Introduction to Modeling and Simulation, Spring 2002, MIT
(1.992, 2.993, 3.04, 10.94, 18.996, 22.091)

Problem Set 3

Problem 1

Write a brief essay explaining in simple physical terms what is the technique of molecular dynamics (MD) simulation. Include in your discussion considerations of basic questions such as what is the purpose of this type of simulation, what kind of basic information is required as input and what information is given as output, and the strengths and limitations compared to some other simulation methods, etc.,

Problem 2

Use the MD simulation code given in class to study the atomic structure and motions in condensed matter.

(a) Make simulation run for a **crystal** at the reduced temperature TR = 0.7 and reduced density DR = 1.1 using various values for the number of molecules (NP) and number of time steps after equilibration (MAXKB). Plot, print out and discuss the results for pressure, energy and temperature, <square displacement>, and g(R). Can you tell whether the system has reached equilibrium? What information do you have about atomic structure and atomic motion.

Note: You are encouraged to vary NP, the number of time steps for equilibration NEQ, and MAXKB to see how they affect the results, and decide on what are appropriate values for the problem at hand.

(b) Repeat (a) for a **liquid** at TR = 1.1 and DR = 0.85.

(c) Compare your results for g(R) and <square displacement> from (a) and (b) by commenting on similarities and differences. Based on this comparison, give an atomic-level description of what happens when **a crystal melts**. Can you imagine simulating the melting process directly by MD with the given code? How would you proceed?

Problem 3 (optional, good for extra credit)

Explain briefly what is meant by the following in discussing MD simulation:

equipartition
reversibility
energy conservation
periodic boundary condition
temperature rescaling

How would you go about demonstrating the meaning of each?