06-640: Molecular Simulations
Homework 2
Due date: Thursday 2/3

1. The Lennard-Jones potential for two particles located at $\vec{r}_1 = (x_1, y_1, z_1)$ and $\vec{r}_2 = (x_2, y_2, z_2)$ is $V(\vec{r}_1, \vec{r}_2) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$, where $\vec{r} = \vec{r}_1 - \vec{r}_2$. The force due to a potential energy function is defined by $\vec{F} = -\nabla V$. Note that if we are dealing with two particles, $\vec{F}$ is a six-dimensional vector.

(a) Show that the force on particle 1 due to particle 2 is $\vec{F}_1 = \frac{24\varepsilon}{r^2}\left[2\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]\vec{r}$.

(b) What is the force on particle 2 (Hint: Use Newton's 3rd law)?

(c) Newton's equation of motion for the x-component of particle 2 is $F_{2,x} = m_2 \ddot{x}_2$. Assuming that both of the particles have the same mass, write an explicit expression for this equation of motion in reduced units.

2. (a) The following parameters can be used for a Lennard-Jones potential describing methane: $\varepsilon / k_B = 148$ K and $\sigma = 0.373$ nm. Convert the following quantities from reduced units into the units given: $T^* = 2.5$ into T in K, $\rho^* = 2.5$ into ρ in kg/m^3, $t^* = 450$ into t in s and t in ps, $P^* = 0.35$ into P in atm and P in Pa.

(b) Repeat part (a) for the Lennard-Jones potential for carbon tetraflouride, which has $\varepsilon / k_B = 134$ K and $\sigma = 0.466$ nm.

(c) The critical point of a fluid of Lennard-Jones particles occurs at roughly $T^*_c = 1.35$ and $\rho^*_c = 0.3$. Is the critical temperature of methane higher than carbon tetraflouride? Which of these two species has a higher density at the critical point?

3. This problem requires you to run and make minor adaptations to a MATLAB code. Before starting, review the documents "Accessing UNIX Machines From a Windows PC" and "Introduction to MATLAB" from the course web-page. Then log into an andrew UNIX machine and copy the MATLAB code *ljpot_total.m* into the directory where you will do your work by typing

```
cp /afs/andrew.cmu.edu/course/06/640/ljpot_total.m .
```

at the UNIX prompt. Note that the final period in this command tells the computer to copy the file into the directory you are currently in and give the new file the same name as the old one. This code fills a cubic box with a specified number of Lennard-Jones particles at random locations. It then computes the total potential energy of this set of particles. Note that the total energy will be different each time you run the program, since MATLAB will generate a different set of random numbers for the particle positions.

(a) Run the program 10 times using N = 10 particles in the simulation box. Note that total energy of each run. Explain the results you observe.

(b) Repeat part (a) but use N = 30 particles in the simulation box. Again, explain what you see.
(c) The code has deliberately been written in an inefficient manner. Copy the code into a new file and edit the new file to make it more efficient. Clearly comment the changes you make in the code. You should hand in a clearly commented listing of your revised code and a brief description of which changes were the most important in terms of improving the code's efficiency. Also list the steps you took to ensure that your revised code works correctly (i.e., how you debugged the code).
(d) Revise your code once more by using a Lennard-Jones potential truncated at 3σ. How much does this improve the code's efficiency for N = 30? Again, hand in a commented version of your code and a description of how you debugged the new version.