

Worcester Polytechnic Institute

Physics Minor Capstone Project

Simulation of Gas Kinetics

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# Abstract

The Kinetic Theory of Gasses developed by Maxwell and Boltzmann relates the emergent macroscopic properties of gasses, such as temperature and pressure, to the fundamental kinetic particle interactions as microscopic levels. The Maxwell-Boltzmann distribution for particle velocity is the probability density function that, for a gas with specific macroscopic properties, gives the probability that any given gas particle will have the given velocity. It assumes the components of the three dimensional velocity vector are normally distributed with a mean of zero, such that the gas has zero net momentum in any direction. Related distributions exist for the kinetic energies, momentum, the components of velocity and momentum in a given dimension, and the absolute magnitudes of the velocity and momentum.

# Introduction

The kinetics and interactions of idealized gas particles constrained within a box container are simulated and visualized over time. The momentums and kinetic energies of the particles are recorded and displayed in real-time plots, as are the temperature and pressure of the gas, calculated using kinetic gas theory. These results are compared to the expected behavior from the ideal gas law. In addition, the gas particles are allowed to effuse through a circular opening in one side of the container, and their effusion rate is likewise calculated and displayed. This rate is then compared to that expected by the gas effusion equation.

# Kinetic Theory

The kinetic theory of gasses makes several assumptions: particles obey Newton’s laws of motion, they undergo ideal elastic collisions with other particles and any container, no other forces (electric force between particles, the effect of magnetic fields, gravity, etc.) are considered, and the number of particles is large with sufficiently large space between them.

## Between Two Particles

Completely elastic collision of ideal gas particles in one dimension are governed by two primary laws: the conservation of momentum and the conservation of kinetic energy. For the two particle case, where particle of mass and initial velocity collides with particle of mass and initial velocity , the conservation of momentum states that the total initial momentum after the collision must equal that before the collision.

Similarly, the conservation of kinetic energy states that the sum of the kinetic energies must be constant before and after the collision.

When the masses and initial velocities are known, this system of equations can be solved for the final velocities for each particle (ignoring the trivial case where there is no collision and the final velocities are the same as the initial velocities.)

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For collisions between particles in two or three dimensions, this one dimensional relation holds for the components of the velocities along the line through the centers of mass of the particles (common normal, assuming spherical particles with uniform density.) The other components of each particle’s velocity remain unchanged.

The line is derived from the three dimensional positions of the centers of the particles. The vector connecting the centers is

And the unit in the direction of is then

The component of a particle ’s velocity on to this line is given by vector projection

Or in matrix form for three dimensions

The remaining component of the velocity that is perpendicular to is the vector rejection , the difference between the total velocity and the component along .

The final velocity vectors of each particle after a collision are the sum of the unaffected rejection velocity and the new velocity along the line of collision.

## Particle-Container collisions

Idealized collisions between particles and the walls of the container also obey the conservation of momentum and the conservation of kinetic energy. When the container is fixed, such that its velocity momentum and kinetic energy are always zero, both laws will the same solution for the resulting velocity of the particle: the component of velocity normal to the wall will be inverted after the collision. For a wall with normal along , the component of a colliding particle’s velocity will be

# Pressure

By newton’s law of collisions, the average force on a container wall is equal to

Where is the average particle velocity along the normal vector of the wall, is the distance from that wall to the opposite wall, is the number of particles in the container, and is the mass per particle.

The pressure of a gas in terms of the kinetics of it’s constituent particles is derived from its definition as Force per unit area. For any wall of the container, the pressure at any given time is equal to the average force distributed over its surface area.

# Implementation

The simulation is run over discrete timesteps. For computational simplicity, all physical quantities that are constant over the duration of the simulation are computed with a value of 1 unless otherwise noted. Thus the simulation is not numerically accurate for any particular unit system, but relations between quantities will still hold. At each time step, the following is calculated:

1. Movement update: Particle positions are updated by adding the product of the timestep (1 unit time) and their velocity (unit distance per unit time) to their previous position.
2. Effusion: If effusion is turned on, any particles colliding with the hole are removed
3. Particle-Particle Collisions: Every combination of remaining particle pairs (N choose 2) is checked for the collision condition.

Where is the Euclidian distance between the centers of the particles and is the sum of their radii.

For all pairs of particle, and , that are in collision:

* 1. Calculate the line between the center positions of A and B as
  2. Divide this line vector by it’s normal to get the unit vector from in the direction of .
  3. Project the velocities of each particle on this unit vector to find the components along the line. This is the normalized line vector times the dot product of itself and each velocity.
  4. Find the remaining (rejected) components as the differences of the original velocities and the projected components.
  5. Find the norm of each projected velocity. Because this method of finding scalar projected vectors only produces magnitudes, the signs are adjusted relative to the line vector.
  6. Calculates the corresponding components of the momentums of each particle. These are the particle masses times the signed magnitude of their projected velocities.
  7. Calculate the new projected velocities after collision by the equation derived above.
  8. Calculate the final post-collision velocities as the sum of these new projected components and the old rejected components.

1. Particle-Wall Collisions: Any remaining particles that are in collision with the container have their appropriate velocity components inverted.
2. The particles are rendered as a 3D Scatter plot.
3. The plots of the number of particles and pressure vs. time are updated.
4. The histogram of particle velocity magnitudes is updated.

# Results

# Discussion

# Conclusion

# Future Work

Real-time visual simulator are valuable for providing immediate and understandable indications on the effects certain parameters have on a system and its properties. The more flexible the simulator is in the parameters that are settable and properties that are visualized, the more useful it becomes. As such, adding more controls to this simulator would be the first step for future improvement. This might include:

* A slider bar to control the number of particles in the simulator. New particles would be added with random velocities based on the current average temperature.
* A slider bar to control the temperature of the gas. The velocities of the particles could be scaled to maintain the appropriate distribution by an algorithm similar to histogram equalization.
* Visualization of kinetic temperature in addition to pressure (although they are both proportional to the kinetic energy, which, for a fixed number of pure gas particles, is proportional to the sum of the squares of their velocities.)
* Overlays of the expected temperature, pressure, and particle number density over time based on ideal gas formulas.
* Visualization of effusing particles (They are currently deleted as soon as they escape the container through the hole.)
* Indication of the speed of particles by their color.
* Support multiple types of gas with different masses and particle sizes. This feature would allow for calculation of partial pressures and would serve to demonstrate the relation between particle mass and velocity in a gas mixture of homogeneous temperature. (All particles in a gas have the same average kinetic energy, so lighter particles must have much greater velocities.)
* Particle visualization as true spheres rather than pixel markers. Although this is much more computationally intensive (and was attempted), rendering the particles as sphered gives a much better representation of their position and arrangement in 3D space.
* The overall accuracy of any such simulator increases with the number of particles simulated and the discretization of time and space used (smaller timesteps.)

There are of course numerous computational optimizations to be made to the code and aesthetic/functional improvements to the graphical user interface (GUI.)

Finally, further comparison to empirical and analytic results is needed to further verify the accuracy of the program.

# References