whenever possible. Extend your results to larger N, for example, $N = 12$, 24, and 48. For a given annealing schedule, determine the probability of finding a route of a given length. More suggestions can be found in the references.

(b) The microcanonical Monte Carlo algorithm (demon) discussed in Section 15.3 can also be used to do simulated annealing. The advantages of the demon algorithm are that it is deterministic and allows large temperature fluctuations. One way to implement the analog of simulated annealing is to impose a maximum value on the energy of the demon, $E_{d,\max}$, which is gradually decreased. Guo et al. choose $E_{d,\max}$ to be initially equal to $\sqrt{N}/4$. Their results are comparable to the usual simulated annealing method but require approximately half the CPU time. Apply this method to the same city positions that you considered in part (a) and compare your results. □

15.14 Projects

Many of the original applications of Monte Carlo methods were done for systems of approximately one hundred particles and lattices of order 32^2 spins. It would be instructive 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

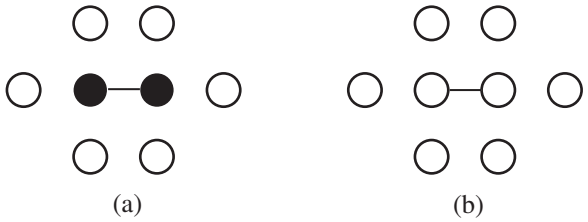

Figure 15.9: (a) A cluster of two up spins. (b) A cluster of two down spins. The filled and open circles represent the up and down spins, respectively. Note the bond between the two spins in the cluster. Adapted from Newman and Barkema.

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

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

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 $p(1-p)^6 e^{-\beta J}e^{-6\beta J}$, 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

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

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.

(a) Modify your program for the Ising model on a square lattice so that single cluster flip dynamics (the Wolff algorithm) is used. Compute the mean energy and magnetization for $L = 16$ as a function of T for $T = 2.0$ to 2.7 in steps of 0.1. Compare your results to those obtained using the Metropolis algorithm. How many cluster flips do you need to obtain comparable accuracy at each temperature? Is the Wolff algorithm more efficient at every temperature near T_c?

(b) Fix T at the critical temperature of the infinite lattice ($T_c = 2/\ln(1+\sqrt{2})$) and use finite size scaling to estimate the values of the various static critical exponents, for example, γ and α. Compare your results to those obtained using the Metropolis algorithm.

(c) Because we are generating site-bond percolation clusters, we can study their geometrical properties as we did for site percolation. For example, measure the distribution sn_s of cluster sizes at $p = p_c$ (see Problem 13.3). How does n_s depend on s for large s (see Project 13.15)? What is the fractal dimension of the clusters in the Ising model at $T = T_c$?

(d) The natural unit of time for single cluster flip dynamics is the number of cluster flips $t_{\rm cf}$. Measure $C_M(t_{\rm cf})$ and/or $C_E(t_{\rm cf})$ and estimate the corresponding correlation time $\tau_{\rm cf}$ for $T = 2.5$, 2.4, 2.3, and T_c for $L = 16$. As discussed in Problem 15.19, $\tau_{\rm cf}$ can be found from the relation, $\tau_{\rm cf} = \sum_{t_{\rm cf}=1} C(t_{\rm cf})$. The sum is cut–off at the first negative value of $C(t_{\rm cf})$. Estimate the value of $z_{\rm cf}$ from the relation $\tau_{\rm cf} = L^{z_{\rm cf}}$.

(e) To compare our results for the Wolff algorithm to our results for the Metropolis algorithm, we should use the same unit of time. Because only a fraction of the spins are updated at each cluster flip, the time $t_{\rm cf}$ is not equal to the usual unit of time, which corresponds to an update of the entire lattice or one Monte Carlo step per spin. We have that τ measured in Monte Carlo steps per spin is related to $\tau_{\rm cf}$ by $\tau = \tau_{\rm cf}\langle c\rangle/L^2$, where $\langle c\rangle$ is the mean number of spins in the single clusters, and L^2 is the number of spins in the entire lattice. Verify that the mean cluster size scales as $\langle c\rangle \sim L^{\gamma/\nu}$ with $\gamma = 7/4$ and $\nu = 1$. (The quantity $\langle c\rangle$ is the same quantity as the mean cluster size S defined in Chapter 12. The exponents characterizing the divergence of the various properties of the clusters are identical to the analogous thermal exponents.)

(f) To obtain the value of z that is directly comparable to the value found for the Metropolis algorithm, we need to rescale the time as in part (e). We have that $\tau \sim L^z \propto L^{z_{\rm cf}} L^{\gamma/\nu} L^{-d}$. Hence, z is related to the measured value of $z_{\rm cf}$ by $z = z_{\rm cf} - (d - \gamma/\nu)$. What is your estimated value of z? (It has been estimated that $z_{\rm cf} \approx 0.50$ for the $d = 2$ Ising model, which would imply that $z \approx 0.25$.)

(g) One of the limitations of the usual implementation of the Metropolis algorithm is that only one spin is flipped at a time. However, there is no reason why we could not choose f spins at random, compute the change in energy ΔE for flipping these f spins, and accepting or rejecting the trial move in the usual way according to the Boltzmann probability. Explain why this generalization of the Metropolis algorithm would be very inefficient, especially if $f >> 1$. We conclude that the groups of spins to be flipped must be chosen with the physics of the system in mind and not simply at random. □

Another cluster algorithm is to assign all bonds between parallel spins with probability p. As usual, no bonds are included between sites that have different spin orientations. From this configuration of bonds, we can form clusters of spins using one of the cluster identification algorithms we discussed in Chapter 12. The smallest cluster contains a single spin. After the clusters have been identified, all the spins in each cluster are flipped with probability 1/2. This algorithm is known as the *Swendsen-Wang* algorithm and preceded the Wolff algorithm. Because the Wolff algorithm is easier to program and gives a smaller value of z than the Swendsen-Wang algorithm for the $d = 3$ and $d = 4$ Ising models, the Wolff algorithm is more commonly used.

Project 15.33. Invaded cluster algorithm

In Problem 13.7 we found that invasion percolation is an example of a self-organized critical phenomenon. In this cluster growth algorithm, random numbers are independently assigned to the bonds of a lattice. The growth starts from the seed sites of the left-most column. At each step the cluster grows by the occupation of the perimeter bond with the smallest random number. The growth continues until the cluster satisfies a stopping condition. We found that if we stop adding sites when the cluster is comparable in extent to the linear dimension L, then the fraction of bonds that are occupied approaches the percolation threshold p_c as $L \to \infty$. The invaded percolation algorithm automatically finds the percolation threshold!

Machta and co-workers have used this idea to find the critical temperature of a spin system without knowing its value in advance. For simplicity, we will discuss their algorithm in the context of the Ising model, although it can be easily generalized to the q-state Potts model (see the references). Consider a lattice on which there is a spin configuration $\{s_i\}$. The bonds of the lattice are assigned a random order. Bonds (i, j) are tested in this assigned order to see if s_i is parallel to s_j. If so, the bond is occupied and spins i and j are a part of the same cluster. Otherwise, the bond is not occupied and is not considered for the remainder of the current Monte Carlo step. The set of occupied bonds partitions the lattice into clusters of connected sites. The clusters can be found using the Newman–Ziff algorithm (see Section 12.3). The cluster structure evolves until a stopping condition is satisfied. Then a new spin configuration is obtained by flipping each cluster with probability 1/2, thus completing one Monte Carlo step. The fraction f of bonds that were occupied during the growth process and the energy of the system are measured. The bonds are then randomly reordered and the process begins again. Note that the temperature is not an input parameter.

If open boundary conditions are used, the appropriate stopping rule is that a cluster spans the lattice (see Chapter 12, page 450). For periodic boundary conditions, the spanning rule discussed in Project 12.17 is appropriate.