PHYS 114 Contemporary Physics II - Rec 4

February 11, 2008

Under Pressure

This is a simple assignment to calculate the temperature dependence on pressure for an ideal gas computationally. To do so, we are going to assume a Maxwell-Boltzmann distribution of speeds:

$$v = v_x\hat{\imath} + v_y\hat{\jmath} + v_z\hat{k} \tag{1}$$

Where each one of the v_x, v_y, v_z are initially drawn from the probability distribution:

$$f(v_x) = \sqrt{\frac{m}{2\pi kT}}\exp\left(-\frac{m}{2kT}v_x^2\right) \tag{2}$$

Which can be rewritten as (with $\sigma = \sqrt{\frac{kT}{m}}$):

$$f(v_x) = \frac{1}{\sigma\sqrt{2\pi}}\exp\left(-\frac{v_x^2}{2\sigma^2}\right) \tag{3}$$

This is clearly a Gaussian distribution. Given a σ, how do we generate random Gaussian numbers? We will be using a trick called the Box-Muller transform. It goes as follows, generate two uniform random numbers between 0 and 1, $a, b = (0, 1]$. Now the generated number c will be drawn from a standard normal distribution:

$$c = \sqrt{-2\ln a}\cos 2\pi b \tag{4}$$

Its ugly, but it works. Lets test this out. Generate 10^5 Gaussian random numbers and plot them from pylab (remember to import!) using the commands:

```
hist(X,30); show()
```

Where X is variable name of your list of random Gaussian numbers. If the plot looks like a Gaussian, you're ready to move on. You'll notice that the numbers generated have $\sigma = 1$ so we need to rescale them. The rescaling of:

$$c' = \sigma c \tag{5}$$

This will give you the distribution of a Gaussian with a standard deviation of σ.

Now generate $N = 350$ hydrogen atoms in a box with a side length of $L = 1m$. Make each component of their velocity a Gaussian random number. Initially set the temperature at $T = 300K$. The atoms will be considered an ideal gas in a vacuum, their only change in momentum should be the collision with the walls. From this I would like you to calculate the average pressure on the box by using the formula:

$$\bar{P} = \frac{\bar{F}}{A} = \frac{\Delta p}{\Delta t}\frac{1}{A} \tag{6}$$

Make the simulation run long enough so that your result is independent of the simulation time. Once you are satisfied with your result, your objective is to plot:

- The dependence of pressure as a function of temperature $T = [300, 1000]$ in intervals of 40K

You will only be graded on the final plot, an animation of the system using visual Python is not necessary (and would take to long!). Your final plot will not be smooth (why?), but it should display a general trend. What could you do to make the plot smooth? Also, what can you conclude about the pressure dependence on temperature?