Homework Assignment #7
(Due Date: Friday, April 09, 10:20 am, in class)

7.1 2D Random Walk (cf. Exercise 7.2 in the textbook) (2+2 pts.)
Write a FORTRAN program to simulate a random walker in 2 dimensions, taking steps of unit length in ±x or ±y direction on a discrete square lattice.

(a) Plot \(\langle x_n \rangle\) and \(\langle (x_n)^2 \rangle\) up to \(n=100\) by averaging over at least \(n_w=10^4\) different walks for each \(n > 3\).

(b) Show that the motion is diffusive, \(\langle r^2 \rangle \propto t\), and determine the value of the diffusion constant (an “eyeball” fit to your numerical data is ok).

7.2 2D Self-Avoiding Walk (cf. Ex. 7.5 in the textbook) (2+2+2 pts.)
Write a FORTRAN program to simulate 2D self-avoiding walks (SAWs) using the “trial” method discussed in class. Make sure that each walk of given step-length \(n\) (polymer with given molecule number, \(n\)) has the same probability i.e., each step direction should always be selected with probability 1/3 (except for the first step).

(a) Defining \(C_n\) as the total number of distinct SAWs for \(n\) steps, the probability for a single SAW simulation surviving after \(n\) steps is given by

\[
P(n) = \frac{C_n}{3^n}\]

which quantifies the numerical attrition in simulating SAWs. Compute (and plot) \(P(n)\) up to \(n=50\) by conducting \(\sim10^6\) trials for each \(n\). Comment on a comparison to the exact results quoted in Table 7.1 of the textbook.

(b) Suppose the large-\(n\) behavior of \(C_n\) is parameterized by

\[C_n \approx C_0 \mu^n n^{-\gamma-1}\]

with parameters \(\mu < 3\) (why?) and \(\gamma\). Show analytically that

\[
\frac{P(n+1)}{P(n)} \approx \frac{\mu}{3} \left(1 + \frac{\gamma - 1}{n}\right)
\]

and plot this relation for your data as a function of \(1/n\) to estimate \(\mu\) and \(\gamma\).

(c) To investigate the diffusive properties of the 2D SAW show analytically that

\[
\frac{\langle r_{n+1}^2 \rangle}{\langle r_n^2 \rangle} = 1 + 2\nu \frac{1}{n}
\]

for large \(n\) using the definition of the Flory exponent, \(\nu\),

\[
\sqrt{\langle r^2(t) \rangle} \equiv At^{\nu}, \ t \text{ large.}
\]

Use the relation (4) to plot your 2D SAW data and determine the value of the Flory exponent.