Homework 4: Introduction to Molecular Dynamics (MD)

1) Influence of the integration timestep

a) Use the input file "Kr_equilibrate.in" to generate a 5x5x5 FCC krypton crystal (with a lattice constant a = 5.0 Å). Using the Lennard-Jones (LJ) potential parameterized for Kr (with a cutoff of 7 Å), perform a "box/relax" minimization to determine the equilibrium lattice constant.

b) Equilibrate the system at 80 K and 0 atm (ensure that the volume and energy reach some plateaus) and save the equilibrated configuration in a data file (Kr_80K.dat).

c) Use the input file "Kr_NVE.in" to restart from the equilibrated configuration (Kr_80K.dat) and perform an NVE simulation with different timesteps varying from 0.1 fs to 50 fs. Check how the timestep affects the conservation of the total energy. Keep a timestep of 1.0 fs for the following. Plot the final total energy of the system as a function of the timestep.

2) Influence of the thermostat and barostat damping parameters

a) Use the input file "Kr_thermostat.in" to perform a sudden change of temperature, from 1 to 120 K with different thermostat damping parameters varying from 1.0 to 1000 fs. Check how the thermostat damping parameter affects how the temperature of the system follows that of the thermostat. Keep a thermostat damping parameter of 100.0 fs for the following.

b) Use the input file "Kr_barostat.in" to perform a sudden change of pressure, from 0 to 10000 atm with different barostat damping parameters varying from 80.0 to 10000 fs. Check how the barostat damping parameter affects how the pressure of the system follows that of the barostat. Keep a barostat damping parameter of 1000.0 fs for the following.

3) Influence of the system size

a) Use the input file "Kr_size.in" to generate various FCC krypton crystals with varying sizes (from 3x3x3 to 8x8x8) equilibrated at 100 K. Plot the simulation time as a function of the number of atoms.

b) Plot the average energy of the system at 100 K as a function of the number of atoms. Conclude.

c) Plot the standard deviation of the temperature of the system at 100 K as a function of the number of atoms. Conclude.

4) Melting of krypton

a) Use the input file "Kr_heat.in" to investigate the melting of Kr from 1 to 150 K under a pressure of 100 atm with a heating rate of 1 K/ps. Save the configuration of the system at 150 K (Kr_150K.dat). Observe how the atomic structure is changing as a function of temperature in VMD.

b) Plot the potential energy and volume as a function of temperature. Identify the melting temperature.
c) Restarting from the configuration of the system at 150 K (Kr_150K.dat), use the input file "Kr_cool.in" to investigate the quenching of Kr from 150 to 1 K under a pressure of 100 atm with a cooling rate of 1 K/ps. On the same plot, show the potential energy (and then volume) of Kr upon heating and subsequent quenching. Observe how the atomic structure is changing as a function of temperature in VMD. What type of phase is obtained after quenching?

5) Pair distribution function

a) Use the input file "Kr_phases.in" to create and save some atomic configurations of Kr in various states: crystal, liquid, gas, and glass. Visualize the structure of Kr in these different states using VMD.
b) Using the input file "Kr_pdf.in", compute the pair distribution function (PDF) of Kr in these states. After the simulation is done, the computed PDF can be found in the "pdf.dat" output file (distance = 2nd column, PDF = 3rd column). Comment on the shape of the PDFs.