**ME 422 Statistical Mechanics for Applications**

# Homework 5–Equally-timed MD sampling & 1D Depletion Force

**due Wednesday, November 7, 2018**

1. You recall from the previous HW, that the $x$- and $y$-positions from the direct and Markov chain MC simulations showed a particular non-uniform distribution. In contrast, the MD simulation results were less clear. In particular, it was not certain whether the MD distributions were the same or different than the MC sampled distributions. HW4's MD distribution was drawn from samples taken at the *events*, that is, when there was a disk-disk or disk-wall collision. This seems suspect, as the event-based samples seem to bias the data taking–for disk-wall collisions–to samples in which at least one disk is close to a wall. Let's then implement a procedure in which the samples are taken at regularly-spaced times.

EventMDEqT.m is included with this HW assignment.

(a) Explain in a few sentences how the Matlab code equally spaces the samples. A sketch would be helpful.

(b) What is the time interval between samples? That is, is it 1? 0.1?, 1/2? . . . ?

(c) The three `Observable` sections each plot a histogram. What is being plotted in these three figures? In particular, for each plot, at what times are the data points drawn?

(d) What can you say about the distribution of positions of the MD simulation compared to those from HW4's MC simulations?

2. Direct1D.m is included with this HW assignment. It computes the configurations for placing $N$ 1D spheres (i.e. bars of length $2\sigma$) along the line of length $L$.

(a) Modify the code to calculate the number of attempts needed to achieve `n_configs` configurations.

(b) Modify the code to save the valid (that is, the non-overlapping) configurations $x$ in a file named $xs$.

(c) Modify the code to make a histogram of the positions of the 1D spheres from the saved configurations.

(d) Modify the code to print to the screen whenever the number of successfully computed configurations passes 0.1, 0.2, ... 0.9, 1.0 of the total `n_configs`.

(e) Include the modified code with your homework.

(f) Produce a histogram of the positions for greater than or equal to `n_configs` $= 10^4$, $N = 5$, and $\sigma = 0.75$. Label the axes appropriately.

(g) In a sentence or two, describe the position behavior seen in the histogram.

(h) For $N = 2, 3, \ldots$ as high as possible, plot the attempts needed per successful configuration.

(i) In a sentence or two, comment on the type of situations for which this code is useful and the situations for which running this code is infeasible. By "type of situations" I mean over the range of values for the parameters $N$ and $\sigma$. That is, how well does the code perform at high and low values of $N$, and high and low values of $\sigma$?