Accelerating Diffusive Nonequilibrium Processes in Discrete Spin Systems

G. T. Barkema and J. F. Marko
Laboratory of Atomic and Solid State Physics, Clark Hall, Cornell University, Ithaca, New York 14853-2501
(Received 26 January 1993; revised manuscript received 30 June 1993)

New Monte Carlo methods are presented for efficient simulation of nonequilibrium processes in spin systems. The elementary moves are flips of connected sets of spins (clusters), subject to constraints. Use of a constraint on the cluster size gives rapid short-wavelength equilibration and accelerated diffusive long-wavelength kinetics; additional constraints can enforce local conservation laws.

PACS numbers: 64.75.+g, 05.70.Ln, 64.60.Ht

The long-wavelength dynamics of nonequilibrium processes are often insensitive to microscopic details, and thus can be categorized into universality classes. Two general examples of such processes are dynamic critical phenomena [1] and phase-ordering kinetics [2]. Simulation studies are both helped and handicapped by this universality: Simple models such as the Ising model can be useful, but large systems must be simulated over long times in order to observe their universal properties. Typically, techniques such as Monte Carlo (MC) simulations using the Metropolis algorithm [3], or integration of discretized Langevin equations [2,4] are used to study nonequilibrium processes. The localized nature of these calculations makes it difficult to simulate the long times required for long-wavelength processes to occur.

For the study of statistical equilibrium of classical spins this problem has been partially overcome with nonlocal MC algorithms, developed by Swendsen and Wang [5] and by Wolff [6]. In these algorithms, a single move groups many neighboring spins into "clusters" which are simultaneously "flipped" from one state to another. The nonlocality of these moves drastically shortens correlation times. However, because such algorithms often flip system-spanning clusters, the resulting long-wavelength dynamics bears no resemblance to physical, e.g., diffusive, transport.

Here, we introduce a new class of *constrained* cluster-flipping algorithms that permit (i) moves of *specified locality*, from single-site spin flips [3] to the highly nonlocal cluster moves accomplished by the Wolff algorithm [6], (ii) imposition of local (i.e., at the scale of the clusters selected) *conservation laws*. Such local-cluster-flip (LCF) algorithms, while maintaining equilibria identical to those of single-site or cluster-flipping MC algorithms, possess a blend of dynamical processes. On the scale of the cluster sizes, there is instantaneous transport: a single move *coherently* rearranges the local state. However, at long scales, conventional diffusion occurs, with a large amplification of the effective transport coefficient relative to single-spin-flip dynamics. Our approach places a hard upper bound on the cluster sizes, in contrast to work on controlling cluster sizes by Niedermayer [7]. In addition, our methods suggest generalization to respect more general cluster-move constraints.

The transport amplification that we obtain makes simulation of spin system dynamics, previously requiring single-spin MC, an attractive alternative to integration of noise-driven discretized partial differential equations (e.g., Langevin equations such as the time-dependent Ginzberg-Landau equation and model B conserved-order-parameter dynamics [2] or related cell-dynamical systems [8]) for the study of order-parameter dynamics. Partial differential equations have been favored in recent studies for two reasons: First, a single site, being a continuous field, is estimated to represent many ($\approx 3^d$) spins [9]; second, various schemes may be employed to boost the time step [8,10]. Both of these factors allow partial differential equations to access later effective times than single-spin MC given a fixed amount of computation. In contrast to single-spin MC, our algorithm allows groups of arbitrarily many spins to be updated at once. In addition, spin systems can be easily studied close to their well-characterized critical points, or in strong or inhomogenous fields, instances where integration of continuum models requires short time steps.

In this paper we apply our ideas to the Q-state Potts model, where spins σ_x take values $0, \ldots, Q-1$ and are located at "sites" x. Nearest-neighbor "links" from site x to y are denoted $\langle x, y\rangle$. The Potts Hamiltonian is

$$-\frac{H}{kT} = \sum_{\langle x,y\rangle} K_{xy}\delta_{\sigma_x,\sigma_y} + \sum_x h_x \delta_{\sigma_x,1}, \qquad (1)$$

where the sums run over all x and links $\langle x, y\rangle$ on the lattice. The coupling constant K_{xy} and the external "magnetic" field h_x may be inhomogeneous. In what follows, we first describe our algorithm, and then we show that its equilibrium is described by the Boltzmann distribution.

In a single cluster move, a group of spins connected by bonds (selected or "activated" links in the language of Wolff [6]) is flipped. We now describe a cluster move in our algorithm without conservation of spin, and with a constraint (e.g., on the cluster size). (i) A site r is chosen at random to be the first spin in cluster C. (ii) Consider the links connecting $x \in C$ to its neighbors $y \notin C$; a previously unconsidered bond $\langle x, y\rangle$ is added to C with probability $\delta_{\sigma_x,\sigma_y}(1 - e^{-K_{xy}})$ if the constraint $c(y, r)$ is

0031-9007/93/71(13)/2070(4)$06.00

true; if $c(y,r)$ is false, the bond is not activated. The constraint $c(y,r)$ may involve any relation between sites y and r defined *without* reference to the spin states. In this paper, we consider the following "distance" constraint: $c(y,r)$ is true if the distance (number of bonds separating y and r on C) is less than R, and false otherwise. (iii) Repeat step (ii) until all links from sites in C have been considered. (iv) Spins in C are flipped to a state $\sigma' \neq \sigma_x \in C$ with probability

$$A = \frac{1}{Q-1}\min\left(1, \prod_{\langle x,\bar{y}\rangle \wedge \overline{c(y,r)}} e^{-K_{xy}\delta_{\sigma,\sigma_y}} \prod_x e^{-h_x\delta_{\sigma,1}}\right), \tag{2}$$

where the product subscript x denotes $x \in C$ and $\bar{y}$ denotes $y \notin C$. Logical "and" ($\wedge$) and the negation of the constraint condition $\overline{c(y,r)}$ are also used. For simplicity, a single magnetic field h_x is considered, coupling to the $\sigma = 1$ state: in general, $Q-1$ such fields are required.

This process of cluster growth and flipping is repeated in the manner of the Wolff algorithm; simulation "time" is measured in attempted cluster moves. We note that when $R = 1$, the constraint $c(y,r)$ is always false, and a cluster of one spin is always formed; the acceptance probability is then just the conventional single-site MC flip probability. When $R = \infty$, the constraint $c(y,r)$ is always true, and the algorithm is that of Wolff [6]. For *any* R, it is always possible for *any* single spin to be flipped to any state, making the algorithm ergodic.

That this algorithm observes detailed balance, and that the probability of a state is given by the Boltzmann distribution appropriate for the Q-state Potts model is easily shown. Consider the probability that a particular cluster (defined by a starting site s and a particular set of links) is constructed and flipped, causing a transition from spin state A to B. This is proportional to a product of factors $1 - e^{-K_{xy}}$ for each link $\langle x,y\rangle \in C$, and factors $e^{-K_{xy}}$ for each link $\langle x,y\rangle$ for which the conditions $x \in C$, $y \notin C$, $\sigma_y = \sigma$, and $c(y,r)$ are all true: these are links which *could* have been made, but were not. This product must be multiplied by the acceptance probability defined in (iv) to give the transition probability t^C_{AB}.

Now consider the *corresponding* reverse process that forms and flips the same cluster (the *same* start site r and links), leading to a transition from B to A. The probability of cluster construction for the reverse move is the product of the *same* factors of $1 - e^{-K_{xy}}$, and the factors $e^{-K_{xy}}$ for each link $\langle x,y\rangle$ for which the conditions $x \in C$, $y \notin C$, $\sigma_y = \sigma'$, and $c(y,r)$ are all true (σ_x refer to state A). When multiplied by the acceptance probability (1), this gives a nonzero reverse transition probability t^C_{BA}.

The ratio of these corresponding transition probabilities is

$$\frac{t^C_{AB}}{t^C_{BA}} = \frac{\prod_{\langle x,\bar{y}\rangle\wedge c(y,r)\wedge(\sigma_y=\sigma)} e^{-K_{xy}} \min\left(1, \prod_x e^{-h_x\delta_{\sigma,1}} \prod_{\langle x,\bar{y}\rangle\wedge\overline{c(y,r)}} e^{-K_{xy}\delta_{\sigma,\sigma_y}}\right)}{\prod_{\langle x,\bar{y}\rangle\wedge c(y,r)\wedge(\sigma_y=\sigma')} e^{-K_{xy}} \min\left(1, \prod_x e^{-h_x\delta_{\sigma',1}} \prod_{\langle x,\bar{y}\rangle\wedge\overline{c(y,r)}} e^{-K_{xy}\delta_{\sigma',\sigma_y}}\right)}, \tag{3}$$

where identical terms in the numerator and denominator have been canceled. This ratio reduces to

$$\frac{t^C_{AB}}{t^C_{BA}} = \prod_x e^{h_x(\delta_{\sigma',1}-\delta_{\sigma,1})} \prod_{\langle x,\bar{y}\rangle} e^{K_{xy}(\delta_{\sigma',\sigma_y}-\delta_{\sigma,\sigma_y})}, \tag{4}$$

just the ratio of the Boltzmann weights of states B and A for the Hamiltonian (1).

Since this ratio is the same for *all* moves C that result in such transitions between A and B, and since there are corresponding reverses for every cluster move, the ratio of the *total* forward and reverse transition probabilities is

$$\frac{T_{AB}}{T_{BA}} = \frac{\sum_C t^C_{AB}}{\sum_C t^C_{BA}} = \exp\frac{H(A)-H(B)}{kT}; \tag{5}$$

the algorithm thus satisfies detailed balance, and the probability of observing a state is given by the Boltzmann distribution for the Hamiltonian (1).

We will now show that increasing the cluster size R can accelerate a spin simulation without affecting the universal properties of the dynamics on scales larger than R. Above the critical temperature $K_c = \ln(1+\sqrt{2}) = 0.8813\ldots$ of the two-dimensional square-lattice $Q = 2$ Potts (Ising) model in zero magnetic field, we have studied spin relaxation in order to determine the nature of transport at long wavelengths. Ising spins are defined as $s_x = 2\sigma_x - 1$. The momentum components of the spins, $\hat{s}_k \equiv \sum_x e^{ikx} s_x$, may be used to form correlation functions $c_k(t) = (M^2T)^{-1}\int_0^T dt'\, \hat{s}_k(t')\hat{s}_{-k}(t+t')$, where t denotes simulation time in cluster flips per lattice site, and M^2 is the number of sites.

If the long-wavelength transport is diffusive (expected for k^{-1} larger than the equilibrium correlation length ξ), we expect $c_k(t) = c_k(0)e^{-t/\tau_k}$, where $c_k(0) = 1/[a + k^2 + O(k^4)]$ is the equilibrium correlation function, and where $\tau_k = c_k(0)/D$. The proportionality constant D is the effective diffusion constant. In the inset of Fig. 1, we plot $c_k(t)/c_k(0)$ as a function of $t/c_k(0)$ for data taken from 4×10^7 cluster flips of a 128^2 square lattice with $K_{xy} = 0.70$ ($\xi \approx 3.6$), and with cluster size $R = 4$; the collapse of these correlation functions for different k indicates that a single diffusion constant D describes long-wavelength relaxation.

We have measured D as a function of coupling K and cluster size R: Our data are shown in Fig. 1, with diffusion constants normalized to those for $R = 1$ (single-spin

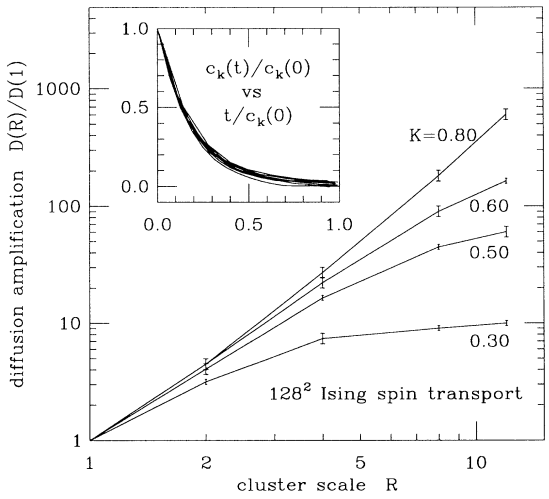

FIG. 1. Diffusion constant $D(R)$ in 128^2 square-lattice Ising model with K =0.3, 0.5, 0.6, 0.8, as a function of cluster size R, normalized to the case $R = 1$. Inset shows the rescaled correlation function $c_k(t)/c_k(0)$ vs $t/c_k(0)$ at large wavelengths, for $K = 0.7$ and wave numbers $k = i/128$, $i = 0$ to 9. The collapse indicates that a single diffusion constant describes the long-wavelength relaxation.

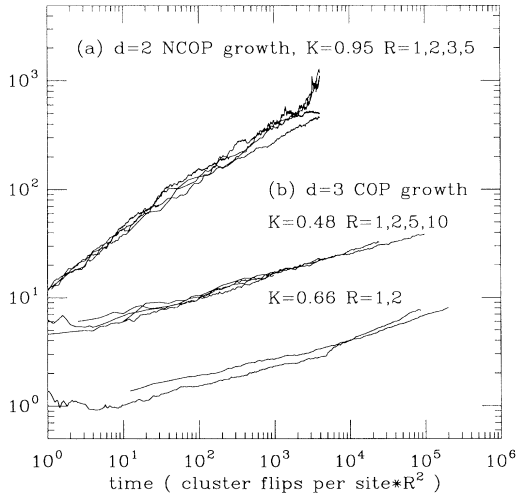

FIG. 2. LCF domain growth. (a) Nonconserved-spin 1024^2 square-lattice Ising model, cluster size $R = 1, 2, 3, 5$ quenched from $K = 0$ to $K = 0.95$ at $t = 0$. For clarity, $10L(t)$ is plotted. (b) Conserved-spin 64^3 simple-cubic Ising model, cluster size $R = 1, 2, 5, 10$ quenched to $K = 0.48$; also shown are data for $R = 1, 2$ quenched to $K = 0.66$. For the two couplings, $5L(t)$ and $L(t)$ are plotted, respectively. In each case, overlap of the curves after scaling simulation time by R^2 indicates an effective diffusion constant $D \approx R^2$.

MC) for each temperature. We observe that for each K, $D(R)$ grows initially as R^n with $n \approx 2.5$. For large R, $D(R)$ saturates: increasing R beyond the percolation length (which is finite above the magnetic phase transition for the $d = 2$ Ising model [11]) will not affect the cluster sizes that are formed, and therefore will not affect the diffusion. As the critical temperature is approached, the percolation length increases, and a larger regime of power-law behavior of $D(R)$ is observed. One can argue that at criticality, the exponent n is larger than 2.1: for the critical $d = 2$ Ising model, critical slowing down is eliminated by the Wolff algorithm ($R \approx L$); for the Metropolis algorithm ($R = 1$), the correlation time is $L^{2.1}$ [6]. Consequently, we expect that the correlation time is less than $(L/R)^{2.1}$, and that the diffusion constant is greater than $R^{2.1}/L^{0.1}$.

Since the LCF moves generate diffusive transport at lengths larger than R, they are suitable for the study of nonequilibrium processes *below* the critical temperature, where ordered phases will condense. We have studied the 1024^2 square-lattice Ising model, measuring the equal-time correlator $C_k(t) = \hat{s}_k(t)\hat{s}_{-k}(t)$ as a function of simulation time t after a quench from infinite temperature to $K = 0.95$ at $t = 0$. This may be Fourier transformed to yield the real-space correlator $C(r, t)$. Solution of $C(0, t) = 2.718C(L, t)$ defines a mean domain size L at any time t. Scaling arguments [12] suggest that domain growth with nonconserved diffusive dynamics should approach a power law $L(t) = (Dt)^{1/2}$, where D is the effective diffusion constant for order parameter fluctuations. The upper curves (a) of Fig. 2 show $10L(t)$ for single runs with $R = 1, 2, 3, 5$: each case shows $t^{1/2}$ growth, with effective diffusion scaling as $D(R) \approx R^2$.

We have also devised a LCF algorithm for Potts models with conserved order-parameter dynamics: (i) Start with a *pair* (r_1, r_2) of neighboring sites with different spins. (ii) Form a cluster around r_1 using the distance constraint described above. (iii) Form a cluster around r_2 using the constraint that the number of sites in cluster 2 is not allowed to exceed the number of sites in cluster 1. (iv) Reject the move if the number of sites in clusters 1 and 2 differ; otherwise, accept the move with an acceptance ratio

$$A = \frac{1}{Q-1}\min\left(1, \frac{P(\{\sigma\})}{P(\{\sigma'\})} \prod_{\langle x,\bar{y}\rangle \wedge \overline{c(y,r)}} e^{-K_{xy}\delta_{\sigma,\sigma_y}} \prod_x e^{-h_x\delta_{\sigma,1}}\right), \tag{6}$$

which equals 1, multiplied by a factor that corrects for fluctuations in the number of links connecting unequal spins $P(\{\sigma\}) \equiv \sum_{<x,y>}(1 - \delta_{\sigma_x,\sigma_y})$ that can be selected in step (i). As before, $\{\sigma'\}$ are the spins *after* the proposed move.

We have studied the growth of ordered domains in the three-dimensional simple-cubic 64^3 Ising model with zero total spin, quenched from $K = 0$ to K larger than the critical coupling $K_c = 0.4432\ldots$ at time $t = 0$ using our spin-conserving LCF algorithm. The correlator $C(r,t)$ is defined as before; $L(t)$ is defined as the smallest solution of $C(L,t) = 0$. The lower curves of Fig. 2 show $5L(t)$ vs tR^2 for $R = 1, 2, 5, 10$ and $K = 1.0829K_c = 0.48$, averaged over eight runs and $L(t)$ vs tR^2 for $R = 1, 2$ and $K = 1.5K_c = 0.6649$, averaged over four runs. For both of these quenches, the thermal correlation length ξ is less than one lattice constant [13]. The four curves for the shallower quench and the two curves for the deep quench superimpose over a large time range, indicating that the effective diffusion scales as $D \approx R^2$, even in the regime $L < R$. For the deep quench, simulations performed with $R > 2$ could not be superimposed by a multiplicative time scaling. For the shallower quench, $R = 20$ failed to scale, indicating that the range of R over which this scaling holds grows as T_c is approached. We note that for both quenches, the growth is slower than the theoretically expected asymptotic result $R \propto t^{1/3}$, especially for the shallower quench. A reduction of the apparent exponent for conserved order-parameter growth near T_c is consistent with earlier studies [14]. In this paper, more important than any specific growth law is the result that the data may be superimposed by simple multiplicative time scaling even before the asymptotic regime is reached.

In all of these growth kinetics studies, we have observed an increase in the *computation* required per cluster flip that increases roughly linearly in R. Since we observe a time rescaling of order R^2 (in units of LCF/site), the real computer time required to reach a given *effective time* decreases roughly as $1/R$. This suggests that with different cluster sizes, growth dynamics over a large range of time scales may be studied. Slightly above the critical temperature in the two-dimensional Ising model without spin conservation, we have observed an even greater reduction in computational effort due to the scaling of the diffusion constant as $D(R) \approx R^{5/2}$. We do not fully understand these exponents, or their dependence on the phase structure at scales smaller than R.

As indicated above, random bonds and fields are easily studied with LCF algorithms. Whether or not acceleration of the dynamics of these glassy systems with LCF algorithms is possible is an open problem. Similar classes of problems that LCF methods may be well suited for are problems involving (possibly inhomogeneous) boundary fields [15], and order-parameter kinetics in porous media [16]. A final, practical advantage of the LCF algorithm (even for equilibrium studies) over the Wolff algorithm is that it is naturally parallelized: the lattice can be divided into sublattices, each one treated by one processor. Constraints limiting clusters to the sublattice interiors allow interprocessor communication to be avoided; ergodicity is obtained by intermittently shifting the boundaries between sublattices.

We thank J. P. Sethna for helpful comments. This work was supported by the National Science Foundation under Contract No. DMR-91-21654 through the MRL Program, the Materials Science Center, and the Cornell National Supercomputer Facility.

[1] P. C. Hohenberg and B. I. Halperin, Rev. Mod. Phys. **49**, 435 (1977).
[2] J. D. Gunton, M. San Miguel, and P. S. Sahni, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. Lebowitz (Academic Press, London, 1983), Vol. 8.
[3] N. Metropolis *et al.*, J. Chem. Phys. **21**, 1087 (1953).
[4] T. M. Rogers, K. R. Elder, and R. C. Desai, Phys. Rev. B **37**, 9638 (1988).
[5] R. H. Swendsen and J. S. Wang, Phys. Rev. Lett. **58**, 86 (1987).
[6] U. Wolff, Phys. Rev. Lett. **62** 361 (1989).
[7] F. Niedermayer, Phys. Rev. Lett. **61**, 2026 (1988).
[8] Y. Oono and S. Puri, Phys. Rev. Lett. **58**, 836 (1987); Phys. Rev. A **38**, 434 (1988); A. Shinozaki and Y. Oono, Phys. Rev. Lett. **66**, 173 (1991).
[9] S. Puri and Y. Oono, Phys. Rev. A **38**, 1542 (1988).
[10] O. T. Valls and G. F. Mazenko, Phys. Rev. B **34**, 7941 (1986).
[11] A. Coniglio and F. Peruggi, J. Phys. A **15**, 1873 (1982).
[12] I. M. Lifshitz, Zh. Eksp. Teor. Fiz. **42**, 1354 (1962) [Sov. Phys. JETP **15**, 939 (1962)]; S. M. Allen and J. W. Cahn, Acta Metall. **27**, 1085 (1979).
[13] A. J. Liu and M. E. Fisher, Physica (Amsterdam) **156A**, 35 (1989).
[14] D. A. Huse, Phys. Rev. B **34**, 7845 (1986).
[15] R. C. Ball and R. L. H. Essery, J. Phys. Condens. Matter **2**, 10303 (1990); G. Brown and A. Chakrabarti, Phys. Rev. A **46**, 4829 (1992).
[16] S. B. Dierker and P. Wiltzius, Phys. Rev. Lett. **66**, 1185 (1991).