$N = 64$ and place the particles initially on a triangular lattice with $L_x = 10$ and $L_y = \sqrt{3}L_x/2$. Plot the instantaneous temperature defined as in (8.5) and compute the average temperature. Estimate the magnitude of the temperature fluctuations. Repeat your simulation for some other initial configurations.

(b) Modify your program to use the Andersen thermostat at a constant temperature set equal to 1.0. Set `collisionProbability` $= 0.0001$. Repeat the calculations of part (a) and compare them. Discuss the differences. Do the results change significantly?

(c) Modify your program to do a simple constant kinetic energy ensemble where the velocities are rescaled after every time step so that the total kinetic energy does not change. What is the final temperature now? How do your results compare with parts (a) and (b)? Are the differences in the computed thermodynamic averages statistically significant?

(d) Compute the velocity probability distribution for each case. How do they compare? Consider `collisionProbability` $= 0.001$ and 0.00001.

(e) A deterministic algorithm for constant temperature molecular dynamics is the Nosé–Hoover thermostat. The idea is to introduce an additional degree of freedom s that plays the role of the heat bath. The derivation of the appropriate equations of motion is an excellent example of the Lagrangian formulation of mechanics. The equations of motion of Nosé–Hoover dynamics are

$$\frac{d\mathbf{p}_i}{dt} = \mathbf{F}_i(t) - s\mathbf{p}_i \tag{8.54}$$

$$\frac{ds}{dt} = \frac{1}{M}\left[\sum_i \frac{p_i^2}{m_i} - dNkT\right], \tag{8.55}$$

where T is the desired temperature, and M is a parameter that can be interpreted as the mass associated with the extra degree of freedom. Equation (8.54) is similar to Newton's equations of motion with an additional friction term. However, the coefficient s can be positive or negative. Equation (8.55) defines the way s is changed to control the temperature. Apply the Nosé–Hoover algorithm to simulate a simple harmonic oscillator at constant temperature. Plot the phase space trajectory. If the energy was constant, the trajectory would be an ellipse. How does the shape of the trajectory depend on M? Choose M so that the period of any oscillations due to the finite value of M is much longer than the period of the system. ■

Project 8.25 Simulations on the surface of a sphere

Because of the long-range nature of the Coulomb potential, we have to sum all the periodic images of the particles to compute the force on a given particle. Although there are special methods to do these sums so that they converge quickly (Ewald sums), the simulation of systems of charged particles is more difficult than systems with short-range potentials. An alternative approach that avoids periodic boundary conditions is to not have any boundaries at all. For example, if we wish to simulate a two-dimensional system, we can consider the motion of the particles on the surface of a sphere. If the radius of the sphere is sufficiently large, the curvature of the surface can be neglected. Of course, there is a price—the coordinate system is no longer Cartesian.

Although this approach can also be applied to systems with short-range interactions, it is more interesting to apply it to charged particles. The simplest system of interest is a model of charged particles moving in a uniform background of opposite charge to ensure overall charge neutrality, the one-component plasma (OCP). In two dimensions this system is a simplified model of electrons on the surface of liquid Helium. The properties of the OCP are determined by the dimensionless parameter Γ given by the ratio of the potential energy between nearest neighbor particles to the mean kinetic energy of a particle, $\Gamma = (e^2/a)/kT$, where $\rho\pi a^2 = 1$ and ρ is the number density. Systems with $\Gamma \gg 1$ are called strongly coupled. For $\Gamma \sim 100$ in two dimensions, the system forms a solid. Strongly coupled one-component plasmas in three dimensions are models of dense astrophysical matter.

Assume that the origin of the coordinate system is at the center of the sphere and that $\mathbf{u}_i$ is a unit vector from the origin to the position of particle i on the sphere. Then $R\theta_{ij}$ is the length of the chord joining particle i and j, where $\cos\theta_{ij} = \mathbf{u}_i \cdot \mathbf{u}_j$. Newton's equation of motion for the ith electron has the form

$$m\ddot{\mathbf{u}}_i = -\frac{e^2}{R^2}\sum_{j\neq i}\frac{1}{\theta_{ij}^2 \sin\theta_{ij}}[\mathbf{u}_j - \cos\theta_{ij}\mathbf{u}_i]. \tag{8.56}$$

Note that the unit vector $\mathbf{w}_{ij} = [\mathbf{u}_j - \cos\theta_{ij}\mathbf{u}_i]/\sin\theta_{ij}$ is orthogonal to $\mathbf{u}_i$. In addition, we must take into account that the particles must stay on the surface of the sphere, so there is an additional force on particle i toward the center of magnitude $m|\dot{\mathbf{u}}_i|^2/R$.

(a) What are the appropriate units for length, time, and the self-diffusion constant?

(b) Write a program to compute the velocity correlation function given by

$$C(t) = \frac{1}{v_0^2}\overline{\dot{\mathbf{u}}(t)\cdot\dot{\mathbf{u}}(0)}, \tag{8.57}$$

where $v_0^2 = \overline{\dot{\mathbf{u}}(0)\cdot\dot{\mathbf{u}}(0)}$. To compute the self-diffusion constant D, we let $\cos\theta(t) = \mathbf{u}(t)\cdot\mathbf{u}(0)$, so that $R\theta$ is the circular arc from the initial position of a particle to its position on the sphere at time t. We then define

$$D(t) = \frac{1}{a^2}\frac{\overline{\theta^2(t)}}{4t}, \tag{8.58}$$

where D and t are dimensionless variables. The self-diffusion constant D corresponds to the limit $t \to \infty$. Choose $N = 104$ and a radius R corresponding to $\Gamma \approx 36$ as in the original simulations by Hansen et al. and then consider bigger systems. Can you conclude that the self-diffusion exists for the two-dimensional OCP?

*(c) Use a similar procedure to compute the velocity autocorrelation function and the self-difusion constant D for a two-dimensional system of Lennard–Jones particles. Can you conclude that the self-diffusion exists for this two-dimensional system? ■

Project 8.26 Granular matter

Recently, physicists have become very interested in granular matter such as sand. The key difference between molecular systems and granular systems is that the interparticle