06-640: Molecular Simulations
Homework 5
Due Date: Tuesday 4/21

This aim of this homework is for you to run a Gibbs ensemble MC code for a system of Lennard-Jones spheres using Case Study 16 from Frenkel and Smit. You may wish to refer back to homework 3 for some general details about running the Frenkel and Smit case studies.

Compiling The Case Study Source Code
Log in to your andrew account on one of the unix.andrew.cmu.edu machines. While in your home directory, execute the following commands
```
cd Frenkel_Smit/CaseStudy_16/Source
rm *.o
make
```
These commands compile the Gibbs MC source code.

Running Case Study 16

1. To run the code, move into the appropriate directory,
```
cd ~/Frenkel_Smit/CaseStudy_16/Run
```
and then type `./run` . This command executes a script that runs the main code and moves around some of the output files. A line of output should appear on your screen that contains information about how long it took to run the code, such as
```
1.6u 0.0s 0:03 54% 0+0k 0+1io 0pf+ 0w.
```
The meaning of this information was explained in homework 3 – it mainly describes how long the code took to run.

2. Running the code creates three output files, `out`, `lj.res,` and `lj.xy`. We will exclusively use the last of these files, `lj.xy` to analyze our results. You may also want to look at some of the information in `out` (a general purpose output file), but this will not be absolutely necessary. Important: Note that if you run the code multiple times, the new results are appended to the end of the existing `lj.xy` file. You can avoid having multiple data sets in a single file by renaming the file after each run. For example, the rename the file `new.name`, type
```
mv lj.xy new.name
```

3. For future reference, it is a good idea to make copies of the original input and output files so you can always recreate the state of the original distribution. To do this:
```
cp out out.original
cp run run.original
```

Editing The `run` Script

To perform Gibbs MC simulations at a variety of different conditions, you must edit the script that runs the code, `run`. The entire script is shown below in its original form, with comments indicating the variables that you will need to change.

```csh
#! /bin/csh -f

foreach temp (0.8 )            Sets the temperature (reduced units)
  echo " --- temp ${temp} "
  echo " --- temp ${temp} "   >> out
  cat > fort.15  <<endofdata                  nequil = # of equilibration cycles
  ibeg  , nequil  , lmax    nsamp  iseed       lmax = # of MC cycles after equilibration
   0        100        200     1     48573478  iseed = seed for ran. # generator
  dr       vmax   succ
  0.09     0.01   50.
  ndispl   nvol nswap        These variables set the ratios of particle displacements:
  200       2      20        volume exchanges:particle swaps to 100:1:10
npart temp rho      p  lattice           npart =total  # of particles
256    ${temp} .31    32.2    'cubic'    rho = initial density
rv
3.0
endofdata
 cp lj.res              fort.11
  cp lj.model           fort.25
 time  ../Source/Gibbs  >>&   out
 cp fort.21        lj.res
 mv fort.66        lj.prt
 cat fort.44      >>           lj.xy
 #perform block analysis
  cp lj.prth            fort.31
  mv  lj.prt            fort.32
 ../../Appendix/block   >>   out
 rm fort.*
end
exit
```

This script runs the code by initially creating two simulation volumes of equal size each containing 128 particles at density $\rho = 0.31$ in a cubic lattice. Reduced units are used for all quantities. During each MC cycle, 200 particle displacement moves, 2 volume exchange moves, and 20 particle exchange moves are attempted.

Interpreting The Output

The output file obtained by running the script above, `lj.xy`, is 200 lines long, one line of output for each MC cycle after the equilibration cycles are complete. The last few lines are

```
  118     438.15    138     387.65
  118     440.91    138     384.90
  118     447.41    138     378.40
  118     443.04    138     382.76
  118     443.04    138     382.76
```

These four columns are the number of particles in box 1, the volume of box 1, the number of particles in box 2, and the volume of box 2, respectively. We see that at the end of this run, the densities of the two simulation volumes were $\rho_1 = 0.266$ and $\rho_2 = 0.361$. This file contains all the information necessary to make plots analogous to Figs. 8.3 and 8.5 in Frenkel and Smit. All of your data analysis in the exercises below will be based on the data in this output file.

Exercises for Case Study 16

1. Set the number of equilibration cycles, `nequil,` to zero and run the simulation for 3000 MC cycles at T = 0.8. Plot your result in the same was as in Frenkel and Smit's Figs. 8.3 and 8.5. Explain what you see. Use your results to determine an appropriate number of equilibration cycles for this system and thus determine the gas and liquid densities at the coexistence point at this temperature.

2. Repeat your simulation at T = 0.8 using 3 different seeds for the random number. The random number seed must be a positive integer. Is the identity of box 1 at the end of each simulation the same? Why or why not?

3. Perform Gibbs MC simulations to compute the densities of coexisting phases for T = 0.6, 0.8, 1.0, 1.2, and 1.4. At each temperature, you should follow a procedure similar to the one outlined in exercise 1. Use your data to plot the vapor-liquid coexistence curve for the Lennard-Jones fluid as a function of density and temperature.