Exercises

(Section 2.1)

(2.1) Implement Alg. 2.2 (`pair-time`) and incorporate it into a test program generating two random positions $\{\mathbf{x}_1, \mathbf{x}_2\}$ with $|\Delta_\mathbf{x}| > 2\sigma$, and two random velocities with $(\Delta_\mathbf{x} \cdot \Delta_\mathbf{v}) < 0$. Propagate both disks up to the time t_{pair}, if finite, and check that they indeed touch. Otherwise, if $t_{\text{pair}} = \infty$, propagate the disks up to their time of closest encounter and check that, then, $(\Delta_\mathbf{x} \cdot \Delta_\mathbf{v}) = 0$. Run this test program for at least 1×10^7 iterations.

(2.2) Show that Alg. 2.3 (`pair-collision`) is correct in the center-of-mass frame, but that it can also be used in the lab frame. Implement it and incorporate it into a test program generating two random positions $\{\mathbf{x}_1, \mathbf{x}_2\}$ with $|\Delta_\mathbf{x}| = 2\sigma$, and two random velocities $\{\mathbf{v}_1, \mathbf{v}_2\}$ with $(\Delta_\mathbf{x} \cdot \Delta_\mathbf{v}) < 0$. Check that the total momentum and energy are conserved (so that initial velocities $\mathbf{v}_{1,2}$ and final velocities $\mathbf{v}'_{1,2}$ satisfy $\mathbf{v}_1 + \mathbf{v}_2 = \mathbf{v}'_1 + \mathbf{v}'_2$ and $\mathbf{v}_1^2 + \mathbf{v}_2^2 = \mathbf{v}_1'^2 + \mathbf{v}_2'^2$). Run this test program for at least 1×10^7 iterations.

(2.3) (Uses Exerc. 2.1 and 2.2.) Implement Alg. 2.1 (`event-disks`) for disks in a square box without periodic boundary conditions. Start from a legal initial condition. If possible, handle the initial conditions as discussed in Exerc. 1.3. Stop the program at regular time-intervals (as in Alg. 2.4 (`event-disks(patch)`)). Generate a histogram of the projected density in one of the coordinates. In addition, generate histograms of velocities v_x and of the absolute velocity $v = \sqrt{v_x^2 + v_y^2}$.

(2.4) Consider Sinai's system of two large disks in a square box with periodic boundary conditions ($L_x/4 < \sigma < L_x/2$). Show that in the reference frame of a stationary disk (remaining at position $\{0, 0\}$), the center of the moving disk reflects off the stationary one as in geometric optics, with the incoming angle equal to the outgoing angle. Implement the time evolution of this system, with stops at regular time intervals. Compute the two-dimensional histogram of positions, $\pi(x, y)$, and determine from it the histogram of projected densities.

(2.5) Find out whether your programming language allows you to treat real variables and constants using different precision levels (such as single precision and double precision). Then, for real variables $x = 1$ and $y = 2^{-k}$, compute $x + y$ in both cases, where $k \in \{\dots, -2, -1, 0, 1, 2, \dots\}$. Interpret the results of this basic numerical operation in the light of the discussion of numerical precision, in Subsection 2.1.2.

(Section 2.2)

(2.6) Directly sample, using Alg. 2.7 (`direct-disks`), the positions of four disks in a square box without periodic boundary conditions, for different covering densities. Run it until you have data for a high-quality histogram of x-values (this determines the projected densities in x, compare with Fig. 2.9). If possible, confront this histogram to data from your own molecular dynamics simulation (see Exerc. 2.3), thus providing a simple "experimental" test of the equiprobability principle.

(2.7) Write a version of Alg. 2.7 (`direct-disks`) with periodic boundary conditions. First implement Alg. 2.5 (`box-it`) and Alg. 2.6 (`diff-vec`), and check them thoroughly. Verify correctness of the program by running it for Sinai's two-disk system: compute histograms $\pi(x_k, y_k)$ for the position $\mathbf{x}_k = \{x_k, y_k\}$ of disk k, and for the distance $\pi(\Delta_x, \Delta_y)$ between the two particles.

(2.8) Implement Alg. 2.9 (`markov-disks`) for four disks in a square box without periodic boundary conditions (use the same covering densities as in Exerc. 2.6). Start from a legal initial condition. If possible, implement initial conditions as in Exerc. 1.3. Generate a high-quality histogram of x-values. If possible, compare this histogram to the one obtained by molecular dynamics (see Exerc. 2.3), or by direct sampling (see Exerc. 2.6).

(2.9) Implement Alg. 2.8 (`direct-disks-any`), in order to determine the acceptance rate of Alg. 2.7 (`direct-disks`). Modify the algorithm, with the aim of avoiding use of histograms (which lose information). Sort the N output samples for $\eta_{\max}$, such that $\eta_{\max,1} \le \dots \le \eta_{\max,N}$. Determine the rejection rate of Alg. 2.7 (`direct-disks`) directly from the ordered vector $\{\eta_{\max,1}, \dots, \eta_{\max,N}\}$.

(2.10) Implement Alg. 2.9 (`markov-disks`), with periodic boundary conditions, for four disks. If possible, use the subroutines tested in Exerc. 2.7. Start your

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simulation from a legal initial condition. Demonstrate explicitly that histograms of projected densities generated by Alg. 2.7 (`direct-disks`), Alg. 2.9, and by Alg. 2.1 agree for very long simulation times.

(2.11) Implement Alg. 2.9 (`markov-disks`) with periodic boundary conditions, as in Exerc. 2.10, but for a larger number of disks, in a box with aspect ratio $L_x/L_y = \sqrt{3}/2$. Set up a subroutine for generating initial conditions from a hexagonal arrangement. If possible, handle initial conditions as in Exerc. 1.3 (subsequent runs of the program start from the final output of a previous run). Run this program for a very large number of iterations, at various densities. How can you best convince yourself that the hard-disk system undergoes a liquid–solid phase transition?
NB: The grid/cell scheme of Subsection 2.4.1 need not be implemented.

(Section 2.3)

(2.12) Sample the gamma distribution $\Gamma_N(x)$ using the naive algorithm contained in Alg. 2.13 (`direct-piston-particles`). Likewise, implement Alg. 2.15 (`gamma-cut`). Generate histograms from long runs of both programs to check that the distribution sampled are indeed $\Gamma_N(x)$ and $\Gamma_N^{\text{cut}}(x, x_{\text{cut}})$. Histograms have a free parameter, the number of bins. For the same set of data, generate one histogram with very few bins and another one with very many bins, and discuss merits and disadvantages of each choice. Next, analyze data by sorting $\{x_1, \ldots, x_N\}$ in ascending order $\{\tilde{x}_1, \ldots, \tilde{x}_k, \ldots, \tilde{x}_N\}$ (compare with Exerc. 2.9). Show that the plot of k/N against $\tilde{x}_k$ can be compared directly with the integral of the considered distribution function, without any binning. Look up information about the Kolmogorov–Smirnov test, the standard statistical test for integrated probability distributions.

(2.13) Implement Alg. 2.11 (`naive-piston-particles`) and Alg. 2.12 (`naive-piston-particles(patch)`), and compare these Markov-chain programs to Alg. 2.13 (`direct-piston-particles`). Discuss whether outcomes should be identical, or whether small differences can be expected. Back up your conclusion with high-precision calculations of the mean box volume $\langle L \rangle$, and with histograms of $\pi(L)$, from all three programs. Generalize the direct-sampling algorithm to the case of two-dimensional hard disks with periodic boundary conditions (see Alg. 2.14 (`direct-p-disks`)). Plot the equation of state (mean volume vs. pressure) to sufficient precision to see deviations from the ideal gas law.

(2.14) (Uses Exerc. 2.3.) Verify that Maxwell boundary conditions can be implemented with the sum of Gaussian random numbers, as in eqn (2.13), or alternatively by rescaling an exponentially distributed variable, as in Alg. 2.10 (`maxwell-boundary`). Incorporate Maxwell boundary conditions into a molecular dynamics simulation with Alg. 2.1 (`event-disks`) in a rectangular box of sides $\{L_x, L_y\}$, a tube with $L_x \gg L_y$ (see Exerc. 2.3). Set up regular reflection conditions on the horizontal walls (the sides of the tube), and Maxwell boundary conditions on the vertical walls (the ends of the tube). Make sure that positive x-velocities are generated at the left wall, and negative x-velocities at the other one. Let the two Maxwell conditions correspond to different temperatures, T_{left}, and T_{right}. Can you measure the temperature distribution along x in the tube?

(2.15) In the piston-and-plate system of Subsection 2.3.2, the validity of the Boltzmann distribution was proved for a piston subject to a constant force (constant pressure). Prove the validity of the Boltzmann distribution for a more general piston energy

$$E(L) = L^\alpha$$

(earlier we used $\alpha = 1$). Specifically show that the piston is at position L, and at velocity v with the Boltzmann probability

$$\pi(L, v)\,\mathrm{d}L\ \mathrm{d}v \propto \exp\left[-\beta E(L, v)\right]\,\mathrm{d}L\ \mathrm{d}v.$$

First determine the time of flight, and compute the density of state $\mathcal{N}(E)$ in the potential h^α. Then show that at constant energy, each phase space element $\mathrm{d}L\ \mathrm{d}v$ appears with equal probability.
NB: A general formula for the time of flight follows from the conservation of energy $E = \frac{1}{2}v^2 + L^\alpha$:

$$\frac{\mathrm{d}L}{\mathrm{d}t} = \sqrt{2\,(E - L^\alpha)},$$

which can be integrated by separation of variables.

(Section 2.4)

(2.16) (Uses Exerc. 2.11.) Include Alg. 2.15 (`gamma-cut`) (see Exerc. 2.12) into a simulation of hard disks at a constant pressure. Use this program to compute the equation of state. Concentrate most of the computational effort at high pressure.

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