In this problem set, you will do only one problem.

However, your solution is to be a video/screencast/voice-over that gives a “how-to” to solve the problem you have chosen. The video should be about 6 minutes long: Some of the first four minutes should describe how you set up the problem and solved it; at least the last two minutes should be used to give a visualization of the physical problem that you have solved.

You should upload your video to your MIT athena webpage. This is accessed like this example: [http://mit.edu/~ccarter/www/](http://mit.edu/~ccarter/www/) You would use your own athena username of course. The video should be placed in the www directory on your athena account [http://stuff.mit.edu/doc/how-to-hp.html](http://stuff.mit.edu/doc/how-to-hp.html).

The videos will be based on several criteria including:

- Clarity of explanation.
- Quality of teaching to the audience.
- Creative use of graphics.
- Quality of video.
- Ability to capture interest and inspire the audience.
- Accuracy and facts of the video content.

I will select several winners for based on various merits of the videos. I will screen selected videos during a pizza night during finals week—as well as some other short science videos that Rachel and I like. If you would would like me to post your videos, please send me an email giving me explicit permission to do so.

There is no group problem for this problem set.

Some advice for software can be found here: [http://www.makeuseof.com/tag/how-to-create-a-screencast-pro-6-free-online-tools/](http://www.makeuseof.com/tag/how-to-create-a-screencast-pro-6-free-online-tools/)

On a mac, there are tools like iMovie and QuicktimePlayer to help you combine screencasts and video. There are some online tools such as [http://www.screencast-o-matic.com/](http://www.screencast-o-matic.com/) I don’t
know what tools are available specifically for Windows. The class can make a proposal for some specialized software, and I will see if we can purchase a license for everyone to use.

I will select several winners for based on various merits of the videos. I will screen selected videos during a pizza night during finals week—and Rachel and I will show some other examples of short science videos with which we have been involved. If you would like me to post your videos, please send me an email giving me explicit permission to do so.

There is no group problem for this problem set.

The following two problems are examples of the kinds of problems you might solve. You could choose one of these two. However, I encourage you to construct your own problem which you will describe and present in your video. The following problems are representative of the complexity and length that you use as a guide to select your own problem.

Your video will be worth 400 points.
Example Problem I

Part 1

The purpose of this exercise is to simulate the motion of a buoy in a tidal basin. As a model, consider the following figure.

![Tank with Bouy Diagram](image)

A tank with a bouy floating on top of a volume of water.

Water is pumped in a rate given by $V(t) = A \sin(\omega t)$. The density of the bouy is a fraction $\phi$ that of the water. At time $t = 0$, the bouy is at its equilibrium position and $b(t) = 4\lambda$ and $h(t) = 8\lambda$ where $\lambda$ is the length of the bouy. The radius of the tank is $R$ and the radius of the bouy is $r$. This problem begs to be non-dimensionalized.

Find the equations of motion of the bouy and the height of the water. Assume that there are no viscous effects. Plot a $\beta(t)$ on a vertical axis and $h(t)$ on the horizontal axis. Characterize the case conditions and time that the bouy leaves the surface of the water.

Part 1

The purpose of this exercise is to simulate the motion of a buoy in a basin with a viscous buffer. As a model, consider the following figure:

![Inlet Tank and Basin Diagram](image)

An inlet tank (left) connected to a basin (right) with a porous filter. A bouy and the right basin have the same properties as the above.

The inlet tank has radius $\lambda/2$ and is initially filled to a height $\lambda$. Water flows from the left tank to the right tank according to Darcy’s law: $\dot{V}_{\text{trans}} = \alpha (P_{\text{left}} - P_{\text{left}})$.

Find the equations of motion of the bouy and the height of the water. Plot a $\beta(t)$ on a vertical axis and $h(t)$ on the horizontal axis. Characterize the case conditions and time that the bouy leaves the surface of the water.
Example Problem II

The purpose of this problem is to compute entropy and Helmholtz free energy for a fairly simple system.

Consider a square lattice where each lattice point can be occupied by an atom or a vacancy. We will develop a simple model for the energy of the lattice based on the following rules:

- If two atoms are located side-by-side (i.e., up-down or left-right) then the system has bonding energy of -1.
- If two atoms are located corner-to-corner (i.e., diagonally) then the system has bonding energy of -1/2.
- If two atoms are not touching along the side or corner, then the energy is zero.

![Energy counting scheme for square lattice model.](image)

Suppose the square lattice is \( N \times N \) and that less than 25\% of the sites are filled with atoms.

This problem can be computationally intensive—the time will become large quickly with \( N \) and with the concentration of atoms. A clever energy counting algorithm will help very much.

The first goal is to calculate the internal energies for a given configuration of a given concentration of filled sites on a square lattice. All of the internal energy is assumed to be due to the bonds. It is easier to ignore edge effects (i.e., what happens when a filled site lies at the edge of a square lattice), although you should explain how you treated the edges.

The second goal is to calculate the energies for very many random samples of a fixed concentration and keep track of the energies. Here is an example:

![Histogram of the number of states near each energy for a \( 50 \times 50 \) square lattice with 200 filled sites obtained from 5000 random samples. This calculation took about 10 minutes for WCC to calculate using ParallelTable.](image)
Boltzmann’s formula for entropy is

\[ S(U) = k \log \Omega(U) \]

where \( \Omega(U) \) is the number of ways the system can be arranged and have internal energy \( U \). Therefore, the histogram provides a way to compute the system’s entropy. Because it would take a very very long time to calculate the energy of all possible configurations, this entropy can be estimated by obtaining many random samples and assuming that enough random samples produces a curve that is similar to the complete set of configurations.

In this problem, we will only pay attention to the part of the histogram where the number of states is increasing with energy. (The part where \( \partial \log(\Omega) / \partial U \) is negative corresponds to negative temperatures—which is a real effect, but derives from the fact that we are dealing with a small finite system).

From these internal energies, the entropy will be calculated from Boltzmann’s formula. Derivatives of entropy with respect to internal energy will be used to determine the temperature. From the temperature, entropy, and internal energy, the Helmholtz free energy will be computed: \( F = U - TS \).

\( i \): It would be very tedious to work out a formula for all the possible energy states for a selected number of atoms \( M \), it will be much easier to simulate it. Each random sample is called ‘trial’. Repeat this process over and over until you have constructed a distribution (histogram) of energies as that illustrated above.

\( ii \): Turn your histograms into probability distributions by dividing by the total number of trials; thus the area under the curve must be 1. Fit the probability distribution with an appropriate function to find a form for \( p(U, X_+) \) for several values of \( X_+ \).

\( iii \): The total number of configurations of \( M \) objects and \( N^2 - M \) vacancies is given by:

\[
\text{configurations}(M) = \frac{(N^2)!}{M!(N^2 - M)!}
\]

\[
\log(\text{configurations}(M)) = \log(N^2!) - \log((N^2 - M)!) - \log(M!)
\]

which can be approximated with Stirling’s formula: \( \log N! \approx N \log N - N \). Therefore, \( \Omega(U, M) = p(U, M)\text{configurations}(M) \)

\( iv \): Fit the portion of the curve where the number of states is increasing with energy, and for that portion of the curve find a relationship between the equilibrium temperature, entropy, and internal energy.

\( v \): Plot the equilibrium values internal energy (\( U \)), entropy (\( S \)), and Helmholtz free energy (\( F = U - TS \)) as a function of temperature \( T \).

\( vi \): Visualize example configurations for different temperatures and explain the correlations between the microstructure and the temperature.