This is consistent with the finding $z \approx 0.85$ for a related approach discussed in Ref. [5].

A certain reduction of autocorrelation times is also observed in the high-temperature paramagnetic and low-temperature ordered phases with this approach. The irreversible dynamics does not lead to a significant increase in tunneling events between the symmetric peaks in the ordered phase, however. These results will be discussed elsewhere [10].

3. Two-dimensional Ising model

For general short-range models and appropriate reaction coordinates such as, e.g., energy and magnetization for spin systems, the equivalence of microstates at fixed $E$ or $M$ seen in the mean-field model is lost. Consequently, representing phase space in analogous such as, e.g., energy and magnetization for spin systems, 2. Two-dimensional Ising model discussed elsewhere [10].

Depending on which of the chains the system currently is in, we either pick one of the up or one of the down spins at random and propose a spin flip. Due to the different a priori probabilities for choosing a spin before and after the flip, we again get additional symmetry factors in the acceptance probabilities for the transition $M \mapsto M \pm 2$,

$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j$,

(8)

where spins are located on the sites of an $L \times L$ square lattice. We studied two types of non-reversible simulations, using either the magnetization $M$ or the energy $E$ as the projection coordinate.

For the case of the magnetization, again two chains, one increasing $M \mapsto M + 2$ and one decreasing $M \mapsto M - 2$, are sufficient. Depending on which of the chains the system currently is in, we either pick one of the up or one of the down spins at random and propose a spin flip. The effect of this changeover from diffusive to quasi-ballistic evolution of the magnetization is corroborated by an analysis of the integrated autocorrelation times $\tau_{\text{int}}$. From a binning analysis [9], we determine $\tau_{\text{int}}(M)$ from the original time series data from the limit of large block lengths, where some care has to be taken due to the fact that the autocorrelation function does not simply decay exponentially, but features a superimposed oscillatory behavior resulting from the zig-zag pattern of the time series shown in Fig. 3. Estimating the autocorrelation times for a range of different system sizes results in the dynamical scaling data presented in Fig. 4. Fits of the expected functional form

$$\tau_{\text{int}} = AN^z$$

(7)

to the data for a range of successively smaller values of the replica-change parameter $\theta$ show a gradual reduction of the effective dynamical critical exponent $z$ from its value $z = 1.4390(33)$ for the reversible dynamics down to $z = 0.833(13)$ for the irreversible dynamics in the limit $\theta \to 0$. This is consistent with the finding $z \approx 0.85$ for a related approach discussed in Ref. [5].

A certain reduction of autocorrelation times is also observed in the high-temperature paramagnetic and low-temperature ordered phases with this approach. The irreversible dynamics does not lead to a significant increase in tunneling events between the symmetric peaks in the ordered phase, however. These results will be discussed elsewhere [10].

3. Two-dimensional Ising model

For general short-range models and appropriate reaction coordinates such as, e.g., energy and magnetization for spin systems, the equivalence of microstates at fixed $E$ or $M$ seen in the mean-field model is lost. Consequently, representing phase space in analogy to Fig. 1 corresponds to a projection, not an identity. Here, we consider non-reversible simulations of the ferromagnetic, nearest-neighbor Ising model with Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j,$$

(8)

where spins are located on the sites of an $L \times L$ square lattice. We studied two types of non-reversible simulations, using either the magnetization $M$ or the energy $E$ as the projection coordinate.

For the case of the magnetization, again two chains, one increasing $M \mapsto M + 2$ and one decreasing $M \mapsto M - 2$, are sufficient. Depending on which of the chains the system currently is in, we either pick one of the up or one of the down spins at random and propose a spin flip. Due to the different a priori probabilities for choosing a spin before and after the flip, we again get additional symmetry factors in the acceptance probabilities for the transition $M \mapsto M \pm 2$,

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j,$$

(8)

where spins are located on the sites of an $L \times L$ square lattice. We studied two types of non-reversible simulations, using either the magnetization $M$ or the energy $E$ as the projection coordinate.

For the case of the magnetization, again two chains, one increasing $M \mapsto M + 2$ and one decreasing $M \mapsto M - 2$, are sufficient. Depending on which of the chains the system currently is in, we either pick one of the up or one of the down spins at random and propose a spin flip. Due to the different a priori probabilities for choosing a spin before and after the flip, we again get additional symmetry factors in the acceptance probabilities for the transition $M \mapsto M \pm 2$,

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j,$$

(8)

where spins are located on the sites of an $L \times L$ square lattice. We studied two types of non-reversible simulations, using either the magnetization $M$ or the energy $E$ as the projection coordinate.

For the case of the magnetization, again two chains, one increasing $M \mapsto M + 2$ and one decreasing $M \mapsto M - 2$, are sufficient. Depending on which of the chains the system currently is in, we either pick one of the up or one of the down spins at random and propose a spin flip. Due to the different a priori probabilities for choosing a spin before and after the flip, we again get additional symmetry factors in the acceptance probabilities for the transition $M \mapsto M \pm 2$,

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j,$$

(8)

where spins are located on the sites of an $L \times L$ square lattice. We studied two types of non-reversible simulations, using either the magnetization $M$ or the energy $E$ as the projection coordinate.

For the case of the magnetization, again two chains, one increasing $M \mapsto M + 2$ and one decreasing $M \mapsto M - 2$, are sufficient. Depending on which of the chains the system currently is in, we either pick one of the up or one of the down spins at random and propose a spin flip. Due to the different a priori probabilities for choosing a spin before and after the flip, we again get additional symmetry factors in the acceptance probabilities for the transition $M \mapsto M \pm 2$,

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j,$$

(8)

where spins are located on the sites of an $L \times L$ square lattice. We studied two types of non-reversible simulations, using either the magnetization $M$ or the energy $E$ as the projection coordinate.

For the case of the magnetization, again two chains, one increasing $M \mapsto M + 2$ and one decreasing $M \mapsto M - 2$, are sufficient. Depending on which of the chains the system currently is in, we either pick one of the up or one of the down spins at random and propose a spin flip. Due to the different a priori probabilities for choosing a spin before and after the flip, we again get additional symmetry factors in the acceptance probabilities for the transition $M \mapsto M \pm 2$,

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j,$$

(8)

where spins are located on the sites of an $L \times L$ square lattice. We studied two types of non-reversible simulations, using either the magnetization $M$ or the energy $E$ as the projection coordinate.

For the case of the magnetization, again two chains, one increasing $M \mapsto M + 2$ and one decreasing $M \mapsto M - 2$, are sufficient. Depending on which of the chains the system currently is in, we either pick one of the up or one of the down spins at random and propose a spin flip. Due to the different a priori probabilities for choosing a spin before and after the flip, we again get additional symmetry factors in the acceptance probabilities for the transition $M \mapsto M \pm 2$,

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j,$$

(8)

where spins are located on the sites of an $L \times L$ square lattice. We studied two types of non-reversible simulations, using either the magnetization $M$ or the energy $E$ as the projection coordinate.
Fig. 5. Finite-size scaling of the integrated autocorrelation times $\tau_{\text{int}}(E)$ and $\tau_{\text{int}}(M)$ of the internal energy and magnetization of non-reversible simulations of the two-dimensional Ising model at criticality using a state-space partition according to the energy $E$. Fits of the functional form $\tau_{\text{int}} = A L^{z}$ to the data yield the estimates $\tau_{\text{int}}(E) = 1.670(52)$ and $\tau_{\text{int}}(M) = 1.980(29)$ for the non-reversible dynamics, to be compared to the estimates $\tau_{\text{int}}(E) = 1.766(24)$ and $\tau_{\text{int}}(M) = 2.121(27)$ for the regular, reversible simulation.

Acknowledgements

The authors acknowledge support by the “Center for Computational Sciences in Mainz” (SRFN). M.W. acknowledges computer time provided by NIC Jülich under grant No. hmz18 and funding by the DFG under contract No. WE4425/1-1.

References