PHY420 Computing Class

Dr. Rhoda Hawkins

1. **Visualising biological molecules.**

   Go to the protein data bank website http://www.rcsb.org/pdb. Click on the link "Structural View of Biology" and choose a category and molecule of interest. Explore the 3D structure of your chosen molecule using the inbuilt java applet Jmol. You may need to click "allow" to activate this. Once the viewer is working you can rotate the molecule, change the way the molecule is displayed, zoom in etc. Look at a couple of different molecules.

2. **Simulate a random walk.**

   Use a programming language of your choice to generate random walks, on a one dimensional (1D) lattice, using a quasi-random number generator. Your random walks should start at the origin and have steps of size 1 that are equally distributed in each direction (left/right). You should record the position a walk has reached after N steps. Use the program to generate data and analyse your numerical experiment in the following ways. You will need to repeat the experiment thousands of times to get good averages (i.e. perform many random walks).

   (a) Consider random walks with $N = 10$ steps. Plot a histogram of the frequency of end positions. For this you need the program to perform a random walk many times, storing the end point of the walk each time. Plot the frequency against position, i.e. the number of times the walk ends at a particular point divided by the total number of times you repeated the random walk. Does the distribution agree with what we talked about in lectures?

   (b) Calculate the spread of the random walk ($R = \sqrt{\langle x^2 \rangle}$). Get good averages for the R as a function of increasing number of steps N. Does the relation agree with that discussed in lectures for diffusion and flexible polymers?

   (c) If you have enjoyed this then try doing the same thing for a random walk on a 2D square lattice. Steps should be equally distributed in 4 directions (North/South/East/West).