```
            state[4*i] = dx*(ix+0.75);
         }
      }
   }
}
```

Problem 8.10 Metastability

If we rapidly lower the temperature of a liquid below its freezing temperature, it is likely that the resulting state will not be an equilibrium crystal, but rather a supercooled liquid. If the properties of the supercooled state do not change with time for a time interval that is sufficiently long to obtain meaningful averages, we say that the system is in a *metastable* state. In general, we must carefully prepare our system so as to minimize the probability that the system becomes trapped in a metastable state. However, there is much interest in metastable states and how they eventually evolve to a more stable state (see Problem 15.20).

(a) What happens if the initial positions of the particles are on the nodes of a square lattice. As we found in Problem 8.9, this symmetry is not consistent with the lowest energy state corresponding to a triangular lattice. If the initial velocities are set to zero, what happens when you run the program? Choose $N = 64$ and $L_x = L_y = 9$.

(b) We can show that the system in part (a) is in a metastable state by giving the particles a small random initial velocity in the interval $[-0.5, +0.5]$. Does the symmetry of the lattice immediately change or is there a delay? When do you begin to see local structure that resembles a triangular lattice?

(c) Repeat part (b) with random velocities in the interval $[-0.1, +0.1]$. ■

Problem 8.11 The solid state and melting

(a) Choose $N = 64$, $L_x = 8$, and $L_y = \sqrt{3}L_x/2$ and place the particles on the nodes of a triangular lattice. Give each particle zero initial velocity. What is the total energy of the system? Do a simulation and measure the temperature and pressure as a function of time. Does the system remain a solid?

(b) Give each particle a random velocity in the interval $[-0.5, +0.5]$. What is the total energy? Equilibrate the system and determine the mean temperature and pressure. Describe the trajectories of the particles. Are the particles localized? Is the system a solid? Save an equilibrium configuration for use in part (c).

(c) Choose the initial configuration to be an equilibrium configuration from part (b) and gradually increase the kinetic energy by a factor of two. What is the new total energy? Describe the qualitative behavior of the motion of the particles. What is the equilibrium temperature and pressure of the system? After equilibrium is reached, increase the temperature again by rescaling the velocities in the same way. Repeat this rescaling and measure $P(T)$ and $E(T)$ for several different temperatures.

(d) Use your results from part (c) to plot $E(T) - E(0)$ and $P(T)$ as a function of T. Is the difference $E(T) - E(0)$ proportional to T? What is the mean potential energy for a harmonic solid? What is its heat capacity?

(e) Choose an equilibrium configuration from part (b) and decrease the density by rescaling L_x, L_y, and the particle positions by a factor of 1.1. What is the nature of the trajectories? Decrease the density of the system until the system melts. What is your qualitative criterion for melting? ■

Problem 8.12 Microscopic model of friction

In introductory physics texts, sliding friction is usually described by the empirical law

$$f = \mu F_N, \tag{8.13}$$

where f is the magnitude of the friction force, F_N is the normal force acting on the sliding object, and μ is the coefficient of friction. If the object is not moving, then (8.13), with μ equal to the static coefficient of friction, represents the frictional force needed to start the motion. If the object is moving, then (8.13), with μ equal to the kinetic coefficient of friction, represents the kinetic frictional force, which is assumed to be independent of the speed of the sliding object.

In this problem we explore a simple model discussed by Ringlein and Robbins to investigate the microscopic origin of friction. The stationary surface is modeled by a line of fixed atoms spaced a distance of $a = 2^{1/6}$ apart as shown in Figure 8.6. The sliding object is modeled by two rows of atoms in a triangular lattice configuration initially spaced a distance $2a$ from each other. The bottom row of atoms in the sliding object is a vertical distance a from the line of fixed atoms. The interaction between all the atoms in the two objects occurs via the Lennard–Jones potential. To keep the sliding object together, stiff springs with a spring constant of 500 (in reduced units) connect each atom to its nearest neighbors on the triangular lattice. The left-most atom on the bottom row has a damping force equal to $-10(v_x\hat{x} + v_y\hat{y})$ to help stabilize the motion. In addition, there is an external horizontal spring with spring constant equal to unity attached to the right-most atom on the bottom row. This spring is pulled at a constant rate causing this force on the atom to increase linearly. When this spring force is sufficiently large, the atoms start to move and the spring force suddenly drops. The point at which this decrease occurs defines the magnitude of the static frictional force.

(a) Modify your molecular dynamics program to simulate this model. Choose the sliding object to consist of 13 atoms, 7 on the bottom row and 6 on the top row. Place this system of 13 atoms on the middle of a stationary surface of fixed atoms (100 such atoms should be more than enough). Your program should show the pulling force due to the spring on the right-most atom as a function of time, and a visual display of the atoms in the system. A reasonable rate for pulling the spring is 0.1; that is, the external horizontal spring force is $0.1t - u$, where u is the horizontal displacement of the right-most atom from its initial position.

(b) As the system evolves, you should see the spring force suddenly drop when it reaches a value of about 14. Try different pulling rates and determine if the rate affects your results or the static friction force.

(c) Add a load that is equivalent to increasing the normal force. To add a load W to the system, add a vertical force of $-W/N$ to each of the $N = 13$ atoms in the sliding object. Find the static friction force, f_s as a function of W for W between -20 and