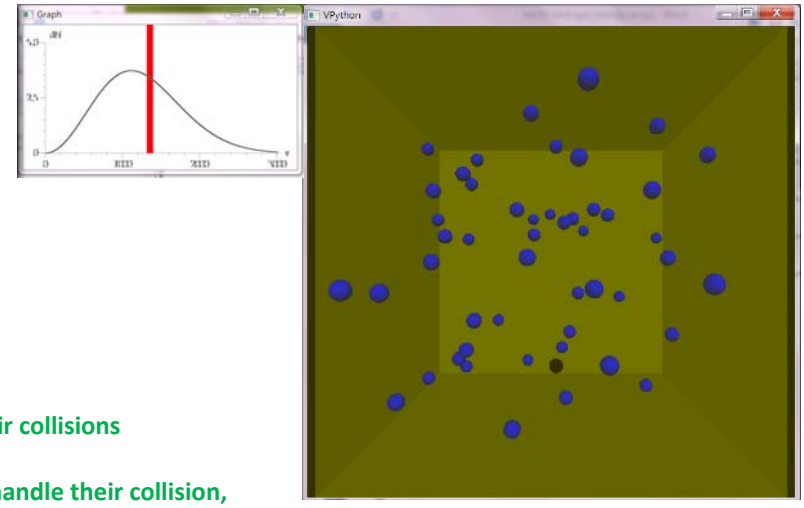
Computer Work Unit 10 Gas, Pressure and mean-free-path

In the homework we will simulate a gas system consisted 50 He atoms in a box of side length *L* at temperature *T*. Your mission is to find the pressure, and the mean free path between collisions of the atoms. The following is the template code.

```
from visual import *
from random import random                    # random module for generate random numbers
from visual.graph import *

N = 50                                       # number of the He atoms
L = ((24.4E-3/(6E23))*N)**(1/3.0)/2          # side length of the cubic container box
m, size = 4E-3/6E23, 310E-12                 # He atoms mass, radius are made 10 times bigger for easiear collision
L_size = L-size                              # L – size, used many times in the program
k, T = 1.38E-23, 298.0                       # k = Boltzmann constant, and T = temperature in unit K
t, dt = 0, 0.5E-13                           # dt = 0.5E-13 second
vrms = (3*k*T/m)**0.5                        # root mean square velocity at T
atoms = []                                   # list to contain the 50 atoms

# histogram initialization, more on this see http://vpython.org/contents/docs/graph.html
deltav = 100.
vdist = gdisplay(x=800, y=0, ymax = N*deltav/1000.,width=500, height=300, xtitle='v', ytitle='dN')
theory = gcurve(color=color.cyan)            # This line and the following 3 are to plot the theoretical speed distribution
dv = 10.
for v in arange(0.,3001.+dv,dv):
    theory.plot(pos=(v,(deltav/dv)*N*4.*pi*((m/(2.*pi*k*T))**1.5)*exp((-0.5*m*v**2)/(k*T))*v**2*dv))
observation = ghistogram(bins=arange(0.,3000.,deltav),accumulate=1, average=1, color=color.red)    # setup for histogram

# initialization of display, setting up for the random position distribution and random velocity direction of atoms
scene = display(width=800, height=800,background=(0.2,0.2,0))
container = box(length = 2*L, height = 2*L, width = 2*L,    opacity=0.2, color = color.yellow )
for i in range(N):
    position = vector(-L_size+2*L_size*random(),-L_size+2*L_size*random(),-L_size+2*L_size*random())
    if i== N-1:
        atom = sphere(pos=position, radius = size, color=color.yellow, make_trail = True, retain = 600)
    else:
        atom = sphere(pos=position, radius = size, color=(random(), random(), random()))
    ra, rb = pi*random(), 2*pi*random()
    atom.m, atom.v = m, vector(vrms*sin(ra)*cos(rb), vrms*sin(ra)*sin(rb), vrms*cos(ra))
    atoms.append(atom)

def vcollision(a1,a2):                       # function to find the velocities of atoms after each collision
    v1prime = a1.v - 2 * a2.m/(a1.m+a2.m) *(a1.pos-a2.pos)    * dot (a1.v-a2.v, a1.pos-a2.pos) / abs(a1.pos-a2.pos)**2
    v2prime = a2.v - 2 * a1.m/(a1.m+a2.m) *(a2.pos-a1.pos)    * dot (a2.v-a1.v, a2.pos-a1.pos) / abs(a2.pos-a1.pos)**2
    return v1prime, v2prime

while True:
    t += dt
    rate(1000)

#calculate new positions for all atoms and plot histogram
    v=[]
    for i in range(N):
        #### calculate new positions for atoms
        v.append(mag(atoms[i].v))
    observation.plot(data=v)

#### find collisions between atoms, and then handle their collisions

#### find collisions between atoms and walls, and then handle their collision,
####       and then you will calculate the momentum transferred to the walls and obtain the resulted pressure

#### print the averaged pressure on the walls every 1000*dt
```



Homework submission:
Step (1): Finish the codes marked by ####. You will find:
1. The pressure is around 107000 (unit: Pa). This is larger than the pressure for idea gas at this temperature and density. The reason is that we use larger size of atoms. You can modify the atom size to the real size of He atom of 31 pm (31E-12) and get a better result, but then the atoms rarely collide and it takes very long time to reach the equilibrium state.
2. You will see that the speed distribution histogram approaches the theoretical Maxwell distribution when the gas reaches the equilibrium.

Step (2): Add some codes to find the mean free path of the atoms. Free path is the distance one atom travels between two consecutive collisions with other atoms (this means that the collisions of the atoms with the walls are not considered for calculating the free path). Obtain every free path of all atoms, average them, and print the mean free path every 1000*dt. Compare your mean free path to the theoretical result $\ell = \frac{V}{\sqrt{2}\pi d^2 N}$, where V is the volume of the container, N the number of particles contained, d =2*size= the diameter of the atoms.

Note (not for submission): What do you find from this simulation? You can add or test many other features to this program, such as
(1) adding interaction force between atoms
(2) adding gravitational potential
(3) changing the size of the atoms
(4) compose pairs of atoms to make molecules