Problem set 6, part I
IM/S Spring 2006

Topic: Basic molecular dynamics (MD)

For the following questions, provide a short paragraph or two of discussion, possibly with a few equations. Part I of problem set 6 will be weighted approximately equally with part II. You are expected to have clear, concise explanations for both parts. For those who are unfamiliar with including plots in your writeups, you may provide plots (or illustrations) as separate pages, but make sure they are well labeled.

1. How do you choose the spatial discretization in molecular dynamics modeling? Discuss the differences between a solid and liquid system.

2. In the *Verlet Central Difference Method*, how would you obtain the current velocities? Start with writing down the algorithm to update coordinates, as discussed in the lecture.

3. What scaling behavior does an MD scheme have with respect to the total number of particles N, without applying techniques such as neighbor lists or bins, and why? Provide an example for this scaling behavior with some pseudocode.

4. For a molecular dynamics simulation of a crystalline material, according to what criterion would you choose the integration time step? Assume that the crystal is in mechanical equilibrium with relaxed stresses, at finite temperature. Sketch the displacements of atoms over time.

5. Using the JAVA applet (http://polymer.bu.edu/java/java/LJ/index.html), determine the critical temperature at which the system starts to melt, *i.e.* the initial crystalline order disappears. Set the parameters in the model to describe a bulk system, at constant temperature. Leave all parameters for molecular interactions as they are initially. Describe the procedure you used to determine the critical melting temperature. Hint: Use the "trajectory" visualization scheme. ("Color Particles - Trajectories").