to redo many of these applications with much better statistics and with larger system sizes. In the following, we discuss some additional recent developments, but we have omitted other important topics such as Brownian dynamics and umbrella sampling. More ideas for projects can be found in the references.

Project 15.32 Overcoming critical slowing down

The usual limiting factor of most simulations is the speed of the computer. Of course, one way to overcome this problem is to use a faster computer. Near a continuous phase transition, the most important limiting factor on even the fastest available computers is the existence of critical slowing down (see Problem 15.19). In this project we discuss the nature of critical slowing down and ways of overcoming it in the context of the Ising model.

As we have mentioned, the existence of critical slowing down is related to the fact that the size of the correlated regions of spins becomes very large near the critical point. The large size of the correlated regions and the corresponding divergent behavior of the correlation length ξ near T_c implies that the time τ required for a region to lose its coherence becomes very long if a *local* dynamics is used. At $T = T_c$, $\tau \sim L^z$ for $L \gg 1$. For single spin flip algorithms, $z \approx 2$ and τ becomes very large for $L \gg 1$. On a serial computer, the CPU time needed to obtain n configurations increases as L^2, the time needed to visit L^2 spins. This factor of L^2 is expected and not a problem because a larger system contains proportionally more information. However, the time needed to obtain n approximately *independent* configurations is of order $\tau L^2 \sim L^{2+z} \approx L^4$ for the Metropolis algorithm. We conclude that an increase of L by a factor of 10 requires 10^4 more computing time. Hence, the existence of critical slowing down limits the maximum value of L that can be considered.

If we are interested only in the static properties of the Ising model, the choice of dynamics is irrelevant as long as the transition probability satisfies the detailed balance condition (15.18). It is reasonable to look for a *global* algorithm for which groups or *clusters* of spins are flipped simultaneously. We are already familiar with cluster properties in the context of percolation (see Chapter 12). A naive definition of a cluster of spins might be a domain of parallel nearest neighbor spins. We can make this definition explicit by introducing a bond between any two nearest neighbor spins that are parallel. The introduction of a bond between parallel spins defines a site-bond percolation problem. More generally, we may assume that such a bond exists with probability p and that this bond probability depends on the temperature T.

The dependence of p on T can be determined by requiring that the percolation transition of the clusters occurs at the Ising critical point and by requiring that the critical exponents associated with the clusters be identical to the analogous thermal exponents. For example, we can define a critical exponent ν_p to characterize the divergence of the connectedness length of the clusters near p_c. The analogous thermal exponent ν quantifies the divergence of the thermal correlation length ξ near T_c. We will argue in the following that these (and other) critical exponents are identical if we define the bond probability as

$$p = 1 - e^{-2J/kT} \quad \text{(bond probability)}. \qquad (15.79)$$

The relation (15.79) holds for any spatial dimension. What is the value of p at $T = T_c$ for the two-dimensional Ising model on the square lattice?

A simple argument for the temperature dependence of p in (15.79) is as follows. Consider the two configurations in Figure 15.9 which differ from one another by the flip of the cluster of two spins. In Figure 15.9(a) the six nearest neighbor spins of the cluster are in the opposite direction and, hence, are not part of the cluster. Thus, the probability of this configuration with a cluster of two spins is $p\,e^{-\beta J}e^{6\beta J}$, where p is the probability of a bond between the two up spins, $e^{-\beta J}$ is proportional to the probability that these two spins are parallel, and $e^{6\beta J}$ is proportional to the probability that the six nearest neighbors are antiparallel. In Figure 15.9(b) the cluster spins have been flipped, and the possible bonds between the cluster spins and its nearest neighbors have to be "broken." The probability of this configuration with a cluster of two (down) spins is $p(1-p)^6e^{-\beta J}e^{-6\beta J}$, where the factor of $(1-p)^6$ is the probability that the six nearest neighbor spins are not part of the cluster. Because we want the probability that a cluster is flipped to be unity, we need to have the probability of the two configurations and their corresponding clusters be the same. Hence, we must have

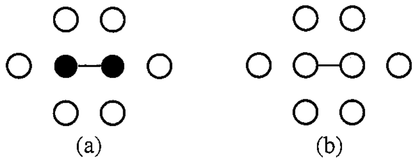

Figure 15.9 (a) A cluster of two up spins. (b) A cluster of two down spins. The filled and open circles represent the up and down spins, respectively. Note the bond between the two spins in the cluster. Adapted from Newman and Barkema.

$$pe^{-\beta J}e^{6\beta J} = p(1-p)^6e^{-\beta J}e^{-6\beta J}, \qquad (15.80)$$

or $(1-p)^6 = e^{-12\beta J}$. It is straightforward to solve for p and obtain the relation (15.79).

Now that we know how to generate clusters of spins, we can use these clusters to construct a global dynamics instead of only flipping one spin at a time as in the Metropolis algorithm. The idea is to grow a single (site-bond) percolation cluster in a way that is analogous to the single (site) percolation cluster algorithm discussed in Section 13.1. The algorithm can be implemented by the following steps:

(i) Choose a seed spin at random. Its four nearest neighbor sites (on the square lattice) are the perimeter sites. Form an ordered array corresponding to the perimeter spins that are parallel to the seed spin and define a counter for the total number of perimeter spins.

(ii) Choose the first spin in the ordered perimeter array. Remove it from the array and replace it by the last spin in the array. Generate a random number r. If $r \leq p$, the bond exists between the two spins, and the perimeter spin is added to the cluster.

(iii) If the spin is added to the cluster, inspect its parallel perimeter spins. If any of these spins are not already a part of the cluster, add them to the end of the array of perimeter spins.

(iv) Repeat steps (ii) and (iii) until no perimeter spins remain.

(v) Flip all the spins in the single cluster.

This algorithm is known as single cluster flip or *Wolff* dynamics. Note that bonds, rather than sites, are tested so that a spin might have more than one chance to join a cluster. In the following, we consider both the static and dynamical properties of the two-dimensional Ising model using the Wolff algorithm to generate the configurations.