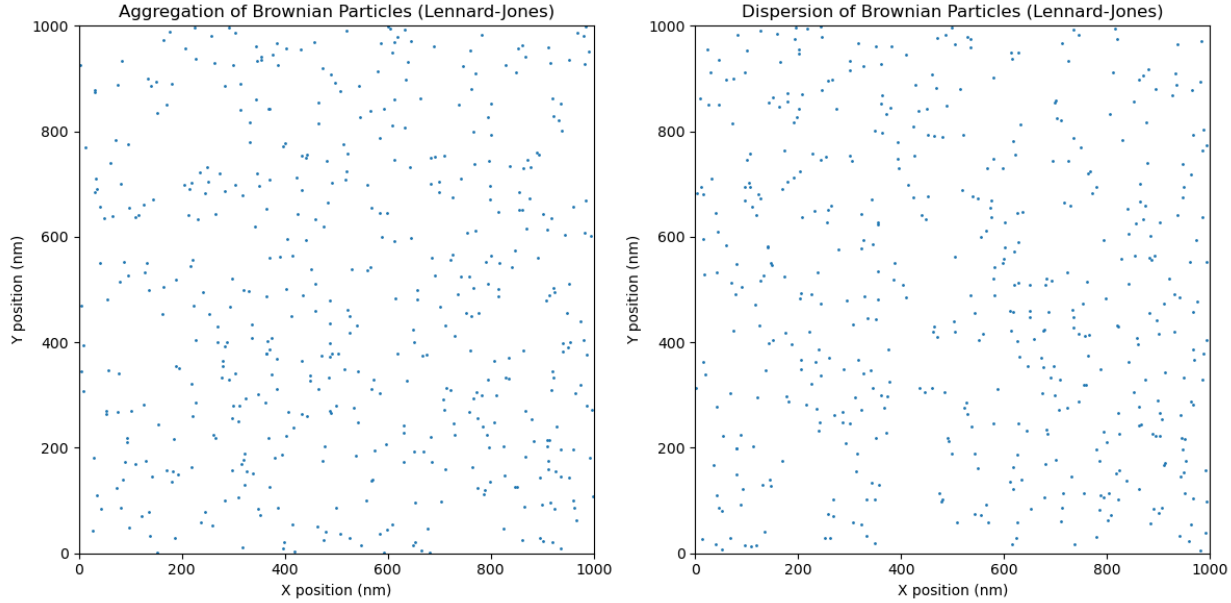
1. If the depth of the potential well in the Lennard-Jones potential is greater than a few k_BT, then thermal energy does not often produce fluctuations that can pull the particles apart. We expect the particles to eventually aggregate for these cases (Do you see why?) For what values of σ and ε do we expect to get aggregation?

- First, I'll rewrite the equation for Lennard-Jones potential: $U(r) = 4\varepsilon[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^{6}]$.
- As the problem mentioned, we need the depth of the potential well aka ε to be a few kBT for the particles to aggregate (a few I would say $3k_B$T and above). This is because when the depth of the potential well gets deep enough, the particles' random thermal motion gets "trapped" and unable to overcome the potential depth, resulting in them sticking together.
- Since the particles are aggregated together, σ should be relatively similar to the diameter of a particle as that is the distance they are apart from each other.

2. For particles with a radius of 10 nm, what is a good choice for the time step to use in a simulation? Hint: What is the largest distance you want a particle to travel over one time step? Explain your reasoning.

- As I have explained above, we don't want the particle to travel a distance larger than its diameter (so for a 10nm, we want the limit to be around 20nm at most).
- Having said that, 20nm is still too large of a timestep as we can sometimes "overwalk" causing it to break the law of physics and make weird errors.
- In this case, the smaller the better, I will just use dt = 1 nm for my timestep to look at more detailed movement.

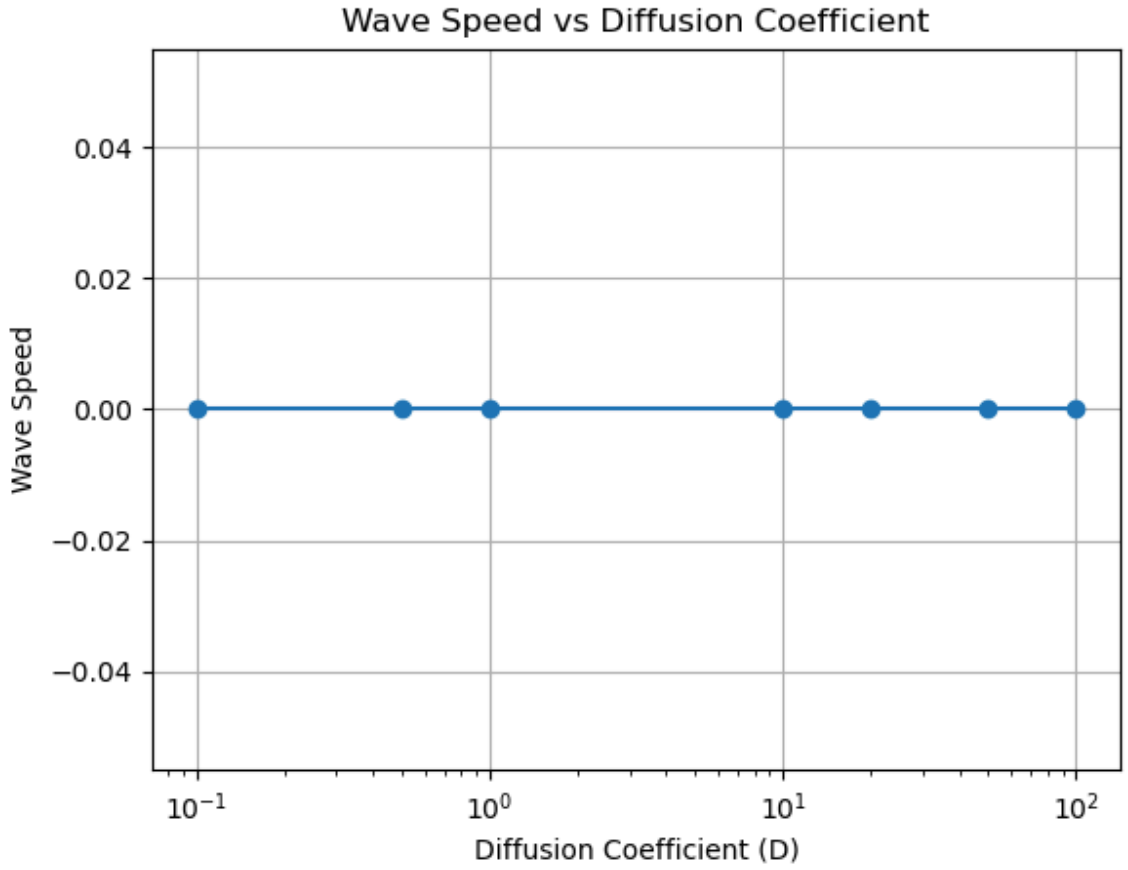
3.



- My epsilon value is 0.012 (3kBT), and my sigma value is 20 nm (diameter of the particle).

- As you can see on the plot above, although the aggregation plot has a bit more “clusters” compared to the dispersion plot, it really doesn’t look that much different.
- I even tried with higher epsilon values because, in theory, higher potential depth value leads to the particles sticking closer together as they cannot escape the potential well. I even try up to value 100 for eps_agg or reduced eps_dis up to 0.00001 but nothing too significant happens. I wonder if my code is actually correct…

4.



- This graph is weird since I thought the Diffusion Coefficient was supposed to increase as wave speed increases since they are proportional to each other. However, the speed stays the same regardless of the values for D (I tried so many different values, but nothing works). I also try to fix the code back and forth but it still looks similar-ish. I wonder what have I done wrong here.
- I have plotted the graph in different time as well but they also look very similar, same old flat, horizontal line like this, very disappointing…