Invaded Cluster Algorithm for Equilibrium Critical Points

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A new cluster algorithm based on invasion percolation is described. The algorithm samples the critical point of a spin system without *a priori* knowledge of the critical temperature and provides an efficient way to determine the critical temperature and other observables in the critical region. The method is illustrated for the two- and three-dimensional Ising models. The algorithm equilibrates spin configurations much faster than the closely related Swendsen-Wang algorithm.

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Enormous improvements in simulating systems near critical points have been achieved by using cluster algorithms [1,2]. In the present paper we describe a new cluster method which has the additional property of "self-organized criticality." In particular, the method can be used to sample the critical region of various spin models without the need to fine tune any parameters (or know them in advance). Here, as in other cluster algorithms, bond clusters play a pivotal role in a Markov process, where successive spin configurations are generated using the Fortuin-Kasteleyn [3] representation to identify clusters of spins for flipping. However, the clusters themselves are identified using *invasion percolation*. The new algorithm is closely related to the Swendsen-Wang (SW) algorithm [1] and may be adapted for a wide range of systems. For purposes of illustration, in this work we will consider the Ising model.

Let us first recall the SW algorithm as applied to an Ising system (in the Potts representation). Starting from a spin configuration, satisfied bonds—those connecting spins that are of the same type—are occupied with probability, $p(\beta) = 1 - e^{-\beta}$ where $\beta = J/k_BT$ is the coupling strength. Unsatisfied bonds are never occupied. Clusters of sites connected by occupied bonds are locked into the same spin type, and all clusters (including isolated sites) are independently flipped with probability $1/2$. The SW algorithm samples the canonical ensemble of the spin system at coupling β and/or the random cluster (bond configuration) ensemble with parameter p. At T_c the SW algorithm is far more efficient than single spin-flip methods, because the flipped clusters are also critical droplets [4].

Here we propose using invasion percolation [5–10] to generate the bond clusters for the spin flips. In the usual invasion percolation, random numbers are independently assigned to the bonds of the lattice. Growth starts from one or more seed sites, and at each step the clusters grow by the addition of the perimeter bond with the smallest random number. If a single cluster grows indefinitely on an infinite lattice, its large scale behavior is presumed to be that of the "incipient infinite cluster" of ordinary percolation. In particular, the fraction of perimeter bonds accepted into the growing cluster approaches the percolation threshold p_c [9,10]. Invasion percolation is thus a self-organized critical phenomenon.

For the present, we modify invasion percolation in two ways. First, we initiate cluster growth at *all* lattice sites. Consider this change for ordinary invasion percolation: Every bond is initially a perimeter bond, and the invasion process consists of collecting bonds in a given random order. Initially, every site is a cluster, and in most steps of the growth process two smaller clusters are combined into a single larger cluster. The growth process is terminated when some cluster "spans" (i.e., is of linear dimension that is the scale of) the system. Let $f = f(L)$ be the fraction of bonds accepted during the growth process in a system of scale L. It is intuitively clear—as first discussed in Ref. [5]—that as $L \to \infty$, f approaches p_c, the ordinary percolation threshold for the corresponding lattice [11].

The second modification, which is the cornerstone of this Letter, correlates invasion percolation to an underlying spin configuration. As in the SW algorithm, this is done by allowing cluster growth along only satisfied bonds.

The new method, which we call the invaded cluster (IC) algorithm, works as follows. Starting with an Ising spin configuration S, the bonds of the lattice are given a random order. Correlated invasion percolation clusters are grown as described above until one of the clusters spans the system. After the growth process is terminated, each cluster is flipped with probability $1/2$ yielding a new spin configuration S'. The bonds are then randomly reordered and the process begins anew.

In the present implementation, a cluster is counted as spanning when the maximum separation in one of the d directions for some pair of points in the cluster is the system size L. We have also used a topological spanning

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rule in which clusters are terminated upon winding around the system in some direction. The results [12] are very similar to those presented below.

We tested the algorithm on the nearest neighbor, ferromagnetic Ising model on square and simple cubic lattices with periodic boundary conditions. The computation time per Monte Carlo step scales linearly in the number of spins but with a somewhat larger prefactor than for the SW algorithm. After equilibration for 200 steps starting from the spin up state, statistics were collected on the energy E and the ratio f of the number of accepted bonds to the number of satisfied bonds. For each system size we collected statistics for the order of 10^4 Monte Carlo steps. We first discuss the results for two-dimensional systems with sizes up to 500^2. In Fig. 1 we show the mean and median [13] values of f plotted against $1/L$. A linear fit through the median data extrapolates to 0.5855 compared with the exact value, $p(\beta_c) = 1 - e^{-\beta_c} = 0.58579\ldots$.

In Fig. 2, we plot the standard deviation of f as a function of $1/L$. The solid line is a fit to a function of the form $c_0 + c_1 L^{-1/2} + c_2 L^{-1}$, which yields $c_0 = -0.0014$. Figures 1 and 2 are thus consistent with the hypothesis that the distribution of f approaches a delta function at $p(\beta_c)$ as $L \to \infty$ with a scaling that is given, approximately, by $L^{-1/2}$. The average energy per spin $\langle E \rangle / N$ is shown in Fig. 3 and plotted against the inverse of the system size $1/L$. The best fit by the form $e_0 + e_1 L^{-1} + e_2 L^{-2}$ yields $e_0 = -1.706$ in comparison to the exact result -1.7071. The variance of the total energy divided by the number of spins is shown in the inset of Fig. 3. In the canonical ensemble, $\mathrm{var}(E)/N$ is proportional to the specific heat and diverges logarithmically in L, whereas here we find that this quantity diverges linearly in L. It is clear that the IC algorithm does not sample the canonical ensemble.

The results for the three-dimensional Ising model up to system size 70^3 are qualitatively similar to the two-dimensional results except that the finite size scaling behavior for f is controlled by the three-dimensional Ising correlation length exponent $\nu \simeq 0.63$. In Fig. 1 we plot the mean value of f against $L^{-1/\nu}$. The solid line in the figure is the least-squares linear fit to all the data which yields an intercept at 0.35803 in comparison to the accepted value [14] $p(\beta_c) \simeq 0.35810$. The standard deviation of f vanishes with a leading behavior that is well fitted to $L^{-1/2\nu}$. The mean energy per spin extrapolates to -2.00.

Why does the IC algorithm work? We do not have a rigorous proof that as the system size goes to infinity the distribution for f peaks at $p(\beta_c)$ or that observables such as the energy density converge to their limiting (infinite volume) values at criticality. Nonetheless we can give some heuristic arguments supporting the validity of the algorithm.

The discussion is based on the observation that each iteration of the invaded cluster algorithm is identical to one iteration of the SW algorithm with $p = f$. Suppose we start with an infinite (or huge) spin configuration that is already typical of the critical point. On the basis of current understanding, $p(\beta_c)$ corresponds to the threshold for the formation of large-scale bond clusters in the associated correlated bond percolation problem on this

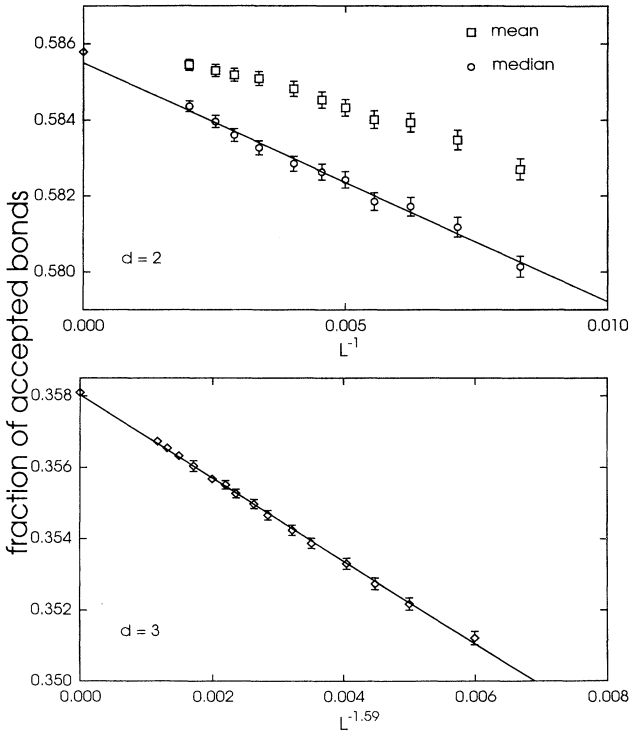

FIG. 1. The fraction of accepted bonds for two and three dimensions vs $L^{-1/\nu}$. For two dimensions the mean and median values of f are shown. The solid lines are linear fits through the data, and the known values of $p(\beta_c)$ are marked on the vertical axes with diamonds.

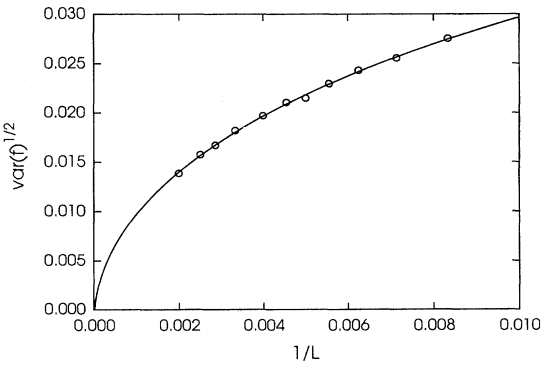

FIG. 2. The standard deviation of f vs $1/L$ for the two-dimensional Ising model. The solid line is the least-squares fit by the form $c_0 + c_1 L^{-1/2} + c_2 L^{-1}$.

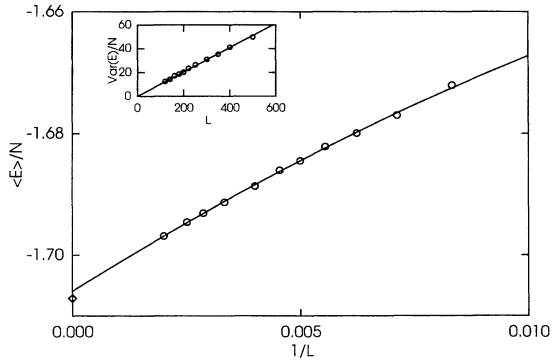

FIG. 3. $\langle E\rangle/N$ vs $1/L$ for the two-dimensional Ising model. The solid line is a fit by the form $e_0 + e_1L^{-1} + e_2L^{-2}$, and the exact infinite volume result is indicated by a diamond on the vertical axis. The inset shows $\mathrm{var}(E)/N$ vs L. The solid line is a linear fit through the data.

configuration. Let us now parallel the arguments given above for uncorrelated invasion percolation. On a finite system, in a critical spin configuration, the fraction f of accepted satisfied bonds will be close to $p(\beta_c)$ when some cluster first spans the system. Hence, when the spin clusters get flipped, the new configuration should still be typical of criticality. It thus follows that if the invaded cluster algorithm starts from a critical spin configuration, it behaves like the SW algorithm with a temperature that fluctuates near T_c and therefore remains near criticality.

It is also clear that the IC algorithm moves the spin configuration toward criticality if it is started in either the high or low temperature phase. Suppose the spin configuration is in the low temperature phase. Here the portion of satisfied bonds is greater than the critical value, and due to this relative abundance, a smaller fraction is needed to produce a spanning cluster than in the case of a critical spin configuration. For example, in the extreme case of the zero temperature configuration, one obtains $f \simeq p_c$, the ordinary percolation point which is, of course, significantly smaller than $p(\beta_c)$. Writing $f = 1 - e^{-\beta}$, this corresponds to an iteration of the SW algorithm at $T > T_c$ and the system is pushed toward higher temperature. Conversely, if the spin system is in the high temperature phase, there are not enough satisfied bonds and spanning will occur for $f > p(\beta_c)$, corresponding to an iteration of the SW algorithm at a temperature less than the critical temperature. We thus have a negative feedback mechanism which warms the spin system when its temperature is below T_c and cools the spin system when its temperature is above T_c.

These arguments suggest that, in finite volume, the stationary distribution of the IC algorithm is close to (although not identical to) the canonical ensemble at β_c and/or the corresponding Fortuin-Kasteleyn random cluster distribution at $p(\beta_c)$. We will refer to the distribution sampled by the algorithm as the invaded cluster ensemble. Let us further suppose that the distribution for f becomes sharp as $L \to \infty$ and that the volume fraction of the spanning cluster tends to zero in this limit. It then follows that in the invaded cluster ensemble, the distribution functions of all local observables, e.g., spin correlation functions or cluster size distributions, will converge to their infinite volume critical point distributions. The critical exponent τ $[= 2 + \beta/(\beta + \gamma)]$ can be obtained from the cluster size distribution. Our measurements of the cluster size distribution for the two- and three-dimensional Ising models are consistent with the accepted values of τ. Another independent exponent can presumably be extracted via finite-size scaling. On the other hand, we must emphasize that finite-volume fluctuations in the invaded cluster ensemble such as $\mathrm{var}(E)$ need not have the same value as in the canonical ensemble and cannot be interpreted as thermodynamic response functions.

We measured the normalized energy and magnetization autocorrelation functions. The energy autocorrelation function is defined by $\langle[E(t) - \langle E\rangle][E(0) - \langle E\rangle]\rangle/\mathrm{var}(E)$ with t the number of iterations of the algorithm. Results for two dimensions are plotted in Fig. 4 and compared to the SW algorithm. The energy and magnetization are almost fully decorrelated in a single Monte Carlo step. Results for the three-dimensional Ising model are similar. The negative overshoot in the energy autocorrelation is consistent with the negative feedback mechanism described above, and the latter suggest why the algorithm is so fast. Consider again the example of an initial spin configuration at zero temperature: one iteration of the SW algorithm at β_c yields a bond percolation configuration at $p(\beta_c) > p_c$, which still maintains a considerable degree of low temperature order. In particular, the average magnetization per site is still appreciable. By contrast, the magnetization after one step of the IC algorithm will have essentially vanished. If the same type of reasoning is applied to more general configurations, the conclusion is that the IC algorithm drives a system to criticality faster than the SW algorithm with $p = p(\beta_c)$. It

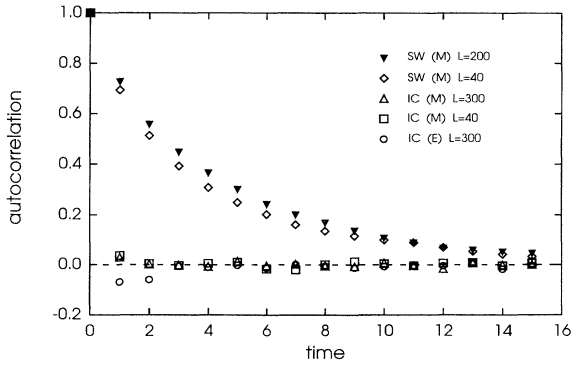

FIG. 4. The normalized magnetization (M) and energy (E) autocorrelation functions for Swendsen-Wang (SW) and invaded cluster (IC) dynamics for the two-dimensional Ising model.

is tempting to speculate that in some cases invaded cluster dynamics has no critical slowing down.

The invaded cluster algorithm should find many uses. The extremely rapid equilibration time suggests it may be the best approach for high precision simulations of the critical region of large spin systems. Using the embedding method of Ref. [2], continuous spin models may be simulated. The algorithm may also be used to study first order transitions, preliminary results for Potts models with first order transitions indicate that the transition temperature is correctly located [12]. The IC algorithm should also prove useful for quenched random ferromagnetic systems where the critical temperature—which depends on the details of the disorder distribution—is often difficult to pin down.

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