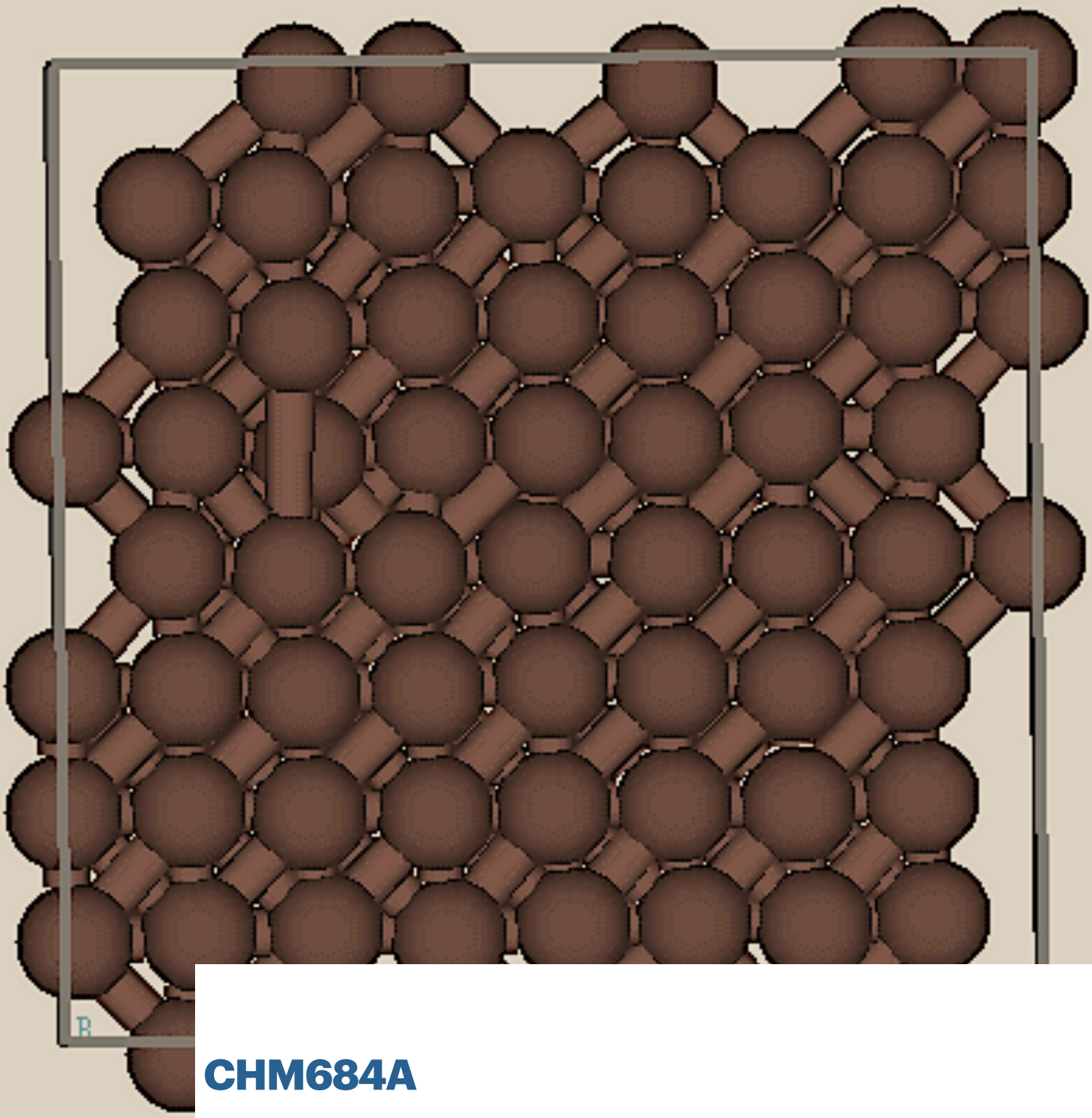
12 OCTOBER 2020



CHM684A

PROJECT-2

SET B

OCT 12, 2020

PHASE TRANSITION IN 2D HARD DISK FLUID

In this project, you will be studying phase transition using a two dimensional hard disk fluid by applying the Monte Carlo (MC) method. Consider a two dimensional periodic box with hard disks undergoing a phase transition with change in density.

The potential energy of the hard disk system is given by

$$V(\mathbf{r}_1, \cdots, \mathbf{r}_N) = \sum_{i}^{N-1} \sum_{j>1} v(r_{ij})$$

with

$$v(r_{ij}) = \begin{cases} 0 & ; \ r_{ij} \geq \sigma \\ \infty & ; \ r_{ij} < \sigma \end{cases}$$

where the inter-particle distance $r_{ij} = \left| \mathbf{r}_i - \mathbf{r}_j \right|$, and σ is the diameter for the disk.

The local structure of a condensed matter system, including fluids, can be understood based on the radial distribution function (RDF), $g(r)$. See Figure 7.4 and 7.5 of D. Chandler's book "Introduction to Modern Statistical Mechanics". RDF defines the distribution of the particles at distance r from a particle. It can be computed by

$$g(r) = \frac{\sum_{j=1}^{N} \sum_{i=1}^{T} n_{ji}(r)}{2\pi r\, dr\, (N-1)T\rho}$$

where N is the number of atoms, T is the number of configurations/frames considered, ρ is the number density, and n_{ji} is the number of particles in the shell r and $r + dr$ from atom j in the frame i. See also Section 7.8 of D. Chandler's book "Introduction to Modern Statistical Mechanics".

When writing out the coordinates periodic boundary condition (PBC) has to be accounted as follows:

```
IF( rx(i) <  −box_size_x * 0.5 )  rx(i) = rx(i) + box_size_x
IF( rx(i) >=   box_size_x * 0.5 )  rx(i) = rx(i) - box_size_x
```

Here rx(i) is the x coordinate of atom i , and box_size_x is the length of the box along the x direction. Similar PBC correction has to be also applied along the y direction as well.

When computing the distance between two atoms, then PBC has to be accounted as follows:

```
dx=rx(i) - rx(j)
IF(dx  >   box_size_x * 0.5 ) dx = dx − box_size_x
IF(dx <= − box_size_x * 0.5 ) dx = dx + box_size_x
```

Similar considerations also has to be accounted for the y-component.
Then,

```
rij=SQRT(dx**2 + dy**2)
```

For more details, see https://en.wikipedia.org/wiki/Periodic_boundary_conditions.

Run MC for various fluid densities and determine $g(r)$ in each case. Then, compute the value of $g(r)$ at contact, $g(r = \sigma)$, from the RDF. Based on this, compute pressure p as

$$\frac{\beta p}{\rho} = 1 + B_2 \rho g(\sigma)$$

with $\beta = 1/k_{\mathrm{B}}T$, ρ is the number density, and B_2 is the second viral coefficient,

$$B_2 = \frac{2\pi}{3}\sigma^3.$$

Your aim is to study the equation of state of hard disks by plotting $\beta p/\rho$ as a function of ρ, and identify the phase transition region.

METHODS

For the MC calculations, use number of particles as 32^2, and number densities 0.1, 0.2, ..., 0.8, 0.94. In every MC step, shift the position of a randomly chosen atom by a random perturbation. The magnitude of the shift can be an input parameter. The move will be rejected if this atom overlaps with any other atom (i.e. their internuclear distance become less than σ).

Note that, the shift parameter has to be wisely chosen for a good acceptance ratio. For low density, large shift is tolerable, while for high density, the shift parameter has to be small.

Periodic boundary conditions (PBC) have to be always applied in the calculations.

Having defined the number density ρ, and number of atoms N, the area A and box length L can be calculated as $A \equiv L^2 = N/\rho$. Consider distances in σ units.

For all densities, calculations have to be started with a regular array (32×32) of hard disks where the distance between any two particles is L/N (and is always greater than or equal to 1σ).

While calculating $g(r)$, the maximum distance $r = r_{\max}$ up to which $g(r)$ has to be calculated is $L/2$ (i.e. half the box length). A suitable value for dr is 0.1σ. Note that, while calculating $g(r)$, PBC have to accounted.

Typically, you one requires $10^5 - 10^6$ steps of MC for obtaining meaningful results.

IMPLEMENTATION

You need to write three Fortran modular programs,: (i) For doing MC , (ii) for the computation of $g(r)$, and (iii) for the computation of pressure for various densities.

The program (i) should contain subroutines for
a) Constructing initial structure (lattice)
a) MC move (accept/reject step)
b) Periodic boundary condition
c) Write XYZ file for all the accepted moves (in the same file, in appended mode)
d) Wrapping coordinates within the box before writing the XYZ file
The program (i) should read in number of atoms, density, step size (for perturbing the coordinates), and number of moves. The output of the program should be % of acceptance (printed every 100 steps) on the screen, and .xyz file of particle coordinates at every accepted move.

For the $g(r)$ code has to read-in the .xyz file written by the program(i). The parameters $r_{\max} = L/2$, dr and box-length have to be read in. A suitable value of dr is 0.1σ. Number of atoms and number of frames in the .xyz files can be read-in directly from the .xyz file.

REPORT

It should contain an introduction to the problem and aim of the project. Subsequently, “Methods and Models” part should give details about the model, algorithm, program

design, and other technical/theoretical details. The details given here should help someone else to reproduce your results. In the "Results" part, explain the results with tables and figures. All the tables and figures should have captions, with figure/table numbers. In this case, generate the figure of snapshots of the last accepted configuration (by visualising .xyz through VMD) and $g(r)$ for every value of ρ considered. A table with $g(\sigma)$, and p for various values of ρ has to be reported. The equation of state should be shown by the plot of $\beta p/\rho$ versus ρ. Final section of the report should be "Conclusion" where you conclude the results of your work. You can add the codes to the report as Appendix.