Physics 281 – Computational Physics

Project 1 Instructions

Grant Wilson - Fall 2013

Project 1 – Simulation of an Ideal Gas

In this project you will construct a simulation of an ideal gas as a random walk process. The background for this project is presented in the lecture notes from Class 10. These instructions provide details on what you will be doing and what must be submitted for grading. There are two final products that you will submit:

1. The main set of simulation code that you write as a group; and
2. A project report that each student writes individually.

The final simulation code for this project will be somewhat complex. It is always a good idea to build-up to a complex final product by performing a series of simpler calculations that you know the answer to. In the instructions that follow I will try to guide you step by step to the final product.

Sub-project 1.1 – simulating a 1-d random walk.

Your first task will be to simulate a 1-d random walk of a single particle. A random walk is a path followed by an object if it chooses its direction at each step randomly. Here we will practice a random walk in 1-dimension. Create a simulation of a particle that has the following properties:

1. It is constrained to move on the x-axis
2. It can only take steps of size d (you choose what d is)
3. In takes steps in the positive-x or negative-x direction randomly and with 50% probability for each direction.

Show that if you do this experiment many times, each time with N-steps, that if you measure the total displacement of the particle each time, the root-mean-square displacement of the particle is $d\sqrt{N}$, that is for step-size d,

$$\sqrt{\frac{1}{N}\sum_{i=0}^{N-1} displacement_i^2} = d\sqrt{N}$$

Show this by making a plot of your simulation results for N=[50,100,500,1000,2000]. For some more reading on 1-d random walks check out:
http://www.mit.edu/~kardar/teaching/projects/chemotaxis(AndreaSchmidt)/random.htm

Sub-project 1.2 – simulating a 2-d random walk.

Now that you've got the 1-d random walk under your belt, try the same thing in 2-d. In this case you will need to keep track of both the x- and y-coordinate of your particle. Again, the step size will be d but you will need to introduce an angle, chosen at each step to be between 0 and 2pi, that will set the direction of the particle after each step.

Perform the following simulation:

1. Start your particle at the origin of your coordinate system.
2. Choose a direction (on the interval [0,2pi)) and move the particle a distance d in that direction.
3. Repeat step 2 N-times.
4. Measure the total displacement of the particle from the origin.
5. Repeat steps 1 through 4 many times and show that the root mean square displacement of the particle after many trials is $d\sqrt{N}$. Again, show this for N=[50,100,500,1000,2000].

Sub-project 1.3 – bouncing a particle off a wall.

In the simulation you will need the machinery to properly reflect a particle off of the walls of your box. Demonstrate that you have this right by doing the following for a single particle and a single wall:

1. Place your particle at x=0, y=0. Place walls in your box at $x = \pm 10$ and $y = \pm 10$.
2. Choose a direction for your particle on the range [0,2pi) where 0 is the x-axis.
3. Move your particle 1000 steps of step-size=0.1, starting in the direction chosen in step 2. Reflect the particle off each wall it hits as described in the class notes.
4. Show the particle trajectory in a plot that convinces the graders that the particle is bouncing properly.

Sub-project 1.4 – calculating Entropy.

The best measure that the particles in your simulation have come to equilibrium is the entropy. A system in equilibrium has constant entropy. To compute the entropy, you will need to divide the area in your box into a number of cells and count the particles in each cell. The probability of finding a particle in a cell at each time step *i* is just the number of particles in the cell divided by the total number of particles. Let P_i be the probability for cell *i*, then the entropy S is:

$$S = -\sum_i P_i \ln(P_i)$$

Build the machinery to calculate the entropy in a 20x20 box with 1000 particles randomly placed inside and using cells that are 2x2 in size. Place the particles in the box in two different ways:

1. Drawing the x and y positons at random from a uniform distribution; and
2. Drawing the x and y positions at random from a normal distribution centered in the center of the box.

Do this many times (placing the particles in the box differently each time) and calculate the mean and standard deviation of the entropy in each of the two cases.

The Main Simulations

There are three main simulations that you will carry out. In each case, the main observables will be the entropy of the gas and the pressure (see the class 10 notes for how to calculate the pressure). The accuracy of your calculations will depend strongly on the number of particles in your simulation. You will need to select a total number of particles that will give an accurate reading for entropy and pressure ... especially pressure since that is what we calculate in the specific cases assigned. Be sure to describe how you determined the number of particles in your simulation in your report.

In each simulation you will use a box of size 20x20 and centered at the origin. Use the time-steps, molecule masses, mean free paths, and velocities described in the class 10 notes.

Simulation 1 – Diffusion of an Ideal Gas

First we want to look at the diffusion of molecules of different mass. We will use the case of hydrogen gas (H_2) and nitrogen gas (N_2). Release each substance at the center of the box and observe the amount of time needed to achieve equilibrium, as measured by the entropy value. Make a plot of the entropy of both H_2 and N_2 as a function of time. Report the results and describe the relationship between this equilibrium time and the mass of the particle.

Simulation 2 – The Ideal Gas Law

Second, we wish to verify that our simulation follows the ideal gas law. In this case you will start off the simulation with all particles having random positions inside the box. There are two aspects to consider:

1. Try your simulation with the same number of particles, but different volumes, and show that pressure is inversely proportional to volume.
2. Try changing the speed of the molecules in several simulations to find the relationship between speed and pressure for a fixed volume. What is that relationship? How does it compare to our understanding of relationship between speed and temperature.

Simulation 3 – The Palladium Membrane

Finally we wish to simulate the problem with the palladium membrane described in class. The membrane allows H2 molecules to pass, but does not allow N2 to pass through the membrane. Start the simulation with pure H2 on one side and pure N2 on the other. What happens to the total Pressure on each side of the Foil membrane? How does the pressure difference between the sides depend on the number of N2 molecules on the left side?

Submitting the Assignment

Your project materials will be submitted in two ways.

1. Group Work – As a group, write the code for the simulations and sub-projects. Submit the final code on the class Moodle page under "Group Submissions."
2. Project Reports – Each person should write up their own project report individually. Project report guidelines are given on the class Moodle page and should be reviewed before your report is produced. Submit your final report by 9am on 17 Oct. using the "Individual Submission" assignment on the class Moodle page.

Getting Help!

If you find you are struggling with any part of the project, contact the TAs and/or Professor Wilson and set up a meeting. Our email addresses are:

- Yuping Tang (yupingt@astro.umass.edu)
- Seunghwan Lim (shlim1206@gmail.com)
- Grant Wilson (Wilson@astro.umass.edu)