ME 422, Fall 2018

Assignment 4.

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Due Oct 31

1. (a) If $k < N - 1$, the next commmand is

   ```
   a = [box_size * rand + sigma, box_size * rand + sigma] ;
   ```

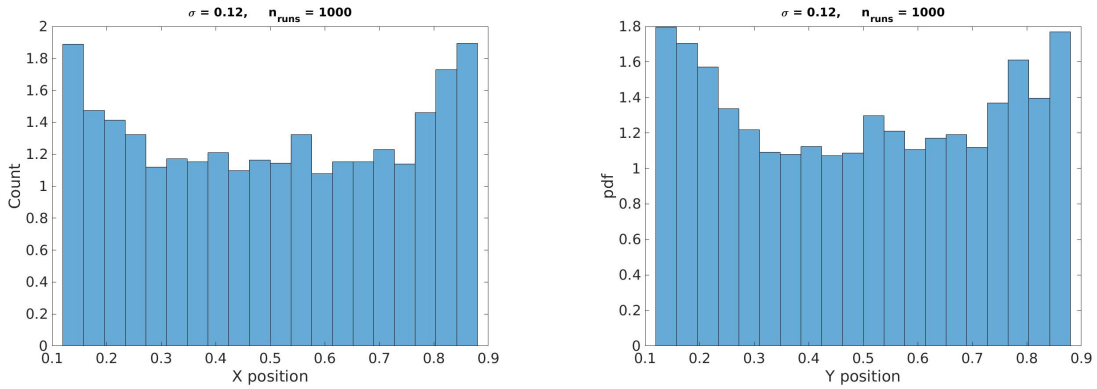
   Else, it is

   ```
   Ls = [Ls,L];
   ```

   (b) The next command is

   ```
   L = [box_size * rand + sigma, box_size * rand + sigma] ;
   ```

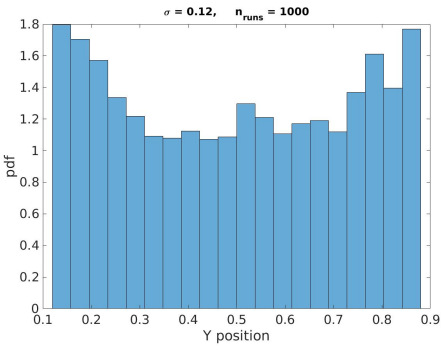
   (c) It looks like the behaviour is similar for x and y. That makes sense logically since our physics and our code is symmetric.



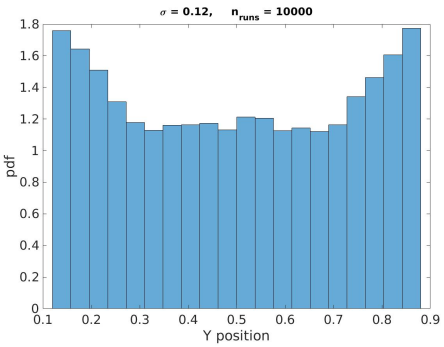
(a) X positions (b) Y positions

Figure 1: Histograms of x and y positions

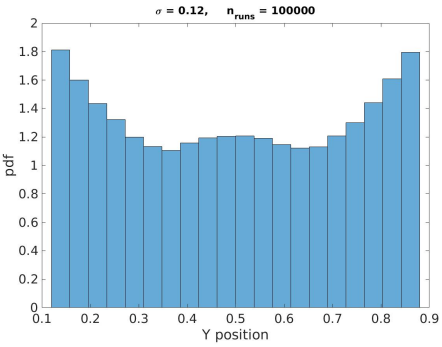
   (d) These are the histograms.



(a) 10^3 runs



(b) 10^4 runs



(c) 10^5 runs

Figure 2: Y behaviour for various runs

2. (a) As the disk size increases, overlaps become more probable

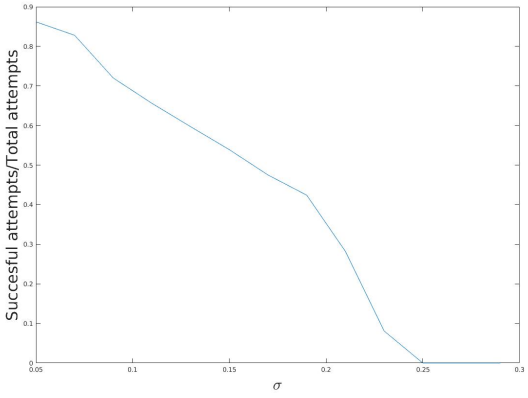
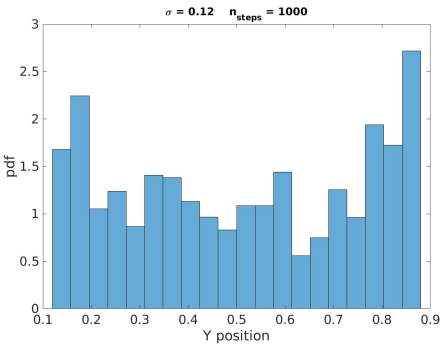
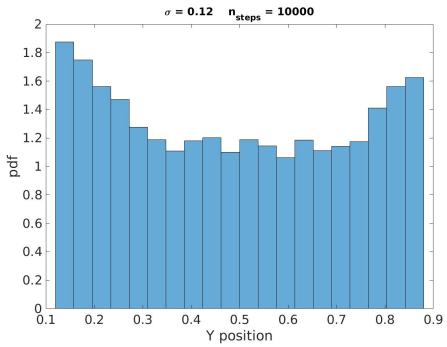


Figure 3: Ratio of succesful attempts vs disk size

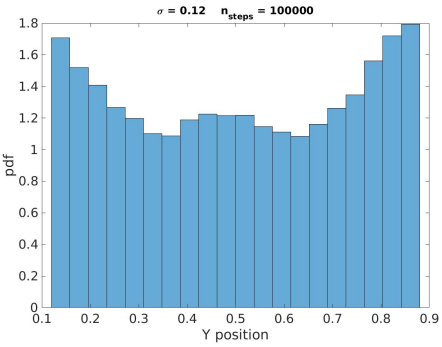
(b) Here is the Y behaviour of various runs



(a) 10^3 runs



(b) 10^4 runs



(c) 10^5 runs

Figure 4: Y behaviour for various runs

3. (a) **singles** is a vector that contains the indices for all the x and y positions of all 4 disks. It is used to identify when a collision will happen with a wall.

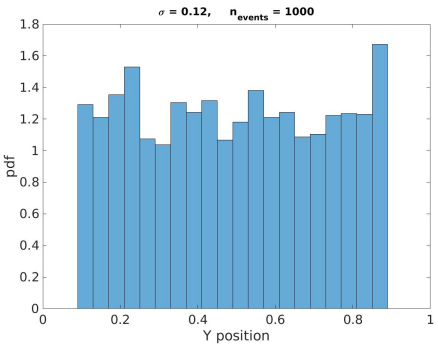
   (b) **pairs** is a vector that compares the positions of all the disks with respect to each other, in order to compute pair wise collision time.

   I would like to point out that parts (a) and (b) are way more obvious from the point of view of the person who wrote the code than the person reading it.

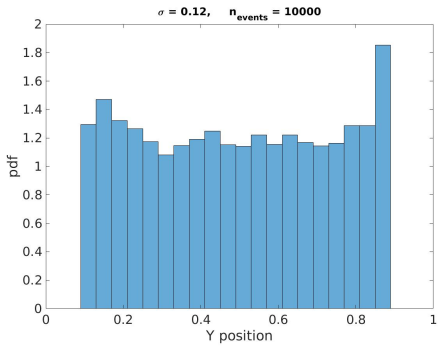
   (c) **e_perp** seems to be the unit displacement vector $(\frac{\Delta x}{|\Delta x|})$.

   (d) **scal** seems to be $\Delta v.\frac{\Delta x}{|\Delta x|}$. It is determined by taking the dot product of **del_v** and **e_perp**

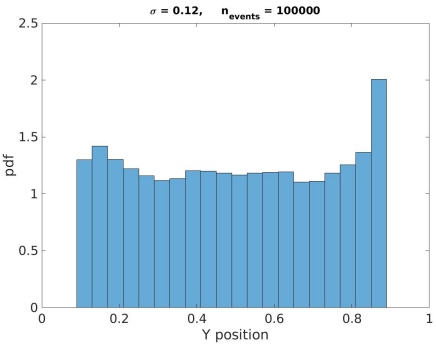
   (e) Here is the Y behaviour of various runs



(a) 10^3 runs



(b) 10^4 runs



(c) 10^5 runs

Figure 5: Y behaviour for various runs

(f)
```
histogram(DFile(:,6:9),20,'Normalization','pdf')
xlabel('Y position', 'FontSize', 24);
ylabel('pdf', 'FontSize', 24);
set(gca, 'FontSize', 24);
title(['\sigma = ', num2str(sigma), ',     n_{events} = ', num2str(n_events)],
```

4. (a) From the histogram from all 3 types of simulations, all configurations are definitely not equally probable. X and Y enjoy symmetry so they have the same kind of probability distribution. It looks like corner and wall positions are more likely than central positions.

   (b) Obviously, the non-uniformity in position arises due to the presence of the two walls. If the boundaries were periodic, perhaps more uniform distributions could be seen.

   (c) Markov chain MC samples the same thing as direct sampling but in a far more efficient way. The molecular dynamics manages to incorporate velocities and collisions very well. So, I would trust MD to best represent what's actually going on.