12-623/24-623 Molecular Simulation
Spring 2014 Assignment - 1

Due: Mon. Jan 27 2013

Problem 1: Write a computer code to compute the force on each particle in a mono-atomic Lennard-Jones system. The code should read in atomic positions from a data file such as the one posted. The first line of the file gives the number of atoms. The next line contains the string "Atoms". Then each line contains one integer giving the "type" of the atom and then the x, y, and z positions of each atom with a tab character ("\t") in between each entry. Your code should output the forces to a text file named "forces.dat". The output file should be in a similar format to the input with each cartesian co-ordinate of position replaced by the corresponding cartesian component of the force vector for that particle. Be sure not to perturb the order of the particles from the input to output file: that is, the n-th line in the output file should represent the force on the n-th line of the input file (that is, the n-th atom). Assume the input positions are expressed in units of σ and write the output forces in units of ε/σ.

Problem 2: Test your code on the attached input file (named "atoms.dat"). Print the contents of your output file to the screen and submit that as part of your assignment.