```
   public Object createObject(XMLControl element) {
      return new LJParticlesApp();
   }

   public void saveObject(XMLControl control, Object obj) {
      LJParticlesApp model = (LJParticlesApp) obj;
      control.setValue("initial_configuration",
                       model.md.initialConfiguration);
      control.setValue("state", model.md.state);
   }

   public Object loadObject(XMLControl control, Object obj) {
      // GUI has been loaded with saved values; now restore LJ state
      LJParticlesApp model = (LJParticlesApp) obj;
      // reads values from the GUI into the LJ model
      model.initialize();
      model.md.initialConfiguration =
           control.getString("initial_configuration");
      model.md.state = (double[]) control.getObject("state");
      int N = (model.md.state.length-1)/4;
      model.md.ax = new double[N];
      model.md.ay = new double[N];
      model.md.computeAcceleration();
      model.md.resetAverages();
      // clears old data from the plot frames
      GUIUtils.clearDrawingFrameData(false);
      return obj;
   }
}
```

Problem 8.3 Approach to equilibrium

(a) Consider $N = 64$ particles interacting via the Lennard–Jones potential in a square central cell of linear dimension $L = 10$. Start the system on a square lattice with an initial temperature corresponding to $T = 1.0$. Let $\Delta t = 0.01$ and run the application to make sure that it is working properly. The total energy should be approximately conserved, and the trajectories of all 64 particles should be seen on the screen.

(b) The kinetic temperature of the system is given by (8.5). View the evolution of the temperature of the system starting from the initial temperature. Does the temperature reach an equilibrium value? That is, does it eventually fluctuate about some mean value? What is the mean value of the temperature for the given total energy of the system?

(c) Modify method `setRectangularLattice` so that all the particles are initially on the left side of a box of linear dimensions $L_x = 20$ and $L_y = 10$. Does the system become more or less random as time increases?

(d) Modify the program so that it computes $n(t)$, the number of particles in the left half of the cell, and plot $n(t)$ as a function of t. What is the qualitative behavior of $n(t)$? What is the mean number of particles on the left half after the system has reached equilibrium? Compare your qualitative results with the results you found in Problem 7.2. ■

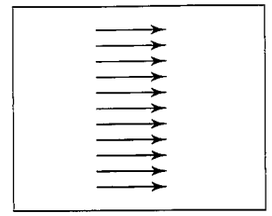

Figure 8.4 Example of a special initial condition; the arrows represent the magnitude and the direction of each particle's velocity.

Problem 8.4 Sensitivity to initial conditions

(a) Modify your program to consider the following initial condition corresponding to $N = 11$ particles moving in the same direction with the same velocity (see Figure 8.4). Choose $L_x = L_y = 10$ and $\Delta t = 0.01$.

```
for (int i = 0; i < N; i++) {
   x[i] = Lx/2;
   y[i] = (i - 0.5)*Ly/N;
   vx[i] = 1;
   vy[i] = 0;
}
```

Does the system eventually reach equilibrium? Why or why not?

(b) Change the velocity of particle 6 so that $v_x(6) = 0.99999$ and $v_y(6) = 0.00001$. Is the behavior of the system qualitatively different than in part (a)? Does the system eventually reach equilibrium? Are the trajectories of the particles sensitive to the initial conditions? Explain why this behavior implies that almost all initial states lead to the same qualitative behavior (for a given total energy).

(c) Modify `LJParticlesApp` so that the application runs for a predetermined time interval, such as 100 time steps, and then continues with the time reversed process, that is, the motion that would occur if the direction of time was reversed. This reversal is equivalent to letting $\mathbf{v} \to -\mathbf{v}$ for all particles or letting $\Delta t \to -\Delta t$. Do the particles return to their original positions? What happens if you reverse the velocities at a later time? What happens if you choose a smaller value of Δt?

(d) Explain why you can conclude that the system is chaotic. Are the computed trajectories the same as the "true" trajectories? ■

From Problems 8.3 and 8.4, we see that from the *microscopic* point of view, the trajectories appear rather complex. In contrast, from the *macroscopic* point of view, the system can be described more simply. For example, in Problem 8.3 we described the approach of the system to equilibrium by specifying $n(t)$, the number of particles in the left half of the cell at time t. Your observations of the macroscopic variable $n(t)$ should be consistent with the following two general properties of systems of many particles:

1. After the removal of an internal constraint, an isolated system changes in time from a "less random" to a "more random" state.