Nonuniversal Critical Dynamics in Monte Carlo Simulations

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A new approach to Monte Carlo simulations is presented, giving a highly efficient method of simulation for large systems near criticality. The algorithm violates dynamic universality at second-order phase transitions, producing unusually small values of the dynamical critical exponent.

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In addition to the intrinsic interest of dynamical critical properties at second-order phase transitions,[1,2] critical slowing down is of crucial importance to computer simulations of phase transitions. Long correlation times at criticality cause severe restrictions on the maximum-size lattice for which we can obtain good statistics.

Increasing the size of the system in a computer simulation has the important advantage of reducing finite-size effects, and in the absence of critical slowing down, would only incur very small penalties. Although the time required for a sweep through the system is proportional to the size of the system, the information contained in a configuration is also proportional to the size.

Although the correlation time, τ, is finite for a finite system, it can be very large at the critical point. As the system size is increased, τ increases as L^z, where L is the linear dimension of the system and z is the dynamical critical exponent. Since z is generally about 2.0 or larger,[3-7] and the simulation time must be much longer than τ for accuracy, this represents a major limitation.

In this paper, we present an unusual type of dynamics, which violates dynamic universality, and greatly reduces relaxation times in the computer simulation of large systems. Large clusters are changed in a single move, so that the process is not local in the usual sense, allowing z to be less than the lower bound of γ/ν.[8] However, it is local in the sense that only local information is required for each step in the algorithm, and the time required for a sweep through the lattice is still proportional to the size of the system. Since relaxation times are much shorter than they are for the usual algorithms, this approach produces very efficient simulations of large systems at the critical point.

The method is most simply described for a Potts model with the Hamiltonian

$$H=K\sum_{\langle i,j\rangle}(\delta_{\sigma_i,\sigma_j}-1), \tag{1}$$

where the spins take on the values $1,2,\ldots,q$, and factors of $-1/k_BT$ have been absorbed into the coupling constant K. Fortuin and Kasteleyn have shown how this model can be mapped onto a general percolation model.[9] Beginning with the partition function

$$Z=\mathrm{Tr}_{\{\sigma\}}e^H, \tag{2}$$

they consider the interaction between sites l and m, and remove it from the Hamiltonian:

$$H_{l,m}=K\sum_{\langle i,j\rangle\neq\langle l,m\rangle}(\delta_{\sigma_i,\sigma_j}-1). \tag{3}$$

Then the restricted sums

$$Z^{\mathrm{same}}_{\langle l,m\rangle}=\mathrm{Tr}_{\{\sigma\}}\exp(H_{\langle l,m\rangle})\delta_{\sigma_l,\sigma_m} \tag{4}$$

and

$$Z^{\mathrm{diff}}_{\langle l,m\rangle}=\mathrm{Tr}_{\{\sigma\}}\exp(H_{\langle l,m\rangle})(1-\delta_{\sigma_l,\sigma_m}) \tag{5}$$

can be defined so that

$$Z=Z^{\mathrm{same}}_{\langle l,m\rangle}+e^{-K}Z^{\mathrm{diff}}_{\langle l,m\rangle}. \tag{6}$$

If we now also introduce

$$Z^{\mathrm{ind}}_{\langle l,m\rangle}=\mathrm{Tr}_{\{\sigma\}}\exp(H_{\langle l,m\rangle})=Z^{\mathrm{same}}_{\langle l,m\rangle}+Z^{\mathrm{diff}}_{\langle l,m\rangle}, \tag{7}$$

we can rewrite Eq. (6) as

$$Z=(1-e^{-K})Z^{\mathrm{same}}_{\langle l,m\rangle}+e^{-K}Z^{\mathrm{ind}}_{\langle l,m\rangle}. \tag{8}$$

Since the first sum contains the restriction that the spins on sites l and m are the same, and the second term contains no restriction on the spins, the weighting factors can be interpreted in terms of the probability, $p=1-\exp(-K)$, of a bond between the two sites.

This procedure is then repeated for all interactions in Eq. (1). For each configuration of bonds, clusters are formed. For each cluster, all the spins are in one of the q states, independent of the states of the other clusters. If there are N_c clusters, this gives Fortuin and Kasteleyn's

result,

$$Z = \mathrm{Tr}_{\{\mathrm{bonds}\}} p^b (1-p)^n q^{N_c}, \quad (9)$$

where b is the number of bonds and n is the number of interactions that did not form a bond.

Carrying out this transformation directly on the spin configurations leads to a Monte Carlo algorithm that satisfies detailed balance.

Beginning with an arbitrary configuration of Potts states, create bonds with a probability $p = 1 - \exp(-K)$ between neighboring states with the same spin. No bonds are present between sites containing different spins. If the original spins are now erased, we are left with a configuration of bonds (and clusters[10]), with the weights found in Eq. (9). Note that some of the original clusters of Potts spins will be split into smaller clusters, since bonds do not occur between all sites with the same spin.

The next step is to assign a new random Potts value to each cluster and the same value to each site in the cluster. By erasing the bonds, we are left with a new Potts configuration. The new configuration can differ substantially from the original one, since large clusters can be changed in a single step.

There are at least two ways to use the theory of Markov processes to see that this procedure produces the equilibrium distribution. The first is to note that there is a nonzero probability of going from any state to any state in a single sweep of the lattice, and [compare Eqs. (1)–(9) with the Monte Carlo algorithm] the equilibrium maps into itself.

Alternatively, to see directly that detailed balance is satisfied, note that every transition between two Potts configurations must pass through some bond configuration in the percolation representation. First consider transitions that pass through a particular bond configuration.

The probability of passing through a particular bond configuration has a factor of p for every bond and a factor of q for every cluster regardless of which Potts configuration we started with. However, the probabilities differ by the number of factors of $1-p = \exp(-K)$ for each missing bond between neighboring spins with the same value. Since the probability is uniform for going from a bond configuration to any Potts configuration consistent with it, the ratio of the transition rates is just the exponential of the difference in the Hamiltonians of the two Potts configurations.

Since detailed balance is satisfied explicitly for every bond configuration the system can pass through during the transition between two Potts configurations, detailed balance is satisfied for the total transition probability.

The procedure is clearly applicable to any lattice in any number of dimensions, as well as to interactions of different strengths between different neighbors. It could even be applied to lattice gauge theories by treating a subset of the operators as interacting through effective two-operator interactions during the updating.

To test the effectiveness of this new algorithm for Monte Carlo simulations, we have studied the relaxation times at criticality for the two- and three-state Potts models in two dimensions and the two-state Potts model (Ising model) in three dimensions.

The results for the two-dimensional Ising model are given in Fig. 1, which shows a plot of the correlation time (obtained from the exponential decay of the long-time behavior of the energy-energy correlation function), as a function of the size of the system. For comparison, we have also shown corresponding data for a standard Monte Carlo simulation, as well as a line with slope equal to the best current estimate of the dynamical critical exponent of the two-dimensional Ising model.[4]

It is clear that the size dependence is not only much less than that of the standard simulation [the dynamical critical exponent z is 0.35(1) instead of 2.125 for standard simulations[4]], but that the new algorithm becomes more efficient for systems as small as 18×18. The new simulation of the Ising model in three dimensions gives $z = 0.75(1)$, as opposed to $z = 2.0$ for standard simulations.[5]

The three-state Potts model in two dimensions shows similar improvement, with $z = 0.6(1)$, as opposed to $z = 2.7(4)$ for standard Monte Carlo.[6]

All of these values of z for the new Monte Carlo algorithm are much lower than the exact lower bound, $z \geq \gamma/\nu$, which holds for single-spin-flip dynamics.[8]

Earlier work by Sweeny presented another way of generating the percolation clusters corresponding to Potts models,[11] based on exactly the same transformation.[9]

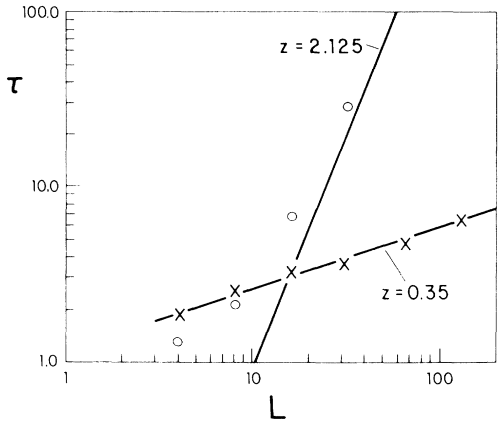

FIG. 1. Log-log plots of correlation times for Monte Carlo simulations of the two-dimensional Ising model at the critical temperature as a function of the linear dimension L. The circles show data for a standard Monte Carlo simulation, and the line marked "$z = 2.125$" gives the expected asymptotic slope (Ref. 4). The crosses show data for the new method, with a least-squares fit labeled with its slope of "$z = 0.35$."

His method had the added advantage that it was applicable to noninteger values of q, while our approach requires the number of states to be an integer. On the other hand, Sweeny's approach is limited to two dimensions, is much more difficult to program, and is not easily generalized to more than nearest-neighbor interactions.

Both Sweeny's method and ours have the advantage of producing explicit percolation configurations corresponding to Eq. (9). The percolation clusters behave as Fisher droplets,[12-14] and contain a great deal of information.

The generalization of our method to include random ferromagnetic interactions and uniform, or even random, magnetic fields is straightforward, either following Fortuin and Kasteleyn's suggestion of using interactions with a dummy spin to represent the magnetic field,[9] or simply choosing the new Potts spin with a probability determined by the magnetic interaction.

The extension to negative interactions for the Ising model is also straightforward, if Z^{same} is eliminated in favor of Z^{diff} and clusters are defined in terms of antibonds connecting opposite spins. This allows the application of this approach to general antiferromagnets and even spin-glasses. However, if the Hamiltonian contains frustrated interactions, percolation generally occurs above the phase transition, limiting the usefulness of the method.

Finally, the generalization to arbitrary spins is straightforward by expression of the interaction in terms of Potts interactions. The algorithm would create a bond with a probability determined by the absolute value of the interaction between the two spins. This has not yet been implemented, and it is not completely clear how efficient it would be.

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[1]P. C. Hohenberg and B. I. Halperin, Rev. Mod. Phys. **49**, 435 (1977).

[2]S. K. Ma, *Modern Theory of Critical Phenomena* (Benjamin, Reading, MA, 1976), Chaps. 11-14.

[3]H. Yahata and M. Suzuki, J. Phys. Soc. Jpn. **27**, 1421 (1969).

[4]J. K. Williams, J. Phys. A **18**, 49 (1985).

[5]C. Kalle, J. Phys. A **17**, L801 (1984).

[6]M. Aydin and M. C. Yalabik, J. Phys. A **17**, 2531 (1984).

[7]G. F. Mazenko, M. J. Nolan, and O. T. Valls, Phys. Rev. Lett. **41**, 500 (1978).

[8]K. Kawasaki, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, New York, 1972), Vol. 2.

[9]P. W. Kasteleyn and C. M. Fortuin, J. Phys. Soc. Jpn. Suppl. **26s**, 11 (1969); C. M. Fortuin and P. W. Kasteleyn, Physica (Utrecht) **57**, 536 (1972).

[10]J. Hoshen and R. Kopelman, Phys. Rev. B **14**, 3438 (1976).

[11]M. Sweeny, Phys. Rev. B **27**, 4445 (1983).

[12]M. E. Fisher, Physics **3**, 255 (1967).

[13]C.-K. Hu, Phys. Rev. B **29**, 5103, 5109 (1984).

[14]A. Coniglio, H. E. Stanley, and W. Klein, Phys. Rev. Lett. **42**, 518 (1979); A. Coniglio and W. Klein, J. Phys. A **13**, 2775 (1980).