Homework Assignment #7

(Due Date: Tuesday, April 02, 05:30 pm, in class)

7.1 Flory Exponent in Random/Self-Avoiding Walks (cf. Ex. 7.5 in textbook) (2+2+2 pts.)
Write a FORTRAN code to simulate random walks on a 2D square lattice starting from the origin.

(a) Simulate unrestricted random walks up to \( n = 100 \) steps, averaging over \( n_w \approx 2 \cdot 10^4 \) walks for each \( n > 3 \). Plot \( \langle r^2_n \rangle \) as function of \( n \) (\( r^2 = x^2 + y^2 \)), and extract the Flory exponent in \( \sqrt{\langle r^2 \rangle} \equiv A t^\nu \) (large), by an eyeball fit.

(b) Simulate a 2D self-avoiding random walk 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). Plot \( \langle r^2_n \rangle \) vs. \( n \). Go to at least \( n = 50 \) and use a sufficiently large \( n_w \). To extract the Flory exponent, first show analytically that

\[
\frac{\langle r^2_{n+1} \rangle}{\langle r^2_n \rangle} = 1 + 2\nu \frac{1}{n}
\]  

for large \( n \). Replot your 2D SAW data using this relation and determine the value of \( \nu \) by an eyeball fit. Re-evaluate \( \nu \) from part (a) with this technique.

(b) Investigate fluctuations of the 2D random walk by extracting the variance, \( \Delta(r^2_n) \), as function of \( n \). Evaluate the exponent \( x \) in \( \sigma(t) \equiv \sqrt{\Delta(r^2(t))} \propto t^x \) by the same technique as in part (b). Sketch the result as a “1-sigma” band around \( \langle r^2 \rangle \) from part (a).

7.2 Diffusion and Central Limit Theorem (cf. Ex. 7.9 in textbook) (3+1 pts.)
Write a FORTRAN program to solve the 1-D diffusion equation using the finite difference method with diffusion constant \( D = 2 \). Start from an initial density profile (e.g., box profile) that is sharply peaked around \( x = 0 \) but still extends over a finite number of grid sites, e.g., 1000 particles in each of the four bins from \( x = -2 \) to +2.

(a) Plot time snapshots of the density distribution when significant changes of the latter have occurred, and show that at later times it can be described a one-parameter fit of a normal distribution.

(b) Plot the extracted width, \( \sigma \), of the distribution as a function of time and compare it to the expected theoretical behavior (plot the latter as a separate line).