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PHYS 305 homework 5 write-up

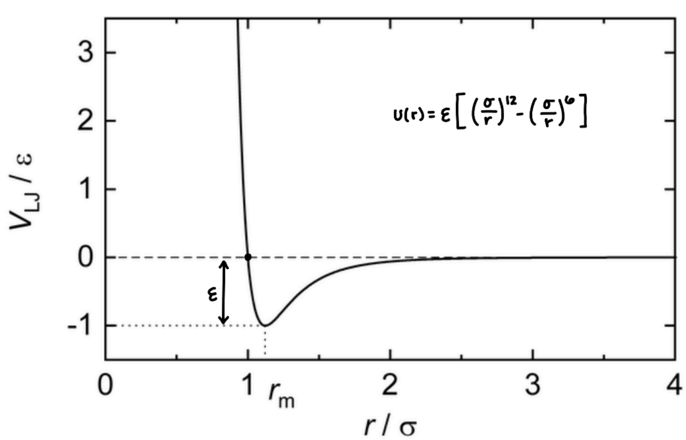
1. The equation for the Lennard-Jones potential is:

$$U(r) = \varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - 2\left(\frac{\sigma}{r}\right)^{6}\right)$$

   Where ε is the depth of the potential well, σ is the distance where the potential energy between the particles is zero, and r is the distance between a set of interacting particles. We know that the potential minimum is:

$$r = r_{min} = 2^{1/6} * \sigma$$

   Concerning the code for problem 3:
   Once the particles escape the well, they will disperse. But they must have a small enough sigma to repel each other because, at moderate distances, the particles will be attracted to each other.



given that the depth of the Lennard-Jones potential is > few K_BT

particle has average $KE \approx \frac{3}{2}K_BT$

∴ let $\boxed{\varepsilon \approx 10\,K_BT}$ so that the potential is large enough that the particles cannot escape the well

repulsion is greatest when the particles are touching (dispersion)

∴ for aggregation: let $\boxed{\sigma \approx R_{particle} = 10\text{ nm}}$ (moderate distance)

∴ for repulsion: let $\sigma < R_{particle}$

2. The largest distance you want a particle to travel over one time step would be 1 nanometer (one-tenth of the particle's diameter).

$$D = \frac{K_BT}{6\pi\eta R} = \frac{4\times10^{-21}\,N\cdot m^{-1}}{6\pi\cdot10^{-3}\,kg\cdot m^{-1}\cdot s^{-1}\cdot10^{-8}\,m} = 2.12206591\times10^{-11}\,m \approx 2.12\times10^{-11}\,m$$

$$\Delta x \approx \sqrt{2D\cdot\Delta t} \rightarrow \Delta t = \frac{(\Delta x)^2}{2D} = \frac{(10^{-9})^2}{2\cdot2.12\times10^{-11}} = 2.356194488\times10^{-8}\,s \approx 2.36\times10^{-8}\,s$$

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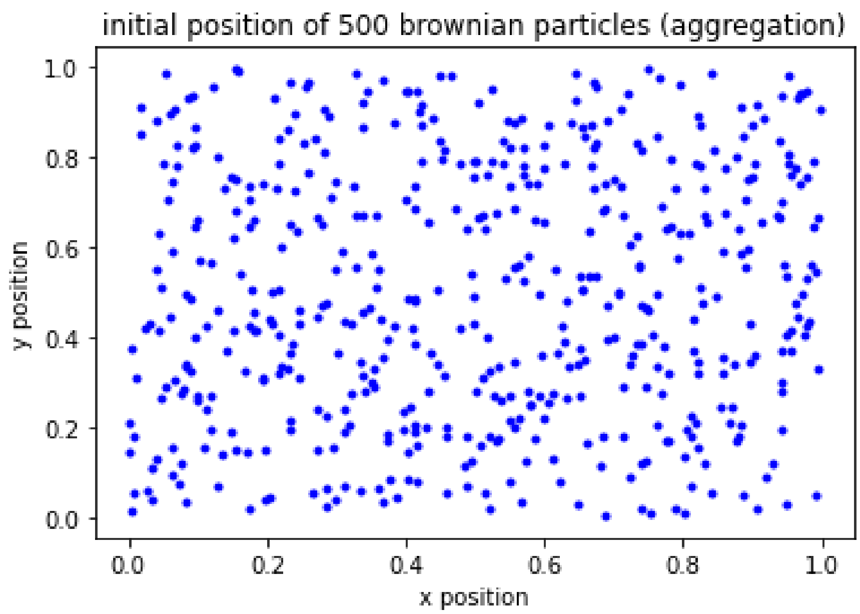
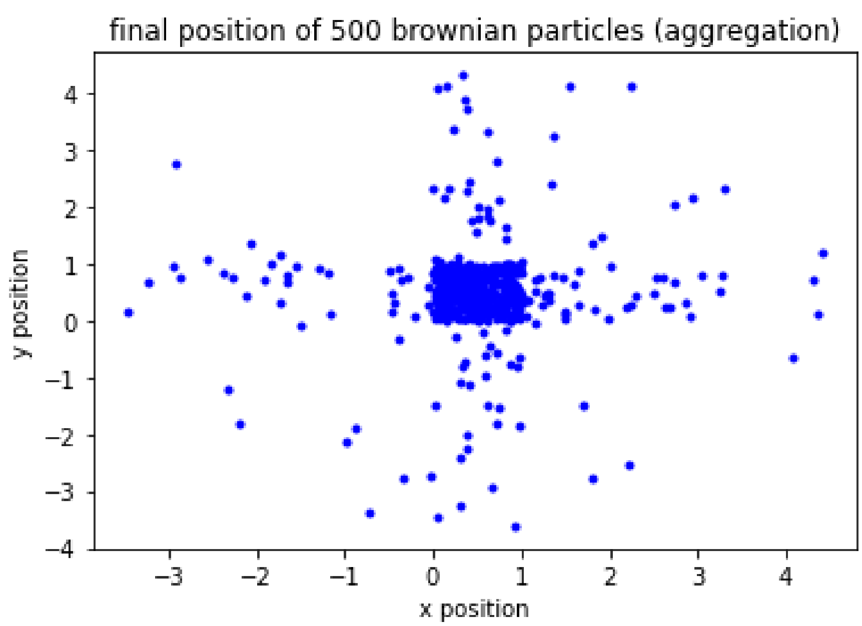
3. (see code)
   In my first submission, I had everything past the force magnitude inside the k loop, so my code would not run and I couldn't figure out why.
   I also previously had kBT to the power of -21. The true power is -14 and I have adjusted the calculations and values within my Brownian Particle function to better match the code from class regarding Brownian particles (multiplied the numerical values from the written work above by 10^6). I also use these bigger numbers when I call the function within main().





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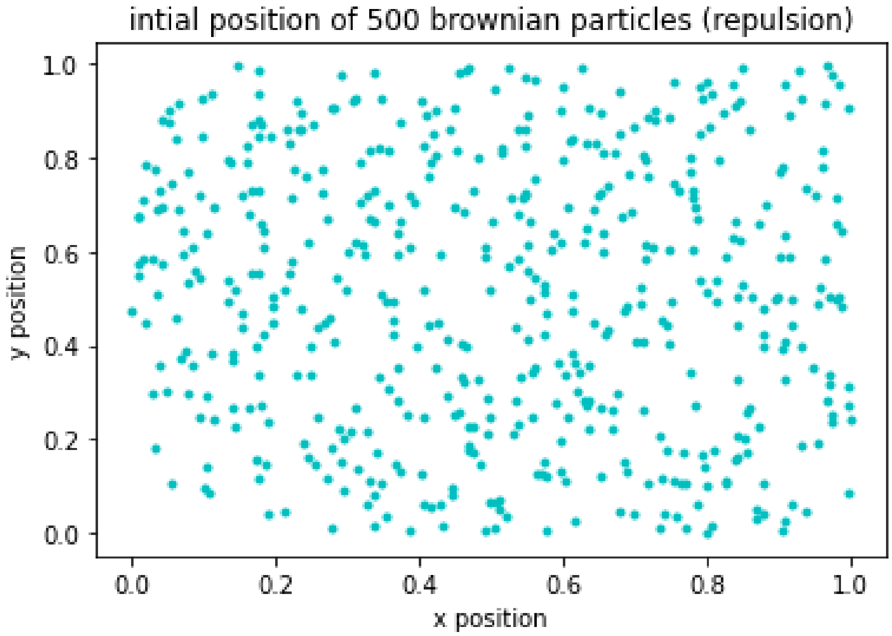

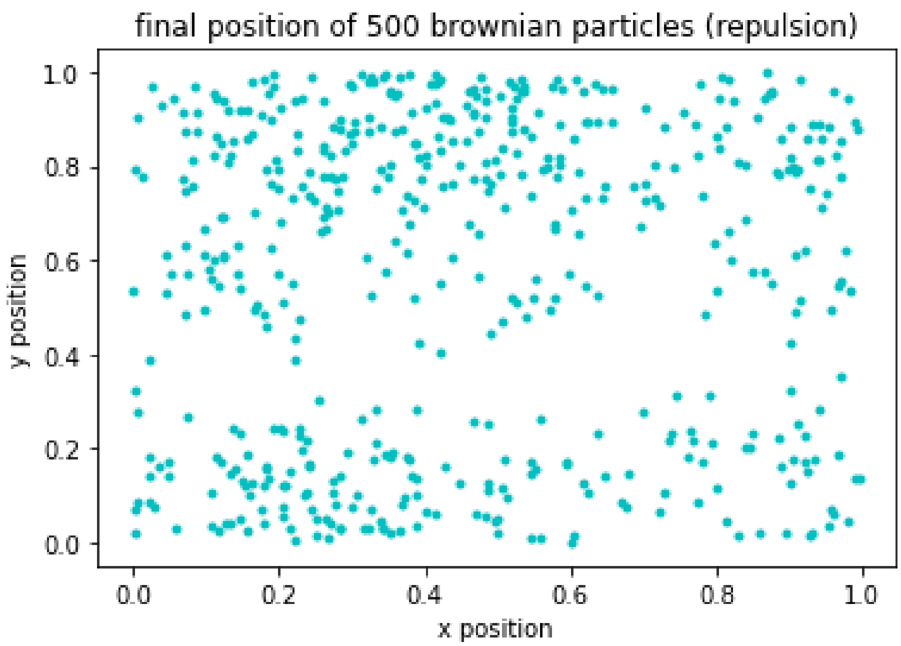

4. Figuring out the time step for Fisher's equation: (also see code)

$$\frac{\partial u}{\partial t} = D \cdot \frac{\partial^2 u}{\partial t^2} + u(1-u)$$

$$\frac{u_i^{j+1} - u_i^j}{\Delta t} = D \cdot \left[\frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{(\Delta x)^2} \right] + u(1-u)$$

$$* \quad u_i^{j+1} = D \cdot \Delta t \cdot \left[\frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{(\Delta x)^2} \right] + u \cdot \Delta t (1-u) \rightarrow \text{need to use BC}: \ u(x=0)=1, \ u(x=10)=0$$

at $x=0$: using the forward derivative:

$$\left.\frac{\partial u}{\partial x}\right|_{x=0} = \frac{1}{\Delta x}(u_1 - u_0), \quad c_0^j = c_1^j$$

at $x=0$: $u_0^{j+1} \approx u_0^j + \frac{D \cdot \Delta t}{(\Delta x)^2}(u_1^j - 2u_0^j + u_{-1}^j) + u \cdot \Delta t (1-u)$

↳ u_{-1} is unknown → set central difference derivative to BC.

$$\frac{u_1^j - u_{-1}^j}{2\Delta x} = 1 \rightarrow u_{-1}^j = u_1^j - 2\Delta x$$

$$u_0^{j+1} \approx u_0^j + \frac{D \cdot \Delta t}{(\Delta x)^2}(u_1^j - 2u_0^j + u_1^j - 2\Delta x) + u \cdot \Delta t (1-u)$$

$$\approx u_0^j + \frac{2D \cdot \Delta t}{\Delta x}(u_1^j - u_0^j) + u \cdot \Delta t (1-u)$$

at $x=10$: using the backward derivative:

$$\left.\frac{\partial u}{\partial x}\right|_{x=10} = \frac{1}{\Delta x}(u_N - u_{N-1}), \quad u_N^j = u_{N-1}^j$$

at $x=10$: $u_{10}^{j+1} \approx u_{10}^j + \frac{D \cdot \Delta t}{(\Delta x)^2}(u_{11}^j - 2u_{10}^j + u_9^j) + u \cdot \Delta t (1-u)$

↳ u_{11} is unknown → set central difference derivative to BC

$$\frac{u_{N+1}^j - u_{N-1}^j}{2\Delta x} = 0 \rightarrow u_{N+1}^j = u_{N-1}^j \rightarrow u_{11}^j = u_9^j$$

$$u_{10}^{j+1} \approx u_{10}^j + \frac{D \cdot \Delta t}{(\Delta x)^2}(u_{11}^j - 2u_{10}^j + u_9^j) + u \cdot \Delta t (1-u)$$

$$\approx u_{10}^j + \frac{2D \cdot \Delta t}{(\Delta x)^2}(u_9^j - u_{10}^j) + u \cdot \Delta t (1-u)$$

The video of the wave propagation at D = 0.01 was submitted to the D2L folder along with this document and the code. With a total time of 50, dt of 0.001 and skip of 100, there was a full movement from one side of the plot to the other.

For this problem involving Fisher's equation, I was unable to produce a curve that I felt made sense (the one below does not seem reasonable). I would expect some sort of linear relationship between the diffusion constant and the velocity and It would make sense for the curve to start at the origin (zero diffusion, zero velocity). I couldn't quite figure out where I was going wrong and how to produce a curve with a somewhat linear relationship.