ChE 548
Homework Assignment II
Spring, 2009

For this homework, each team has been provided with the following codes:

1. md_mix_v22_nompi.for: A code for simulating a mixture of Lennard-Jones particles in the NVT or NpT ensemble. This code contains a thermostat and a barostat.
3. LJ_EOS_pure_TV.for: A code for evaluating the Lennard-Jones Equation of State for single component fluids, given temperature and density.

Each Team Must Complete the following two tasks.

Task 1. Simulate Cl_2 in the gas phase at T = 600 K and 1 atm.

First,

- Use the Lennard-Jones EOS to predict the fluid density at 1 atm. Use this as your initial input for the system density.
- Use the MD simulation to verify that rcut, maxeqb, maxstp, N, Δt are all legitimate values.
- Verify that your simulation is sufficiently long by showing plots of the MSD vs time on both normal and logarithmic axes.
- Explicitly report pressure, self-diffusivity and potential energy with error bars.
- Explicitly report all parameters used in the simulation.

Second,

- Explore temperature dependence of pressure, self-diffusivity and potential energy from 400 K to 700 K at constant density.
- Explore density dependence of pressure, self-diffusivity and potential energy at constant T of 600 K.

Third,

- prepare an oral presentation (powerpoint slides) summarizing your results in an organized manner.
- This report must contain all the tasks listed above summarized in graphical or tabular (or both) form.
- Compare the (i) magnitude and (ii) temperature-dependence of your pressure with the ideal gas law and Lennard-Jones EOS.
- Compare the (i) magnitude, (ii) temperature-dependence, and (iii) pressure dependence of your self-diffusivity with the prediction of Kinetic Theory.

Task 2. Simulate CCl_4 (Carbon Tetrachloride) in the liquid phase at T = 300 K and approximately 1 atm.

First,

- Simulate in the NpT ensemble (using a thermostat and barostat) at this state point.
- Verify that rcut, rnbr, maxeqb, maxstp, N, Δt are all legitimate values.
- Verify that your simulation is sufficiently long by showing plots of the MSD vs time on both normal and logarithmic axes.
- Explicitly report pressure, self-diffusivity and potential energy with error bars.
- Explicitly report all parameters used in the simulation.

Second,

- Explore temperature dependence of pressure, self-diffusivity and potential energy from 100 K to 400 K at constant density.
- Explore density dependence of pressure, self-diffusivity and potential energy in liquid phase at constant T of 300 K.

Third,

- prepare an oral presentation (powerpoint slides) summarizing your results in an organized manner.
- This report must contain all the tasks listed above summarized in graphical or tabular (or both) form.
- Compare the (i) magnitude and (ii) temperature-dependence of your pressure with the Lennard-Jones EOS.
- Compare the (i) magnitude, (ii) temperature-dependence, and (iii) pressure dependence of your self-diffusivity with the prediction from the corresponding states chart in Chapter 17 of BSL 2..