PHYS 305 – Homework #5 **Due: Oct. 28, 2024**

1. If the depth of the potential well in the Lennard-Jones potential is greater than a few $k_B T$, then thermal energy does not often produce fluctuations that can pull the particles apart. For these cases, we expect that the particles will eventually aggregate (Do you see why?) For what values of σ and ε do we expect to get aggregation?
2. For particles of radius 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.
3. Simulate the motion of 500 Brownian particles of radius 10 nm that interact by a Lennard-Jones potential. The particles should be in a 2D box of length 1 μm. Use a cutoff on the force so that the maximum value of the force does not move the particles more than about a tenth of a particle diameter. Determine if the values you found in Problem 1 do indeed lead to aggregation, and whether values outside that range disperse. Provide the code you used and a set of values that lead to aggregation and one that doesn't. Include a plot showing aggregation and one showing dispersion.
4. Fisher's equation

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

describes a simple model for how a replicating species u spreads through space. This equation naturally leads to traveling wave solutions, where a sharp transition in u propagates at constant speed. Solve this equation on a domain of size 10, with boundary conditions $u(x=0) = 1$, and $u(x=10) = 0$ and an initial condition $u(x,0) = 0.5(1 - \tanh(x/0.1))$. Determine how the propagation speed depends on D. You will need to determine how long to run the code in order to determine the propagation velocity. Provide a plot that shows the speed of the wave as a function of D.