06-640: Molecular Simulations
Homework 1
Due date: Tuesday 1/27

Before handing in this assignment, review the guidelines
for homework on the class website.

1. Water at ambient conditions has density 1 g/cc. At supercritical conditions (400 C and 230 bar), the density is reduced to 0.1 g/cc. Your computational resources allow you to perform simulations containing 10000 water molecules. Assuming your simulation domain is a cube with side length L, find L for simulations at ambient and supercritical conditions. How much would L change if you could perform simulations with 10 times as many molecules?

2. You wish to examine collision dynamics of CO_2 molecules by simulating this gas at standard temperature and pressure. You find that by using a cubic box with side length 20 nm, you can follow the molecule's trajectories for 2 ns in a reasonable amount of computer time. How many molecular collisions would you expect to see in this simulation?

3. Read one of the five papers we discussed in class as examples of classical molecular simulations. Write a summary of the paper that describes the main objectives and conclusions of the paper, lists the simulation techniques used in the paper, and briefly lists any limitations of the models that are mentioned in the paper or occur to you as you read. Your summary should be between ½ and 1 page in length (single-spaced). Please review the guidelines on the class website regarding written reports before completing this exercise.