BP205 Molecular Dynamics of the Cell
Problem Set 1
Due January 20th in class.

1. Diffusion of a molecule that is also being consumed by a chemical reaction.

A pill containing molecule P at concentration C floats atop a solution in a very long test tube. P diffuses out of the pill with diffusion constant D and undergoes a chemical reaction in solution at rate K. At steady state, what is the concentration profile as a function of depth of the test tube? Discuss how the concentration profile would differ if no chemical reaction were taking place. What is the flux of P out of the pill at steady state?

2. Interpretation of a Brownian Dynamics simulation.

Brownian Dynamics is used to simulate motion of atoms by incorporating stochastic Brownian forces. The result of the simulation is a series of trajectories: the x, y and z coordinates of each molecule at each time step. A homogeneous population of 153 spheres each with a diffusion constant of 1.839 $Å^2$/ns was simulated for 1 ms, and you have been provided with the first (t0.txt) and last (tf.txt) set of coordinates (in Å). These files can be downloaded at the course website (www.jacobsonlab.org/~monica). Interpret the results of this simulation by answering the following:

a. Is the mean square displacement what you would expect if the system followed normal diffusion (linear with time)?

b. Does the distribution of individual particle displacements around zero compare to the expected probability distribution in three dimensions?