Physics 307 Final Project
Due Tuesday, 15 December

Your final project is intended to be a capstone project both synthesizing the things you have learned and exploring something new.

Here I propose two projects to you in detail: examining the normal mode spectrum of the vibrating membrane, and examining the thermodynamics of a collection of atoms interacting by a simple potential. You can also propose your own projects that have a similar level of depth to these.

Students proposing a particularly in-depth project, or an extension of one of these projects that is in depth, can **omit the final exam**, spending the time they would have spent studying on making something nifty instead.

1 Thermodynamics

Atoms, in general, repel each other very strongly at short distances, but attract each other weakly at intermediate distances. A simple model for this sort of interatomic interaction is the Lennard-Jones potential,

$$V(r) = 4\varepsilon \left[\left(\frac{r_0}{r} \right)^{12} - \left(\frac{r_0}{r} \right)^{6} \right]$$

where ε is the "depth" of the potential well and r_0 is the characteristic distance at which the potential becomes strongly repulsive.

In this project, you will model a collection ($\mathcal{O}(10^2)$) of atoms interacting *via* this potential in a box, and look at values for the pressure and temperature averaged over a long time. For low densities and high temperatures you expect the ideal gas law $P = \frac{NkT}{V}$ to hold; away from this limit you will see departures from the ideal behavior.

The computational approach here is straightforward:

- In your gravity simulation, you learned to simulate two objects interacting by a distance-dependent force;
- In your string simulation, you learned to simulate a large collection of objects
- ... now you just put those two ideas together.

Here is one example of a set of things for you to explore. If you'd like to investigate something else, then we can modify the project as you wish.

1. Make the simulation work. First code it for just a few particles, and verify that it conserves energy. (As always, you will need to empirically determine how small of a timestep you need.) Once you have done this, see how many particles you can simulate before things bog down too much. Note that the work required to simulate N particles is proportional to N^2 per timestep, since you have $N(N-1)/2$ force pairs to evaluate!

2. Modify your program to track the time-averaged temperature and pressure. I will explain how to do this in class.

3. Qualitatively explore what happens as you vary the temperature kT and the particle density. You should see a drastic phase change from gas to liquid as the temperature decreases, and potentially a further one from liquid to solid.

4. Run a simulation at low density and high temperature, and compare your values of P vs. $kT\frac{N}{V}$ to the predictions from the ideal gas law.

5. Now run simulations for a variety of temperatures, going from your high temperature down past the critical point where you see condensation/freezing. Again plot P vs. $kT\frac{N}{V}$, and comment on the limits of validity of the ideal gas law.

6. Finally, run simulations at high temperature but at increasing densities (changing V). Again plot P vs. $kT\frac{N}{V}$, and comment on the limits of validity of the ideal gas law for dense gases. (You may find it interesting to read the Wikipedia page on the "van der Waals gas".)

7. At very low temperature, investigate what happens in the solid phase. There are lots of things you could do here; talk to me about ideas.

8. Simulate in 3D rather than 2D

9. Modify your code to not worry about the forces between particles that are very distant. This can *greatly* speed up your simulation; I will provide you some code to facilitate this. See if you get the same results as with fewer particles.

2 The vibrating membrane

In your previous assignment you simulated a one-dimensional elastic object oscillating in a second dimension. Here you will simulate a two-dimensional elastic object (a membrane) oscillating in a third dimension, and study the frequencies and character of the normal modes for both a square membrane and a circular one.

The square membrane is a straightforward extension of the vibrating string; here you will have a two-dimensional array of masses, with each point connected to its four neighbors.

The circular membrane works the same way. However, here you will need to modify your "boundary conditions"; rather than having only the edges unable to move, you will need to ensure that only points within a circle move.

Again, here is one example of a set of things for you to explore. If you'd like to investigate something else, then we can modify the project as you wish.

1. Simulate the square membrane. Animate your simulation, and verify that energy is conserved.

2. As with the vibrating string, modify the initial conditions of your simulation to simulate a normal mode of your choice. Do so for a variety of normal modes, and note their periods/frequencies. (You can determine the period using the same tricks as for the vibrating string.) What mathematical formula gives you the period of the $(n_x, n_y$ normal mode?)

3. Now, modify your initial conditions to apply a Gaussian deformation, with variable amplitude, width, and location, as your initial condition. Qualitatively, how does the observed behavior depend on these parameters?

4. Now, modify your code to simulate a circular membrane. This is actually not that hard; you can just not move particles outside a central circular region, just like you aren't moving the edges of the square.

5. Investigate the normal modes of the circular membrane. You can do this in one of several ways, which we will discuss in class.