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Readers of this column need little reminder that numerical simulation is a valuable tool for studying many problems in statistical physics.[1] In this column we explore the use of the microcanonical ensemble to study the coexistence of substances that exhibit first-order phase transitions. The most common example of such a substance is water. At 100 °C and normal atmospheric conditions, the liquid and vapor phases coexist and energy is required to transform water into vapor at this temperature. Water vapor can be supercooled to well below 100 °C. In this condition it is metastable and will turn to water (or even ice) if perturbed. We will explore these and other properties of first-order transitions in the following.

The most common Monte Carlo method for simulating a system with many degrees of freedom is the Metropolis algorithm. The main features of this algorithm are that the temperature T is fixed and changes in the configuration of the system are accepted with the Boltzmann probability $\exp(-\beta\Delta E)$, where ΔE is the change in the energy of the system associated with the attempted change, and $\beta = 1/k_B T$. In contrast, the Creutz or *demon* algorithm[2] fixes the energy of the system and the other thermodynamic properties of the system are determined during a run. In particular, the temperature is determined by monitoring the energy of one or more demons that are in thermal contact with the system.

We introduce the simplest version of the demon algorithm in the context of the nearest-neighbor[1] Ising model. In addition to the system of interest, imagine that we also introduce a demon with energy E_d that is constrained to have positive energy but is allowed to exchange energy with the system. The algorithm can be summarized as follows:

0. Establish an initial spin configuration.
1. Choose a spin at random and attempt to flip it.
2. Compute ΔE, the change in the energy of the system associated with the attempted flip.
3. If $\Delta E \leqslant 0$, accept the change, and give the extra energy to the demon, i.e., $E_d = E_d + \Delta E$.
4. If $\Delta E > 0$, accept the change if the demon has sufficient energy to give to the system. In this case $E_d = E_d - \Delta E$. Otherwise the trial change is rejected and the configuration is unchanged.

For the duration of a run the combined energy of the system and the demon is held constant. Steps 1–4 are repeated until thermal equilibrium is established, the demon and the system agree on mean energy for each, and a representative sample of states of the system is obtained. Since the demon is only one degree of freedom in equilibrium with a system of N spins, it has $1/N$ of the total energy so that the most likely energy of the system approximates a microcanonical ensemble.

Since the demon is a small system in thermal equilibrium with a much larger system, it is easy to see that the demon energy distribution $P(E_d)$ is proportional to $\exp(-\beta E_d)$, and the value of β can be extracted from the slope of a semilog plot of $P(E_d)$. If E_d can have a continuum of values, the mean demon energy $\langle E_d \rangle$ is given by $\langle E_d \rangle = 1/\beta$. However, the values of E_d are not continuous for the Ising model, and the relation between $\langle E_d \rangle$ and T for the Ising model in the absence of a magnetic field can be determined from

$$\beta J = \tfrac{1}{4} \ln(1 + 4J/\langle E_d \rangle), \tag{1}$$

where J is the nearest-neighbor exchange interaction. This result comes from the relation $\langle E_d \rangle = \Sigma E_d \times \exp(-\beta E_d) \Sigma \exp(-\beta E_d)$, where the sums are over the possible demon energies, 0, $4J$, $8J$, ...

One advantage of the demon algorithm is that it is inherently faster than the constant temperature Metropolis algorithm because it avoids the calculation of the exponential Boltzmann factors required by the latter. That is, the use of the demon algorithm for the Ising model allows the use of integer programming with consequent increases in speed on many machines. It is suggested that the reader attempt Problem 1 in order to gain experience with the demon algorithm in a simple context.

Another advantage of the demon algorithm, particular to the study of first-order phase transitions, is the possibility of studying the coexistence of phases and aspects of their metastable and even unstable behavior. This advantage is due to the fact that we can fix the energy rather than the temperature and choose the simulation to be done precisely in the part of the coexistence region of interest. In order to understand these ideas, we modify the Ising model so that it exhibits a first-order phase transition.[3] We assume that each spin sees a local field that gives spin-up, $\sigma = 1$, an energy Δ greater than spin-down, $\sigma = -1$. In addition, $\sigma = 1$ is degenerate with degeneracy g. If we interpret the Ising model as a lattice gas for which spin-up and spin-down correspond to the vapor and liquid phases, respectively, we can think of the energy Δ as a pressure and the degeneracy g as the extra degree of freedom of the lattice gas when it is in its vapor phase.

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It is straightforward using the canonical ensemble to show the existence of the first-order transition for the modified Ising model. The partition function differs from the usual Ising model only in that each up spin term carries the factor

$$ge^{-\beta\Delta}, \tag{2a}$$

which can be written as

$$e^{-(\Delta - T\ln g)/T}. \tag{2b}$$

Hence, the additional effective energy of an up spin is $\Delta - T\ln g$, and there is a competition between the extra energy Δ and the entropylike term $T\ln g$. This latter term dominates for $T > T_f$, where T_f is the temperature for the first-order transition, if T_f is less than the critical temperature T_c of the usual Ising model. Hence, we have that

$$T_f = \Delta/\ln g, \quad \text{if } T_f < T_c = 2.269J. \tag{3}$$

Because the first-order transition involves the flipping of every spin in the system, the energy change per spin can be identified as

$$\delta E = \Delta(n\uparrow - n\downarrow) = \Delta m, \tag{4}$$

where $n\uparrow$, $n\downarrow$, and m are, respectively, the fractional numbers of up and down spins and the fractional magnetization evaluated for the usual Ising system at $T = T_f$. This energy is the latent heat of the system. Hence, as $T_f \to T_c$, m and therefore the latent heat become smaller.

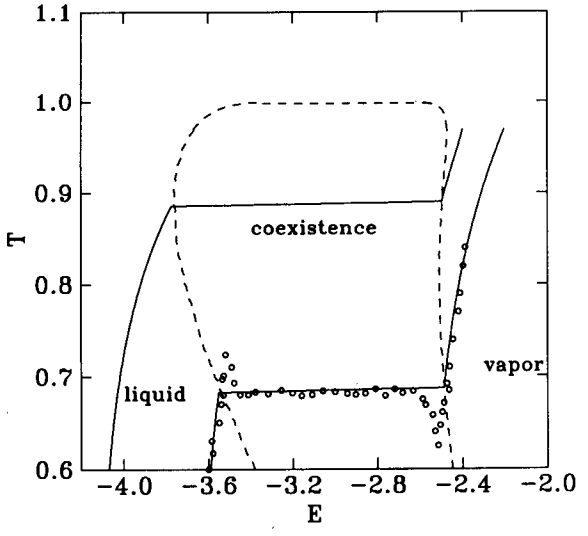

FIG. 1. Phase diagram of a two-dimensional Ising model with a first-order phase transition. The vertical axis is the temperature T and the horizontal axis is the internal energy E. The solid lines are the results of a mean field calculation and connect points having the same value of Δ which we interpret as the pressure. For clarity, we show data only for $\Delta = 1.08J$, so that $T_f = 0.68T_c$. The results were obtained for a 180×180 lattice with 10 000 Monte Carlo Steps (MCS) per spin. The part of the phase diagram enclosing the horizontal lines is the coexistence region and is denoted by a dashed line.

Monte Carlo results using the demon algorithm for the modified Ising model with $g = 2$ are shown in Fig. 1. For low-energy E the system is all liquid and, for larger E, the system is all vapor. Clearly visible are horizontal portions of the constant pressure lines where an increase in E does not change T. All that happens in this case is that an increase in E produces a greater proportion of the vapor phase. The part of the phase diagram enclosing the horizontal lines is known as the coexistence region. The advantage of the microcanonical ensemble is that by fixing Δ and E, we can fix the system at a point inside the coexistence region. In contrast, the Metropolis algorithm allows us only to fix the temperature and to investigate portions of a constant pressure line.

FIG. 2. Typical configuration in the coexistence region. The figure is part of an interface with 1024×64 spins with $T_f = 0.9T_c$. The dark regions correspond to down spins and hence the liquid phase.

A typical configuration of the system in the coexistence region is shown in Fig. 2, where an interface between the two phases has been created by pinning the spins at the top to be up (vapor) and the spins at the bottom to be down (liquid). This pinning is not necessary in principle. The reader who attempts to reproduce these results will likely encounter some interesting problems, especially if the size of the system is smaller than $\sim 10^4$ spins. For small systems, the coexistence region for a given value of Δ will not correspond to a unique temperature and the data will resemble a van der Waals loop.[4] In this case the results can be explained in terms of the energy associated with the interface between the vapor and the liquid. This energy is proportional to the linear size of the system and becomes comparable to the bulk energy, which is proportional to the area, when the system is too small.

There are other configurations in the coexistence region that differ qualitatively from the particular configuration of the system shown in Fig. 2. For example, one can obtain a bubble of liquid surrounded by vapor. An interesting question is how such configurations are formed as the system is cooled from the high-temperature vapor phase above the coexistence region. The study of the nucleation and growth of one phase at the expense of another is very important for materials science. The strength and stability of alloys depend on their microstructure, which in turn depends on the coexistence of different crystal phases.[5] A common experimental situation is when the high-temperature phase of a material is rapidly cooled, or *quenched*, into the coexistence region.

Such experiments can easily be simulated on the computer.[6] In the microcanonical ensemble, for instance, we can begin with a negative demon energy and a previously equilibrated system, so that the system will lose energy and its temperature will decrease. Much of the

interesting physics involves the early stages of growth. It is important to identify the time at which the first nucleating droplets appear, and to study the structure of these droplets as they grow. Monte Carlo results show that the droplets rapidly become compact, and subsequently grow by condensation on their surface in good agreement with classical theories. The results also suggest that the microcanonical method can be used to model *dynamics*, not just equilibrium thermodynamics. This important idea is used in our next application.

Inspection of the configuration shown in Fig. 2 also encourages questions about the nature of the interface. Our perception of the surface of a liquid is that it is smooth, but the interface in the figure is clearly rough. This property of the interface is a consequence of the two-dimensional nature of our system; roughness in three dimensions is much weaker.[7] We can investigate the nature of the roughening process by preparing an interface that is flat and observing how it becomes rougher as the simulation proceeds. Such a study is an excellent test of the dynamics of the demon algorithm, because there are theoretical predictions available with which to compare.[8] The physics of the roughening of interfaces is also of interest to understanding phenomena such as dendritic instabilities, crystal growth, and nucleation.[5] It is known that stable interfaces in two-dimensional Isinglike systems are rough, with a width that depends on the square root of their length. It is also known that the relaxation of flat interfaces to their equilibrium roughened state should display simple power law behavior. After the initial transients have decayed away, but before thermodynamic equilibrium is reached, the width w of an interface should grow as

$$w \propto t^{1/n}, \tag{5}$$

where the time t can be interpreted as the number of Monte Carlo steps per spin. For the usual Ising model with no latent heat, $n = 4$.[9] For a two-dimensional system with latent heat, $n = 6$ after a sufficiently long time. This behavior arises form the transition between rapid early growth of structure at short length scales and slower growth of structure at large length scales. Only the large-scale structure of the interface is sensitive to the latent heat because only then does the diffusion of heat dominate the dynamics.[10,5]

To model the diffusion of heat we must modify the demon algorithm so that instead of one demon for the whole system, there is one demon *per spin*. This use of multiple demons distinguishes demon-type algorithms from the Metropolis algorithm that cannot be modified in any comparable way. The reader will find the basic ideas in Ref. 1. A straightforward application of the use of multiple demons to the determination of the thermal conductivity is discussed in Problem 3 and in Ref. 11. Each demon is responsible for administering the rules of spin flip for a subset of the spin population, and thus mimics the diffusion of heat, as well as measuring the local temperature. To improve the rate of diffusion, we allow each spin to have access to its own demon and to the demons of its nearest neighbors. That is, each time a particular spin is chosen to be updated, we also choose at random the demon with which it can interact. This choice is limited to its own demon and the demons of its four nearest neighbors. Otherwise the algorithm proceeds as before. In this way heat flow is localized, and the simulation can more accurately reflect what happens in an actual system.

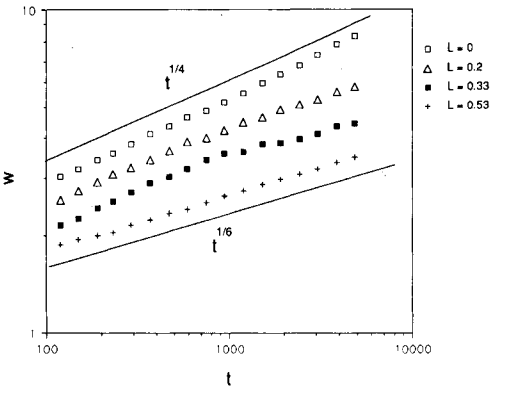

FIG. 3. The time dependence of the mean interface width w for different values of the latent heat L. The latent heat is given in terms of the exchange constant J. The smooth lines are given for comparison and correspond to $t^{1/4}$ and $t^{1/6}$. The time is given in terms of the number of the Monte Carlo steps per spin.

Figure 3 shows the results of simulations of the roughening of an initially flat interface. The simulations were performed on $L_x \times L_y$ systems with $L_x = 1024$ and $L_y = 64$ and values of Δ and g such that $T_f = 0.9T_c$. Each run was performed 50 times to give error bars that are about the size of the data points. The position of an interface parallel to the x axis is determined as a single-valued function $\xi(x)$ by ignoring overhangs and bubbles in the bulk. The interface width w is defined in terms of $\xi(x)$ as $w^2 = \langle(\xi - \langle\xi\rangle)^2\rangle$. The crossover from rapid early growth to slower late time behavior is very apparent and depends upon the latent heat of the model, in agreement with theoretical predictions.

Unfortunately the reader wishing to test these results must tackle several practical problems. To minimize the time for the simulation to reach thermal equilibrium, the demons must be prepared by randomly distributing the energy estimated to place them in thermal equilibrium with the spins (i.e., at T_f).To determine the power laws, it is necessary to observe the growth over an adequate period of time. It is necessary to ensure an adequate interval of time between the early transient behavior and the ultimate saturation of the width at its equilibrium value, and hence large systems must be used. We observed saturation of the roughening in systems with $L_x \leqslant 512$, and consequently choose size with $L_x = 1024$ and $L_y = 64$. These simulations are a task for a supercomputer!

However, the significance of the results shown in Fig. 3 is immense. It appears that a suitably modified demon algorithm does lead to dynamical behavior that mimics real world behavior. Although there remain important questions of principle, for example, the ergodic behavior

of Creutz' original algorithm, there remains little doubt that demon-type algorithms will be of much value for investigating the evolution of complex systems. It will be interesting to follow applications to crystal growth and surface physics, where there are difficult problems of much practical importance.

Suggestions for Further Study

1. Write a program to use the demon algorithm to estimate the critical temperature T_c for the two-dimensional Ising model on the square lattice. A 30×30 array of spins is sufficient. Measure the energy per spin, E, and the temperature in terms of J. Consider E in the range 0.05 to 0.25. Begin with all spins down, and choose E_d so that the total energy is equal to the desired value. Approximately 10 000 MCS are needed to obtain good results for each value of E. Rather than resetting the starting configuration for each desired value of E, use the final configuration at a given energy as the starting point for the next and increase E_d. A new equilibrium will be established quickly, typically within a few hundred MCS. Plot your results for T or β vs E and estimate T_c from the observed inflection point. What is the origin of the inflection point? A simple program for the demon algorithm for the one-dimensional Ising model can be found in Chap. 15 of Ref. 1. More discussion of the two-dimensional case is in Ref. 3.

2. Modify the demon algorithm to simulate the modified Ising model with degeneracy g and field Δ. Add to the system energy the quantity Δ for each up spin. What is the effect of degeneracy on the tests for attempted changes in the spins? To account for the degeneracy when attempting to flip an up spin, we need to keep it up automatically with probability $(g-1)/g$. One way is to compute a random number r between 0 and 1. If $r<1/g$, go to step 2; otherwise the spin remains up and proceed to step 1 (see text). In addition, the relation (1) between $\langle E_d\rangle$ and T is no longer applicable. Inspect the distribution of demon energies and decide how best to extract the temperature. Choose $\Delta=1.08J$ and $g=2$. Consider a 100×100 lattice and begin with all spins down (in the liquid state). In general, 10 000 MCS are needed to obtain good results for each value of E. Raise the energy for each successive run as in Problem 1. Do your results for T vs E correspond to the results shown in Fig. 1? What is the nature of your results near the beginning and the end of the coexistence region? Do you observe any evidence of metastable states?

3. Modify your program so that each spin interacts with q spins rather than the usual $q=4$ nearest neighbors on the square lattice. Consider a 100×100 lattice, choose $q=27$, and verify that superheating becomes *easier* to observe. Can you observe the nucleation and growth of droplets?

4. A discussion of the use of multiple demons to control the distribution of energy throughout the system and hence to determine the thermal conductivity is discussed in Chap. 15 of Ref. 1 for the one-dimensional Ising model and in Ref. 11 for the two-dimensional Ising model. The idea is to use one demon *per spin* to allow the monitoring of the local temperature. The local demon permits a flip of the spin with which it is in contact. In the one-dimensional case, we can maintain a temperature gradient by fixing the temperature at the left and right boundaries. The demons at the boundaries permit spin flips if they receive energy, and permit energetically unfavorable flips with Boltzmann probabilities. The heat flux in the system can be found by determining the average change in the energy of the boundary spins per MCS. When the system has reached local equilibrium, the energies taken up and released, respectively, at the two boundaries should agree within statistical uncertainties. If sufficient computer resources are available, determine the thermal conductivity for the one- and two-dimensional Ising models.

5. Modify the multidemon method in order to simulate the growth of an interface. Develop procedures for tracing the interface and computing its width. Consider a 50×200 system and verify that the width of an interface increases with its length. It is sufficient to consider the usual Ising model. More details can be found in Ref. 8. A similar simulation of a relatively small three-dimensional Ising model ($20\times20\times20$) will show a roughening transition at $\approx0.6T_c$. See Ref. 7 for background information.

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In our next column: An introduction to quantum Monte Carlo methods.