ME 422 Statistical Mechanics for Applications

Homework 4–MD & Monte Carlo for Hard Spheres in a Closed Box

due Wednesday, October 31, 2017

Note: In question 4, you will be comparing results from questions 1 - 3. In making this comparison, you should use the same disk radius σ.

1. The included Matlab script DirectSmpl.m is the direct sampling Monte Carlo algorithm that we discussed in class.

(a) After the commands `overlap = false` and `L = [L;a];`, what is the next command to be executed?

(b) After the commands `overlap = true;` and `break;`, what is the next command to be executed?

(c) The code ends with a section `% Observable`, that plots a histogram (using the default Matlab normalization `Count`) of the x-positions of the disks. Observe the behavior of the histograms for a few values of `n_runs`. Modify the `% Observable` portion of the code to make a histogram of the probability density function (`pdf`) of the y-positions of the disks. (You do not need to hand in the modified code.) Do you observe the same behavior in x?

(d) Show the histograms for the y behavior for `n_runs` $= 10^3, 10^4, 10^5$.

2. The included Matlab script MarkovSmpl.m is the Markov chain sampling Monte Carlo algorithm that we discussed in class. The program ends with a fun visualization section which plots the disk positions at each attempt.

(a) Modify the code to determine the number of attempts needed per non-overlapping configuration. (An *attempt* includes both successful and unsuccessful attempts at making a new configuration.) For `n_runs` $= 10^2$ or higher and a range of values of disk radius, plot (successful configurations/attempts) versus σ.

(b) Modify the program to plot a histogram of the y-positions of the disks. (You do not need to hand in the modified code.) Show the histograms for the y behavior for same values of `n_runs` as you used above for DirectSmpl.m, namely $10^3, 10^4, 10^5$.

3. The molecular dynamics Matlab script EventMD.m is also included. This program solves for the dynamics of four hard spheres in a 2D box. The program ends by plotting the particles as they move along their trajectories. You can observe the trajectories more closely by changing the `pause` statement: `pause` with an argument, such as `pause(0.1)` will pause for a certain number of seconds, here 1/10 of a second, and then move on; `pause` with no argument waits for a keystroke from you. You will not need this section in your HW, but it's fun to follow the trajectories.

(a) What is specified in `singles`?

(b) What is specified in `pairs`?

(c) What is `e_perp`?

(d) What is `scal` and how was it determined?

(e) Modify the code to find the y-positions of the disks. Make histograms of the probability density function of the y-positions for, once again, `n_runs` $= 10^3, 10^4, 10^5$.

(f) Include in your HW the snippet of code that you inserted in EventMD in order to plot the histograms.

4. Comment on the distribution of particles in the box.

(a) Include, in your comments, whether you think that configurations are equally probable, and whether x or y-positions are equally probable.

(b) For x and y positions, try to think of a reason for your observations. To help with your thinking, look at the size of the non-uniformities in position: are they comparable to the disk size? the box size?...? (We'll be discussing these types of behavior for positions in the coming weeks.)

(c) Which program, MD, direct sampling MC, or Markov chain MC is most efficient at showing the non-uniformities in position? That is, which one, for a given number of runs, can most clearly reveal the positional non-uniformities?