SIMPLE TESTS FOR MD PROGRAM

Units: LJ units, unit for energy = ε; unit of length = σ; unit of mass = particle mass (= 1)
Volume of fcc cubic unit cell = a^3, volume per atom = $a^3 / 4$, density = $4 / a^3$.

You can do the following simple tests to make sure your MD code is working.

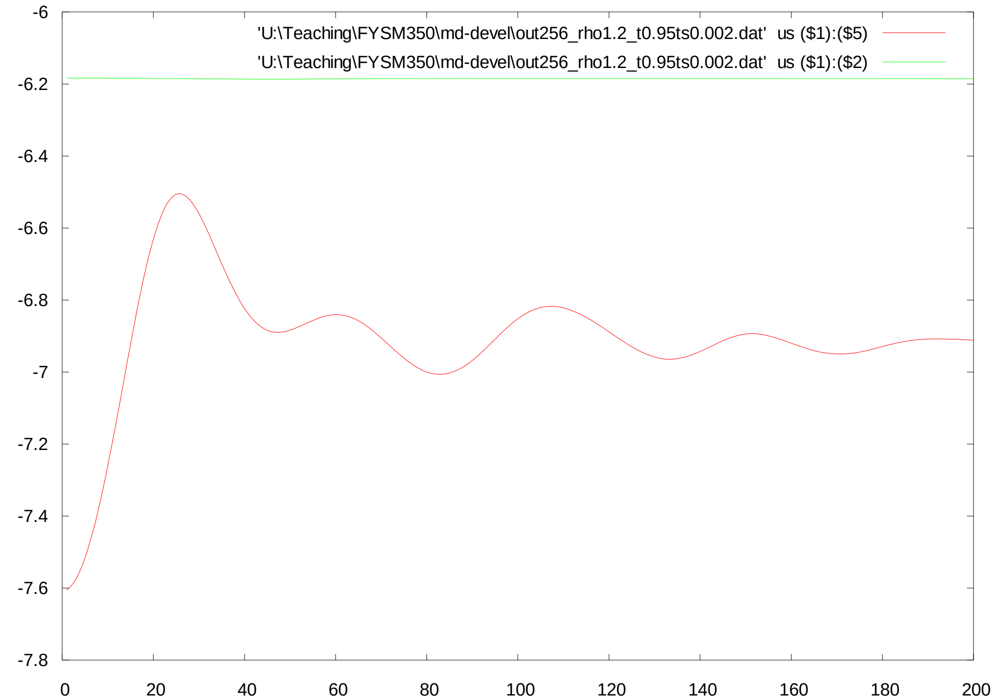
1. Set the density of your fcc lattice (lattice parameter a) equal to sqrt(2)*r_0 ($r_0 = 2^{1/6}$ corresponds to the bottom of LJ potential well where the energy = 1ε) and impose a short cutoff of potential between 1st and 2nd neighbours in fcc lattice (e.g. a cutoff value of 1.2σ). (What is then the scaled density (in units of σ^3)?) With this setup you should be going just over the nearest neighbour pairs in the potential calculation loop and the potential energy per atom in a perfect fcc lattice with periodic boundary conditions is = **(1/2) * 12 ε = -6 ε**. (*Note that the short cutoff is only for testing the potential calculation for a static fcc lattice, you cannot do reliable MD runs with this cutoff since the large discontinuity of forces messes up the dynamics. I recommend a cutoff value of 2.5 σ for real dynamics.*)

2. Check visually (VMD) that your fcc lattice looks OK. A handy way (and one quantity to analyze structure changes of your system in dynamic runs) is to implement an *order parameter calculation*. Let's define an order parameter for fcc lattice:

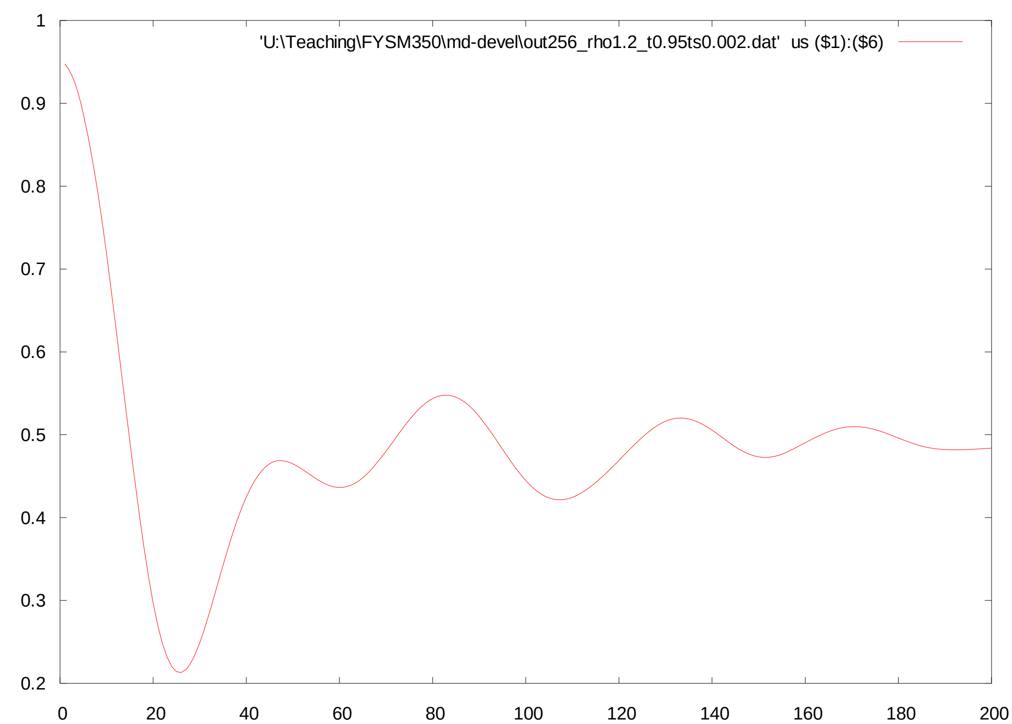
   $$S_{\mathbf{k}} = (1/N) \sum_{j=1,N} \exp(i\mathbf{k} \cdot \mathbf{r_j}) \quad \text{where} \quad \mathbf{k} = (2\pi/a)\,(1,-1,1)$$

   is one of the possible vectors in the reciprocal lattice of fcc and a is the lattice parameter corresponding the density of your system. If your fcc lattice is correct, $| S_{\mathbf{k}} | = 1$. (Hint: write exp-function with cosine and sine.)

3. Set the potential cutoff to 2.5σ. This means you have to create an fcc lattice of at least 256 atoms. (4 unit cells per side). Run a short MD simulation with a time step of 0.001 to 0.004. Your system should start to evolve in a constant total energy surface, and the value of the total energy is set by your initial velocities (kinetic energy). Print out the total energy as a function of time step and plot it. The graphs on the next page show results for a simulation for 256 atoms, initial density = 1.2 σ^3, initial velocities corresponding to temperature of 0.95 ε, time step = 0.002.



x-axis: time in time steps, y-axis, total energy per atom (green), potential energy per atom (red)



x-axis: time in time steps, y-axis, temperature (red)

4. (this test maybe become slow for MATLAB users, if it is prohibitively slow you can skip) The theoretical limit of the potential energy per atom in a static infinite fcc lattice (lattice parameter a = sqrt(2)*1.09 = **1.54149**.., density = **1.092032**…) with Lennard-Jones interactions is **-8.606863… ε.** (For a related discussion see e.g. Ashcroft-Mermin, Chapter 20, p. 401). See how close to this value you can get by increasing the cutoff stepwise and re-calculating the potential energy of a static fcc lattice as a function of the cutoff radius (remember that you have to always make sure that the length of your simulation cell is at least twice the potential cutoff).