# 10 – Project 1 Introduction Simulation of an Ideal Gas

Phys 281 – Class 10

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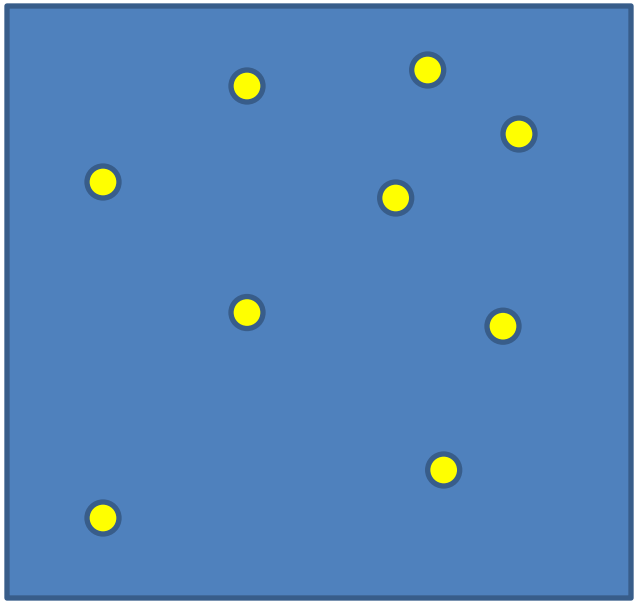
# Project Goals

- Simulate a 2-d random walk of a large number of particles.
- Introduce boundary conditions (walls!)
- Calculate physical quantities of the ensemble of particles based on a statistical representation of a reasonable number of particles.
- Confirm the expected behavior of an ideal gas.

# Our model

- Ignore particle size – treat all particles as points
- Treat collisions between particles in a statistical sense through the random walk, not directly.
- Particles will have elastic collisions with the walls – counting these will lead to our estimate of the pressure.
- Particles will move at a single, constant speed.
- Simulate a 2-dimensional box to keep things simpler.



# Physics to be Included

- Temperature – this is determined by the particle speed.

- Pressure – this results from collisions of the particles with the walls.

- Ideal gas law:

$$P = nkT$$

- The concept of a mean free path (see below)

P = pressure, n = N/V (number density of molecules) and T is temperature.

# Particle-Particle Collisions

- Simulating all the particle collisions would be too big a job. Instead, us the concept of the mean free path.

- The mean free path is the typical distance a molecule travels between collisions.
  - depends on cross-sectional area of molecules
  - density of molecules
  - velocity of molecules

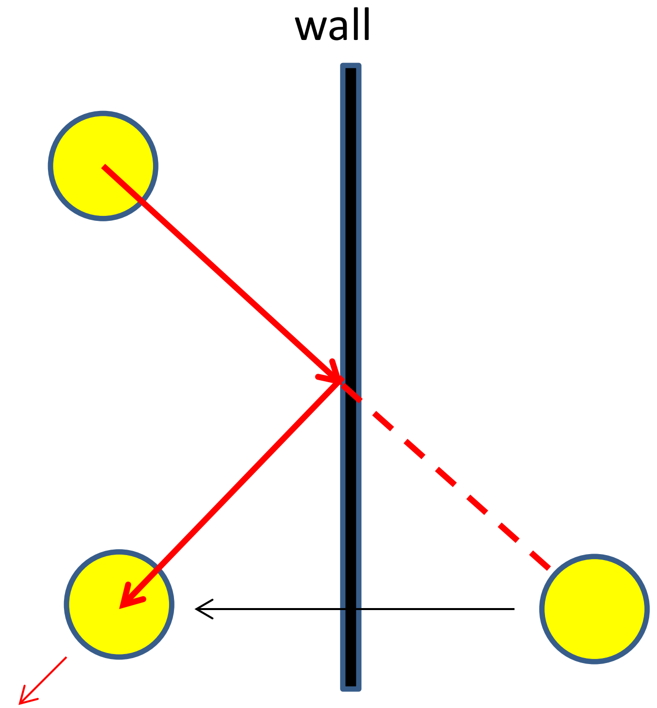
- The probability that a particle will undergo a collision in distance x (where x<<MFP) is

$$p(x) = x/MFP$$

- After collision, the molecule goes off in a random direction and with the same velocity as it had before the collision

# Particle-Wall Collisions

- This we must deal with directly.
- Check the positions of all particle after each time step.
- Any particles beyond the walls must be re-placed inside the box.
- Use reflection (see cartoon) to reset the particle.
- Count the collisions with the walls to calculate the pressure.




Move to mirror image point when step takes molecule beyond the wall. Don't forget to mirror the velocity vector too!

# Particle Velocity

- In an ideal gas of molecules, the particles have a broad distribution of velocities (drawn at random from a Maxwell Boltzmann distribution).
- Here, we will approximate all particle velocities in terms of a single number "c" which we will take to be the velocity of $H_2$ molecules. [NOTE: c is NOT the speed of light!]
- The velocity of other molecules, such as $N_2$, will scale as:

$$v_{\{N2\}} = c\sqrt{\frac{m_{\{H2\}}}{m_{\{N2\}}}}$$

# Simulation Strategy

- This is a time-based simulation, so we will calculate the entire state of the system (all the particle positions, velocities, etc.) in small discrete time steps.

- At t=0, start the simulation with all the particles in the "initial conditions" positions (see below) and random velocity orientations.

- At t=dt, all the particles have moved a distance of $x = cdt$
  - We want this distance to be much smaller than the MFP so that we can honestly model collisions, that is, $x = cdt \ll MFP$
  - Ask two questions of each particle:
    - Has the particle hit another particle?
    - Has the particle hit a wall?

# Has a particle collided with another particle?

- This is a random process so we simulate the probabilities.

- The probability of a collision is $p = \frac{x}{MFP}$

- For each particle, draw a uniform deviate, u, on [0,1).
  - If u<p then  the particle collided with another particle.  Set a new random direction for the particle.
  - Otherwise, continue on in the same direction.

# Has a particle hit a wall?

- This is straightforward, is the particle outside of the box?
  - If so, reflect the particle back into the box and appropriately change its velocity direction.
  - Count the number of particles that hit a particular wall during each time step.

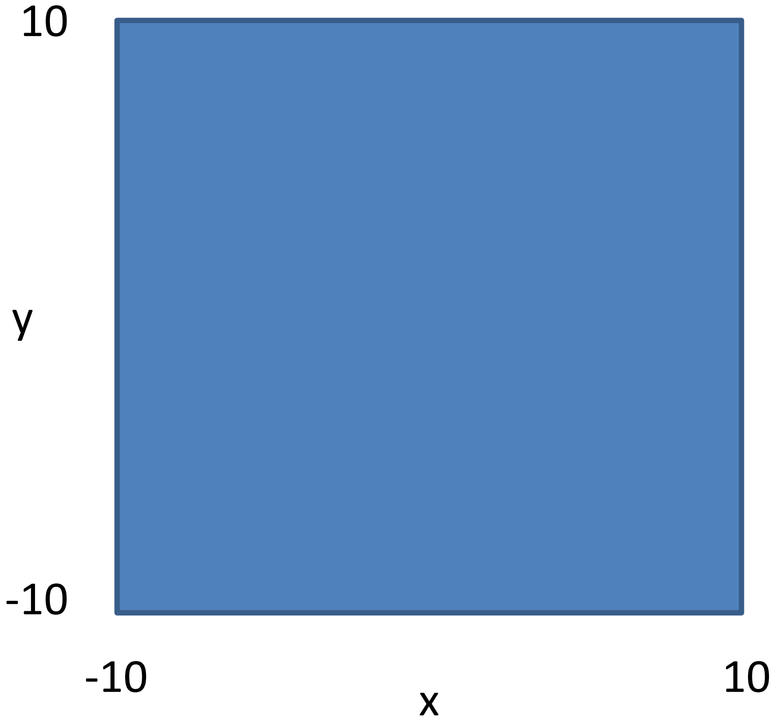
# Units and Values

- Unit of length: MFP of a Hydrogen Molecule
- Unit of time: time it takes H2 to move one MFP = MFP/c. Note that this makes c=1 in these units.
- Each time step, dt, should be small compared to one time unit
  - try $dt = 0.5$ – this makes $dx = cdt = 0.5$ (in MFP units)
  - then probability of collision is $p = \frac{x}{MFP} = 0.5$
- We will also consider $N_2$ whose mass is 14 times that of $H_2$
  - c(N2) = c(H2)/sqrt(14)
  - Probability of collision for $N_2$ is 0.425 times probability of collision for $H_2$ in the same time step based on size and speed of N2 relative to H2.

# The Box

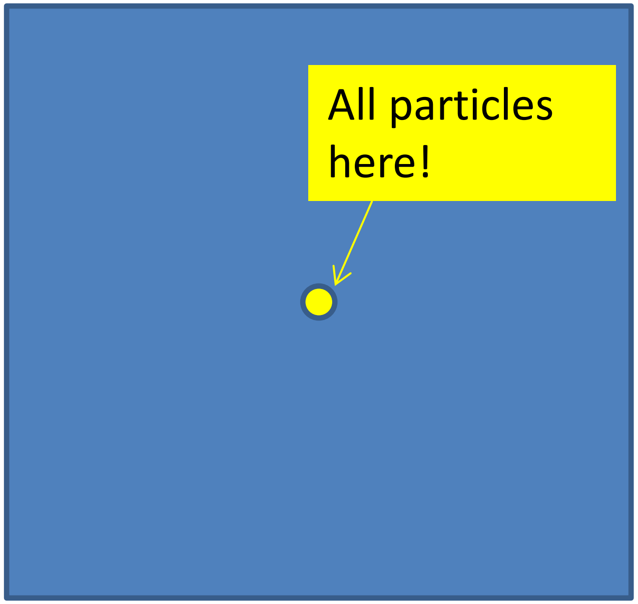
- Us a box with dimensions 20x20 (in MFP units)

- This is small but a larger box would require much longer to compute.

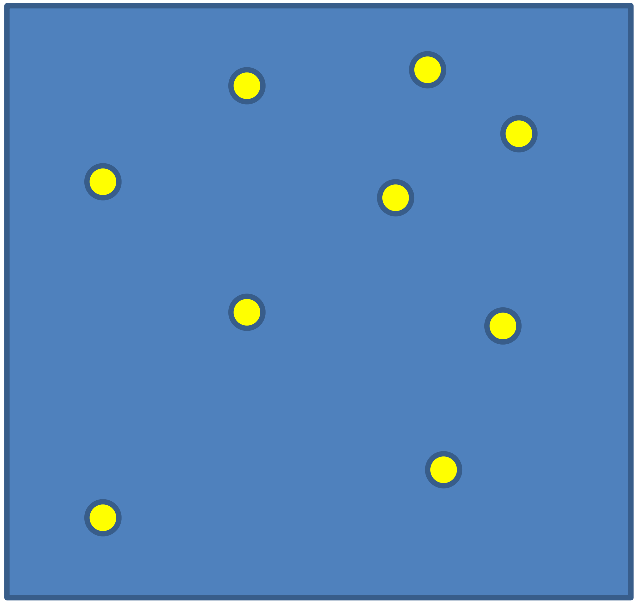


# Initial Conditions

1. Start all molecules at the center of the box, with random initial directions.




2. Place molecules at random positions throughout the box with random initial directions.



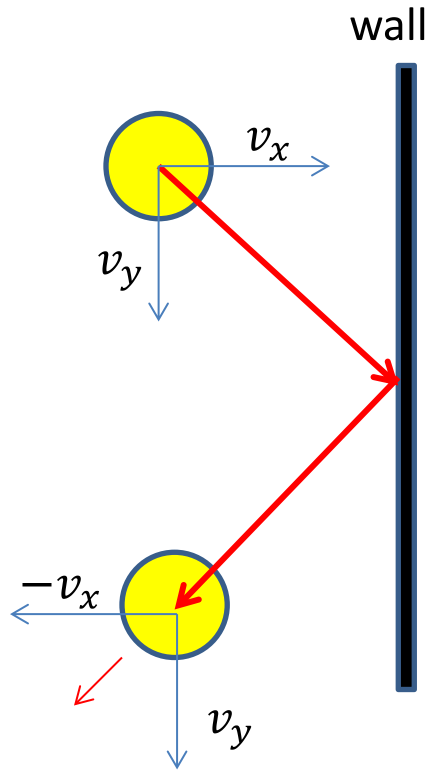
# Measuring Pressure

- Collision with wall results in transfer of momentum between particle and wall.

- For each collision in time step dt, the change in momentum is
$$dp = 2mv_x dt$$

- For N collisions in dt, the force on the wall is
$$F = N\left(\frac{dp}{dt}\right)$$

- Pressure is F/Area of wall

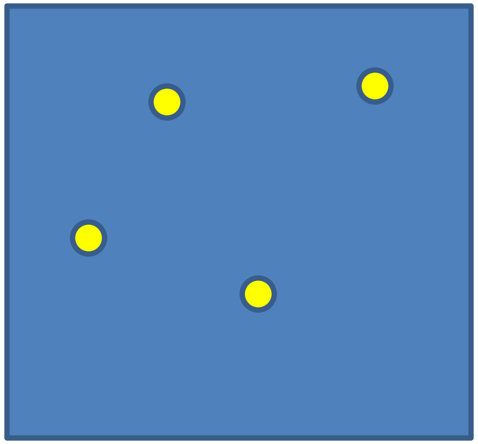


# Entropy

- Entropy is a measure of
  - probability of achieving a particular configuration
  - randomness, or disorder, in the system
- Definition:
  - If there are many different states, i, in our system, let $P_i$ be the probability of a particle being in state i.
  - The system entropy is

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

Not likely - Ordered



More likely - Disordered

# Measuring the Entropy

Consider each small area a state (there are 25 states here)

$N_i$ = # of molecules in subbox *i*

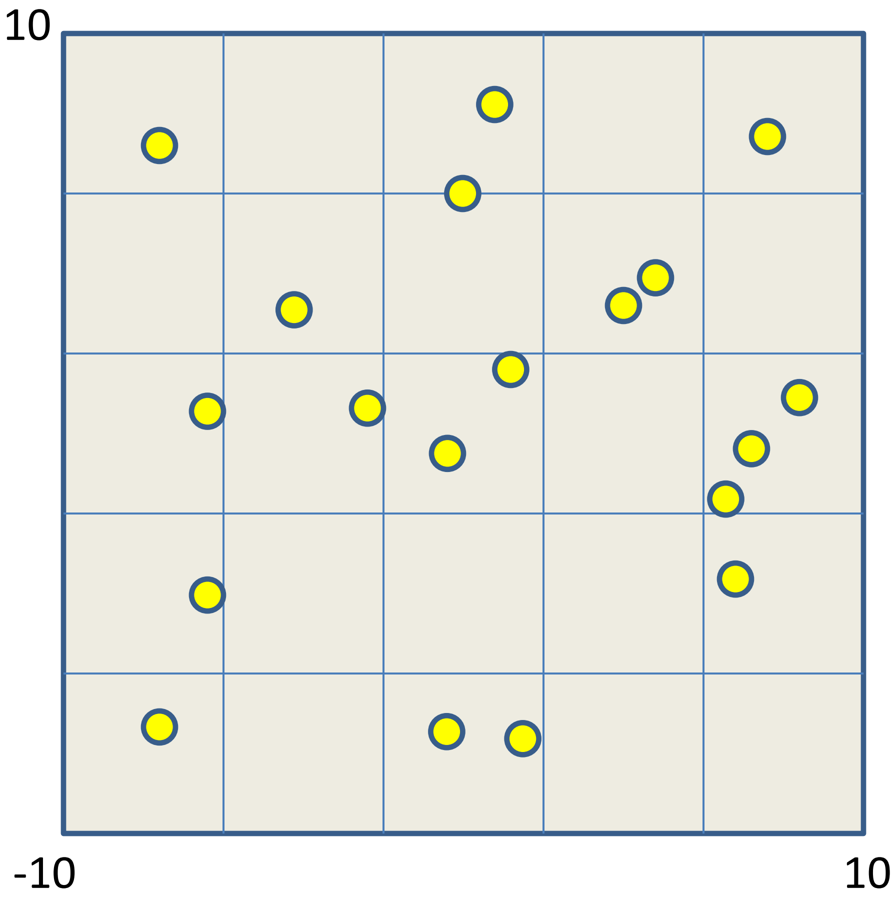
The probability of there being a molecule in subbox *i* is then

$$P_i = \frac{N_i}{N_{total}}$$

The entropy of the system is

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

When the system is in equilibrium, the entropy is constant in time.



# Questions to Answer

1. Time-scales of diffusion of $H_2$ and $N_2$
   - Start with all particles at the center of the box
   - Run the simulation until equilibrium (entropy no longer changing).
   - Note time required to reach equilibrium.  How does this scale with the molecule mass?

2. Confirm the Ideal Gas Law
   1. Show that the pressure is proportional to the number density of molecules in your box.
   2. Show that the pressure depends on the speed of the molecules – what is the proportionality?

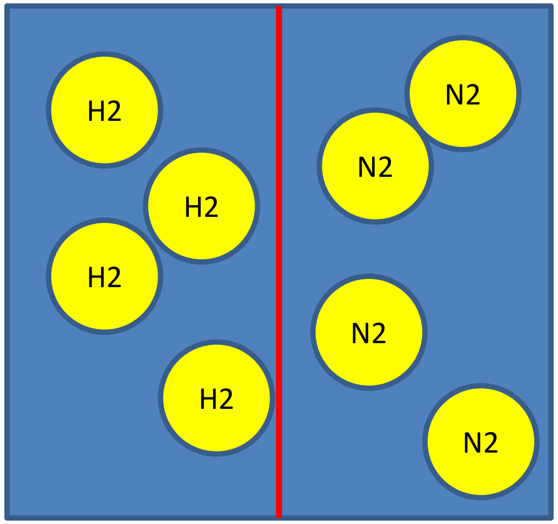
# Questions to Answer (continued)

3. Now reproduce a famous experiment!

   1. Place N2 and H2 molecules on opposite sides of a palladium foil membrane.

   2. Palladium allows H2 to pass through but is a wall to the N2

   3. Run your simulation and report on what happens.




Questions:

1. What happens to the total pressure on each side of the membrane?

2. How does the pressure difference between the sides depend on the number of N2 molecules on the right side?