Singapore-MIT Alliance, CME5233 – Particle Methods and Molecular Dynamics

Monte Carlo Project, due 15 Dec 2006

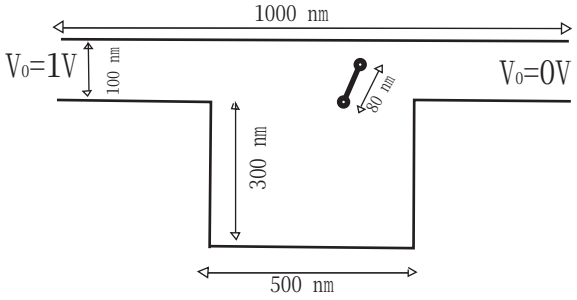
[I may modify the questions based on your feedback as we go on into the detail of the project]

1. Research on the algorithms of random number generators, and pick one for this project. Make sure you know how to use it correctly. Matlab is likely to have one; find its algorithm if you plan to use it.

2. In this project, we model the flow of short DNA molecules in a nano-channel in solution and electric field with a highly simplified model. Our first step is to solve the Laplace equation for electric potential $V(x,y)$ in two dimensions

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} = 0,$$

with the Dirichlet boundary conditions on the two opening (V_0 = 1 Volt, V_1=0 Volt) and von Neumann boundary conditions with the normal derivative $\partial V / \partial n = 0$ on the walls. The geometry of the deep-sallow channel is as follows (1 nm = 10^{-9}m):



Solve the Laplace equation on a grid with any one of the methods.

3. We model the movement of one DNA molecule under the influence of the electric field and the solution. The solution is taking care only implicitly by assuming that it is in thermal equilibrium with a temperature T = 300 Kelvin. Thus the solution causes the DNA molecule making random displacements. We assume that the DNA is a rod with two point charges of magnitude $+q$ at the ends. We'll take the charge q = 0.1e, where e = 1.6×10^{-19} coulomb is the magnitude of the charge of an electron. The length of the rod is L = 80 nanometer. You also need the Boltzmann constant, which is $k_B = 1.38\times10^{-23}$ joule/Kelvin.

   We ignore the kinetic energy (as usual in Monte Carlo) and consider only the electric static potential energy $q\,(\,V(x_1, y_1) + V(x_2, y_2)\,)$ where (x_1, y_1) and (x_2, y_2) are the locations of the charges.

   Discuss the implementation details. In particular, exactly how to make proposals for Monte Carlo moves. [Perhaps we need to fix it for the whole class after some

discussion]. Note that for this non-equilibrium problem, the final results do depend on the proposal matrix T(X ->X').

Adjust the model parameters such as the charge q and rod length L, or temperature T to see any interesting effect.

4. Make a visualization of the movements of the simulation if you can. Compute the average "velocity" $v(x)$ as a function of the horizontal position. Discuss the concept of time in Monte Carlo and how to define reasonably the velocity.

5. Put many rods of same sizes in the system. Introduce interactions between the rods. Compute density profile at the exit of the channel as a function of time. [This part is quite open-ended and can be optional].