Assignment 12: Monte Carlo Simulations

1. **Random Number Generators**. Investigate the types of random number generators available on: (a) your local computing environment and (b) a mathematical package that you frequently use. How good are they? Is either one adequate for long molecular dynamics runs? Suggest how to improve them and test your ideas.

   To understand some of the defects in linear congruential random number generators, consider the sequence defined by the formula $y_{i+1} = (a\,y_i + c) \bmod M$, with $a = 65539$, $M = 2^{31}$, and $c = 0$. (This defines the infamous random number generator known as RANDU developed by IBM in the 1960s, which subsequent research showed to be seriously flawed). A relatively small number of numbers in the sequence (e.g., 2500) can already reveal a structure in three dimensions when triplets of consecutive random numbers are plotted on the unit cube. Specifically, plot consecutive pairs and triplets of numbers in two and three-dimensional plots, respectively, for an increasing number of generated random numbers in the sequence, e.g., 2500, 50,000, and 1 million. (Hint: Figure D.3 shows results from 2500 numbers in the sequence).

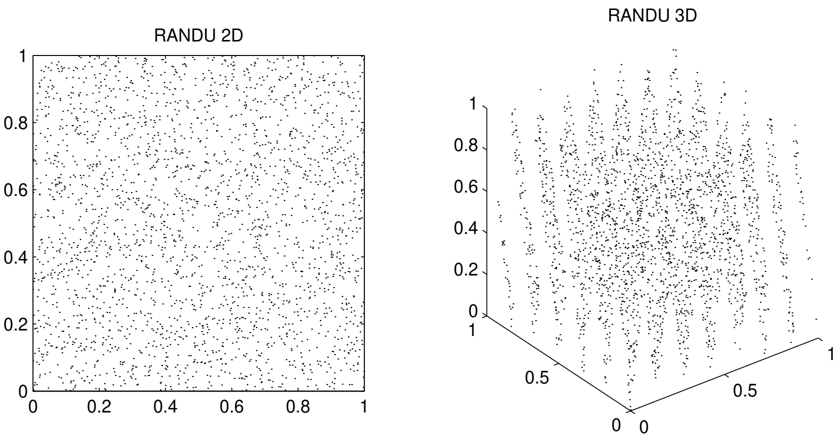

Figure D.3. Plots generated from pairs and triplets of consecutive points in the linear congruential generator known as RANDU defined by $a = 65539$, $M = 2^{31}$, and $c = 0$ when 2500 total points in the sequence are generated.

2. **MC Means**. Propose and implement a Monte Carlo procedure to calculate π based on integration. How many MC data points are needed to yield an answer correct up to 5 decimal places? What is the computational time

involved? Show a table of your results displaying the number of MC steps, the associated π estimate, and the calculated error.

3. **Gaussian Variates**. You are stranded in an airport with your faithful laptop with one hour to spare until the deadline for emailing your homework assignment to your instructor. The assignment (next item) relies on a *Gaussian random number generator*, but you have forgotten the appropriate formulas involved in the commonly used Box/Muller/Marsaglia transformation approach. Fortunately, however, you remember the powerful Central Limit Theorem in basic probability and decide to form a random Gaussian variate by sampling N uniform random variates $\{x_i\}$ on the unit interval as

$$\bar{y} = \sum_{i=1}^{N} x_i \, .$$

You quickly program the expression:

$$y = \sqrt{\frac{1}{\sigma^2(\bar{y})}} \sum_{i=1}^{N} [x_i - \mu(\bar{y})]$$

where above σ^2 is the standard deviation of $\bar{y} = N\sigma^2(x)$ and the mean $\mu(\bar{y}) = N\mu(x)$. [Recall that the uniform distribution has a mean of 1/2 and variance of 1/12].

How large should N be, you wonder. You must finish the assignment in a hurry. To have confidence in your choice, you set up some tests to determine when N is sufficiently large, and send your resulting routine, along with your testing reports, and results for several choices of N.

4. **Brownian Motion**. Now you can use the Gaussian variate generator above for propagating *Brownian motion* for a single particle governed by the biharmonic potential $U(x) = kx^4/4$. Recall that Brownian motion can be mimicked by simulating the following iterative process for the particle's position:

$$x^{n+1} = x^n + \frac{\Delta t}{m\gamma} F^n + R^n$$

where

$$\langle R^i R^j \rangle = \frac{2k_B T \Delta t}{m\gamma} \delta_{ij} , \qquad \langle R^i \rangle = 0 \, .$$

Here m is the particle's mass; γ is the collision frequency, also equal to ξ/m where ξ is the frictional constant; and F is the systematic force. You are required to test the obtained mean square atomic fluctuations against the known result due to Einstein:

$$\langle x^2 \rangle = 2 \left(\frac{k_B T}{m\gamma} \right) t = 2D\, t\,,$$

where D is the diffusion constant.
The following parameters may be useful to simulate a single particle of mass $m = 4 \times 10^{-18}$ kg and radius $a = 100$ nm in water: by Stokes' law, this particle's friction coefficient is $\xi = 6\pi\eta a = 1.9 \times 10^{-9}$ kg/s, and $D = k_B T/\xi = 2.2 \times 10^{-12}$m^2/s. You may, however, need to scale the units appropriately to make the computations reasonable.

Plot the mean square fluctuations of the particle as a function of time, compare to the expected results, and show that for $t \gg 1/\gamma = 2 \times 10^{-9}$ s the particle's motion is well described by random-walk or diffusion process.

Background Reading from Coursepack

- T. Schlick, E. Barth, and M. Mandziuk, "Biomolecular Dynamics at Long Timesteps: Bridging the Timescale Gap Between Simulation and Experimentation", *Ann. Rev. Biophys. Biomol. Struc.* **26**, 179–220 (1997).
- E. Barth and T. Schlick, "Overcoming Stability Limitations in Biomolecular Dynamics: I. Combining Force Splitting via Extrapolation with Langevin Dynamics in LN", *J. Chem. Phys.* **109**, 1617–1632 (1998).
- L. S. D. Caves, J. D. Evanseck, and M. Karplus, "Locally Accessible Conformations of Proteins: Multiple Molecular Dynamics Simulations of Crambin", *Prot. Sci.* **7**, 649–666 (1998).