1/4/10 Homework 1 Polymer Properties (Due 1/11/10 at 5 pm)

1) Write a computer program to simulate random walks of 10,000 steps on a 3d lattice.

2) Use a graphics software to display some of the 3d walks.

3) Calculate R, $\langle R \rangle$, R^2, $\langle R^2 \rangle^{1/2}$ (RMS size) where the averages are taken over a number of walks. (R is the end to end distance)

Comment on the following,

4) What is the range of structures possible for a random walk? (i.e. is a straight line possible, is a 3d block possible etc.)

5) Do you observe clustering of the walk steps in your random walks? Is clustering expected in a random process?

6) What are the expected values for R, $\langle R \rangle$, R^2, $\langle R^2 \rangle^{1/2}$?

7) Do you expect variability from the expected values? Why?

8) How would you expect changing the step length to affect the value of $\langle R^2 \rangle^{1/2}$?

9) For walks of variable length, z, (such as z = 100, 1000, 10000, 100000 etc. steps) how would you expect a plot of $\log(\langle R^2 \rangle^{1/2})$ versus $\log(z)$ to appear?

10) If you include a no-step option in the program will this effect the results?

Hints on how to write program:

You can use any software or compiler that you like. I have used Igor Pro by Wavemetrics for this problem since it can plot and calculate the simulation in the same software. You can use two separate softwares to do the simulation and plotting if you desire.

Your program could involve a random integer generator from 1 to 7 with values specified for positive and negative steps in the x, y and z directions and one choice for a no-step option.

First you set up an array of x, y and z values of length 10,000. The first point is 0,0,0. You go through a loop of 9,999 iterations where you add or subtract 1 to one of the positions (or do nothing for the no step option). The final value is the vector **R**. The scalar R is $(x^2 + y^2 + z^2)^{1/2}$ for this final vector. $\langle R \rangle$ is the mean of a series of **R** vectors then converted to the scalar. The RMS value is the root of the mean of the squares of the values for a series of simulations (say 10 to 100 simulations).