and choose the mesh size so that the acceptance probability for changing the volume by one unit is 40–50%. Do a Monte Carlo simulation of the hard disk system for $L = 10$ ($N = 100$) and $p^* = 7.30$. Published results are for 10^7 Monte Carlo steps. To apply the Lee–Kosterlitz method, smooth $\ln N(v)$ by fitting it to an eighth-order polynomial. Then extrapolate $\ln N(v)$ using the histogram method to determine $p_c^*(L = 10)$, the pressure at which the two peaks of $N(v)$ are of equal height. What is the value of the free energy barrier ΔF? If sufficient computer resources are available, compute ΔF for larger L (published results are for $L = 10$, 12, 14, 16, and 20) and determine if ΔF depends on L. Can you reach any conclusions about the nature of the transition? ■

Project 15.45 Vacancy mediated dynamics in binary alloys

When a binary alloy is rapidly quenched from a high temperature to a low temperature unstable state, a pattern of domain formation called *spinodal decomposition* takes place as the two metals in the alloy separate. This process is of much interest experimentally. Lifshitz and Slyozov have predicted that at long times, the linear domain size increases with time as $R \sim t^{1/3}$. This result is independent of the dimension for $d \geq 2$, and has been verified experimentally and in computer simulations. The behavior is modified for binary fluids due to hydrodynamic effects.

Most of the computer simulations of this growth process have been based on the Ising model with spin exchange dynamics. In this model there is an A or B atom (spin up or spin down) at each site, where A and B represent different metals. The energy of interaction between atoms on two neighboring sites is $-J$ if the two atoms are the same type and $+J$ if they are different. Monte Carlo moves are made by exchanging unlike atoms. (The number of A and B atoms must be conserved.) A typical simulation begins with an equilibrated system at high temperatures. Then the temperature is changed instantaneously to a low temperature below the critical temperature T_c. If there are equal numbers of A and B atoms on the lattice, then spinodal decomposition occurs. If you watch a visualization of the evolution of the system, you will see wavy-like domains of each type of atom thickening with time.

The growth of the domains is very slow if we use spin exchange dynamics. We will see that if simulations are performed with vacancy mediated dynamics, the scaling behavior begins at much earlier times. Because of the large energy barriers that prevent real metallic atoms from exchanging position, it is likely that spinodal decomposition in real alloys also occurs with vacancy mediated dynamics. We can do a realistic simulation by including just one vacancy because the number of vacancies in a real alloy is also very small. In this case the only possible Monte Carlo move on a square lattice is to exchange the vacancy with one of its four neighboring atoms. To implement this algorithm, you will need an array to keep track of which type of atom is at each lattice site and variables to keep track of the location of the single vacancy. The simulation will run very fast because there is little bookkeeping and all the possible trial moves are potentially good ones. In contrast, in standard spin exchange dynamics, it is necessary to either waste computer time checking for unlike nearest neighbor atoms or keep track of where they are.

The major quantity of interest is the growth of the domain size R. One way to determine R is to measure the pair correlation function $C(r) = \langle s_i s_j \rangle$, where $r = |\mathbf{r}_i - \mathbf{r}_j|$, and $s_i = 1$ for an A atom and $s_i = -1$ for a B atom. The first zero in $C(r)$ is a measure of the domain size. An alternative measure of the domain size is the quantity $R = 2/(\langle E \rangle/N + 2)$, where $\langle E \rangle/N$ is the average energy per site and N is the number of sites (see Project 15.39). The quantity R is a rough measure of the length of the perimeter of a domain and is proportional to the domain size.

(a) Write a program to simulate vacancy mediated dynamics. The initial state consists of the random placement of A and B atoms (half of the sites have A and half B atoms); one vacancy replaces one of the atoms. Explain why this configuration corresponds to infinite temperature. Choose a square lattice with $L \geq 50$.

(b) Instantaneously quench the system by running the Metropolis algorithm at a temperature of $T = T_c/2 \approx 1.13$. You should first look at the lattice after every attempted move of the vacancy to see the effect of vacancy dynamics. After you are satisfied that your program is working correctly and that you understand the algorithm, speed up the simulation by only collecting data and showing the lattice at times equal to $t = 2^n$ where $n = 1, 2, 3 \ldots$. Measure the domain size using either the energy or $C(r)$ as a function of time averaged over many different initial configuration quenches.

(c) At what time does the log R versus log t plot become linear? Do both measures of the domain size give the same results? Does the behavior change for different quench temperatures? Try $0.2T_c$ and $0.7T_c$. A log-log plot of the domain size versus time should give the exponent $1/3$.

(d) Repeat the measurements in three dimensions. Do you obtain the same exponent? ■

Project 15.46 Heat flow using the demon algorithm

In our applications of the demon algorithm, one demon shared its energy equally with all the spins. As a result the spins all attained the same mean energy of interaction. Many interesting questions arise when the system is not spatially uniform and is in a nonequilibrium but time-independent (steady) state.

Let us consider heat flow in a one-dimensional Ising model. Suppose that instead of all the sites sharing energy with one demon, each site has its own demon. We can study the flow of heat by requiring the demons at the boundary spins to satisfy different conditions than the demons at the other spins. The demon at spin 0 adds energy to the system by flipping this spin so that it is in its highest energy state, that is, in the opposite direction of spin 1. The demon at spin $N - 1$ removes energy from the system by flipping spin $N - 1$ so that it is in its lowest energy state, that is, in the same direction as spin $N - 2$. As a result, energy flows from site 0 to site $N - 1$ via the demons associated with the intermediate sites. In order that energy not build up at the "hot" end of the Ising chain, we require that spin 0 can only add energy to the system if spin $N - 1$ simultaneously removes energy from the system. Because the demons at the two ends of the lattice satisfy different conditions than the other demons, we do not use periodic boundary conditions.

The temperature is determined by the generalization of the relation (15.10); that is, the temperature at site i is related to the mean energy of the demon at site i. To control the temperature gradient, we can update the end spins at a different rate than the other spins. The maximum temperature gradient occurs if we update the end spins after every update of an internal spin. A smaller temperature gradient occurs if we update the end spins less frequently. The temperature gradient between any two spins can be determined from the temperature profile, the spatial dependence of the temperature. The energy flow can be