Pythonic simulation of Maxwell's Pressure Demon*

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The physics of ideal and non-ideal gases becomes an increasingly more challenging task to model computationally. By using pygame, a python module that is used to code 2D video games in python, I modeled the approximate behavior of Maxwell's Demon while simulating an ideal gas. The focus of this paper is solely an investigation on James Clerk Maxwell's attempt to disprove the second law of thermodynamics using computational methods.

I. INTRODUCTION

Suppose one has a small cup of cream and a larger cup of coffee. As cold cream is put into hot mug of coffee, the duo mixes. The colors of the coffee and the cream change from a deep brown and white to the color of plywood. Moreover, the system also. Simply put, the cream diffuses into the coffee, meaning that the fewer cream molecules relative to the more numerous coffee molecules tend to move into a region of lower concentration. Also, the motion of the coffee molecules or the cream molecules are not preferred to move in a specific direction or method and the energy is exchanged. For the cream, it absorbs the energy given to it by the coffee, and for the coffee it emits energy to the cream. Thus, an object at a higher temperature than another wants to emit energy and another object at a lower temperature than another wants to absorb energy. The ways in which the particles exchange energy is through collisions and electromagnetic radiation.

Suppose that there is a twist to this system: what if in some boundary to the coffee cup that there is a being which sorts the molecules of the coffee and the cream by their speeds? The speeds of the molecules of whatever substance is being studied are proportional to the temperature of the system, as the temperature is directly proportional to the square root of the root mean square of the speeds of the molecules. If a boundary were drawn on some part of the cup and each molecule were kept in a bound volume according to their speeds then that would infer the coffee and cream molecules would be sorted again! This paper dives deep into simulating an ideal and non-ideal gases with a said conundrum called "Maxwell's Demon" whose job principally is to violate the second "law" of thermodynamics classically.

A. Theory of Ideal and Non-Ideal Gases

Particles in a gaseous state have an internal microscopic kinetic due to the equipartition of energy theorem[3] defined to be

$$U = \frac{f}{2} k_B T \tag{1}$$

where k_B is the Boltzmann constant, T is the temperature of the system, and f is the degrees of freedom of the particle. For each degree of freedom increments of $\frac{1}{2}k_B$ are added at a time. A monatomic gas with three degrees of freedom because has motion in the three cardinal directions. Generally speaking, an increase in the temperature of an object will increase the microscopic kinetic energy of the particles inside the objects. If those particles are gaseous and can move freely inside the volume of the container, their individual speeds will increase. For a low density gas, the behavior of the molecules has certain, fundamental assumptions in what is called kinetic theory:

1. The particles do not interact with each other, aside from elastic collisions (see section IV). For the walls of the volume, they are in the particles bounce
2. The particles' motions are explained with Newton's descriptions of motion with the exception that they are not accelerated due to gravity
3. The particles do move in a constant, random direction. They are in diffusive equilibrium.
4. The combined volume of the particles is negligible compared to the volume of the space.

Essentially, due to equipartition of energy, by setting $(3/2)k_BT$ equal to kinetic energy $(1/2)m\bar{v^2}$, the root mean square of the speeds of the particles is obtained to be

$$\bar{v^2} = \frac{3k_BT}{m} \tag{2}$$

$$v_{\rm rms} = \sqrt{\bar{v^2}} = \sqrt{\frac{3k_BT}{m}} \tag{3}$$

By allowing particles to have volume, they are allowed to collide with each other as the total volume of the particles is not negligible to the V of the container. Therefore, if collisions parameters are taken into account, the distribution of the speeds of the particles are given by the

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Maxwell Boltzmann Distribution

$$f(v) = \left(\frac{m}{2\pi k_B T}\right)^{3/2} 4\pi v^2 \exp\left(\frac{mv^2}{2k_B T}\right) \quad (4)$$

which is independent of any sort of container the particles are in nor is it dependent upon the pressure. The ideal curve resembles that of a gaussian distribution multiplied by a quadratic term which creates a tail of the function due to speeds of the particle. A system that has a larger range of speeds has a wider gaussian and a longer tail than a system whose particle speeds vary little.

Free expansion of an ideal gas describes the randomness of the spread of molecules assuming the condition in which the particles are able to collide on top of the assumptions of kinetic theory. The result is a system in which half of the particles are on one side and the other half on the other on average. The states in which the particles are more equally distributed will have a higher probability than those with a less equal distribution. In section II A this will be explored quantitatively.

B. Theory of Maxwell's Demon

Two systems of unequal temperature can be used to do useful work on an object or objects. To summarize the second law of thermodynamics, the amount of entropy, or a quantity that describes the randomness or uncertainty in a system, never decreases. As said previously, the coffee and the cream mix due to the cream molecules diffusing in the environment of the coffee. Entropy was at an all time low when the coffee and the cream were separable. At the instant the duo begin to mix entropy increases; after a period of time the total entropy of the system will increase even more. In the year 1871, James Clerk Maxwell posed a thought experiment: he thought that if there is a being "whose faculties are so sharpened that he can follow every molecule in its course, such a being, whose attributes are as essentially finite as our own would be able to do what is at present impossible to us"[1]. The impossibility he refers to is essentially a reversal of the second law of thermodynamics: the total entropy of a system decreases. In other words, "order" is brought back into existence. From the coffee and cream example, it would mean after mixing one is able to separate the cream and coffee perfectly (and eventually put them back into their respective cups). The original idea for Maxwell's demon is that of raising the temperature of one side of some volume and lowering that of another by allowing a demon to allow molecules of certain speeds to pass through a door. However, a Maxwell's demon cannot be a purely mechanical device[2] that differentiates the speeds of particles as they pass through a spring door. The particles that need to overcome the spring door would need to have a considerable enough momentum to exert work on the spring which opens the door. The door can be assumed to slide without friction to avoid unwanted forces. The demon ought to rely on the knowledge is has about the speeds of the particles before which this simulation contains. Section II B will provide a quantitative exploration of the classical problem of Maxwell's demon in the setting of gas molecules in a two-dimensional container.

II. EXPERIMENTATION

The simulation of the ideal and non-ideal gas and Maxwell's pressure demon is done using "pygame" a 2D graphics module within python. The version used is 2.1.2 as of the date this paper is being written. For the purposes of this project, the borders of the map are analogous to the boundaries of the box in which the gas particles may interact. When ideal_gas.py, the "__main__" module is run the simulation begins! There is a toggle for implementing Maxwell's demon and visual graphics.

A. Simulation I: Ideal Gas

For a two state system that was simulated in python, the gas molecules are free to move under kinetic theory assumptions and may collide, and after a certain a specific particles may be on the left (L) or right (R) region of the box. Due to free expansion of the gas, the total number of ways in which a particle n out of N may be arranged in the L region in this two state system is:

$$\Omega(N, n) = \frac{N!}{(N-n)!}\frac{1}{n!} \quad (5)$$

where N is the total number of particles is and n the number of particles on the L (or R) region of the box. This two state system will generally trend to the more probable microstates with the most probable being when half of the total particles are in the L region, and half in the R region.

According to figure 1, using equation (5), the most probable microstate in which a system of 60 particles has split 30-30 occurs about just over 10% after a certain time for two state system. A pythonic simulation with 2000 trials were done over the course of 600 frames in figure 2. The simulation estimates that a 30-30 state of the 60 particles occurs in just over 200 trials out of 2000, which is just over approximately 10%.

In figure 3, the difference in the two curves shows that the experimental mean of the probability more particles are in the L region is higher than what the theory predicts.

B. Simulation II: Maxwell's Pressure Demon

For a two state system that has the implementation of Maxwell's demon, the focus is also that of where the

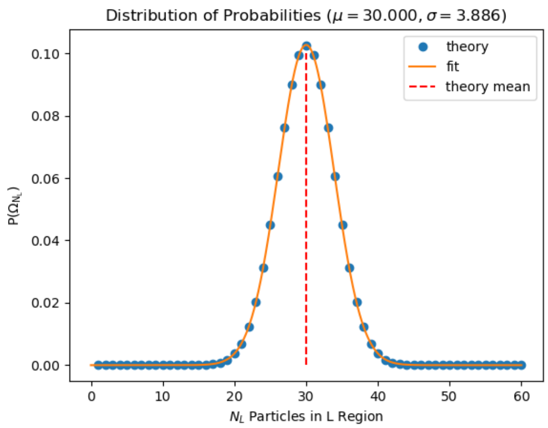

Figure 1. Theory of a distribution in which 60 particles simulated to bounce in a two dimensional box. For 30 particles in the L region equality divided box, that state occurs approximately 10% of the time.

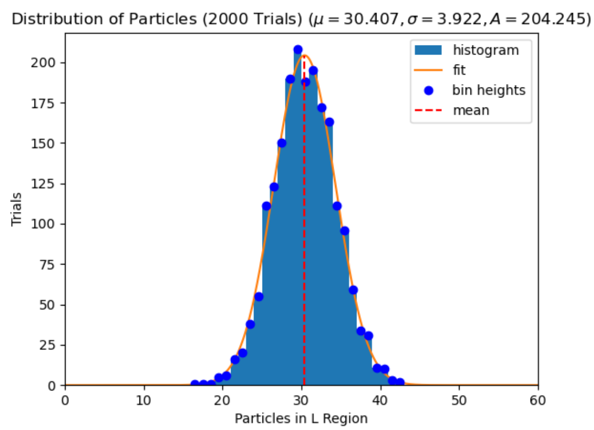

Figure 2. 2000 simulations which build a distribution of number of particles in L region. The theory is roughly matched, as just over 200 trials out of 2000 in which 30 particles are in the L region occur about 10% of the time.

particles are in the box. The box has dimensions of 1300 pixels in width and 700 pixels in height. The demon with its omniscience magical powers is able to detect the speeds of the particles as they pass across midline of the box at 650 pixels. In each scenario, the demon sorts out particles in the L region of the box that have a speed of less than the speed the demon requires. For each of the "speed boundaries" of the demon, a total of 250 trials were run for 4500 frames. The speed boundaries are as follows: 3, 6, 9, 12, 15, 17, 19, 21, 23, 25, 27, and 29 pixels per frame. Much like in section II A, a particle with an initial speed of 20 pixels per second was sent off into motion upon a field of 60 stationary particles. After 4500 frames, a trace of the number of particles in the L region for the different speed boundaries is shown on figure 4. The number of particles in the L region for the

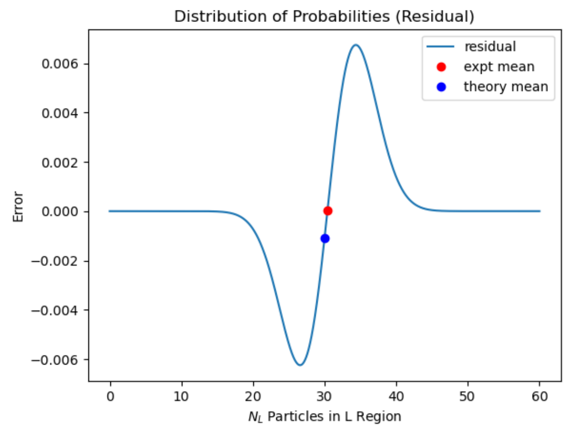

Figure 3. A difference in gaussians of experimentation and theory. The experimental mean is estimated to be highter than that of the theory. A difference of ± 0.006 is probably due to thickness of the experiment histogram bins as 2000 trials would not create a perfectly smooth curve.

lower speeds assumes a normal distribution to begin with as the the number of particles, but as the speed boundary approaches that of the speed of the initial kinetic energy of the first particle set off into motion, the particles begin to cluster in the L region of the box. This is due to the particles not having enough kinetic energy to overcome the hard speed boundary set by the demon. From speed boundary 3 to speed boundary 21, the Gaussian curve shifts to the left, meaning fewer particles on average sit in the L region after 4500 frames, and then the curve flattens. It is only on and after speed boundary 21 that there is a sharp peak at the 60 particles in the L region. For that range of boundaries, by curve fitting a Gaussian and extracting the mean would be an incorrect statistic to use since the number of particles in the L region with the most trials, the mode of the data set, is better to use than any one data point. The mode is a necessary outlier in this physical simulation.

For each speed boundary histogram, a total of 250 trials and 60 particles were used as a representation of what might happen when 15000 particles are simulated on a screen. The speeds of the particles are put into a histogram in figure 5. The x-axis is in pixels per second with the y-axis being the number of particles in that speed. This provides for a more smooth histogram. For each successive speed boundary, after 4500 frames the speed at which most of the particles had decreased with an noticeable spike at 0 pixels per second for almost all the speed boundary simulations. The plots do resemble a Maxwell Boltzmann distribution from equation (4). However, the temperature parameter could not be extracted from a curve fit due to limitations in computational efficiency. Thus, creating a plot of the traces of the root mean square of the speeds of the 15000 particles per speed boundary was necessary and is shown on figure 6. As the speed boundary increase, so does the root mean

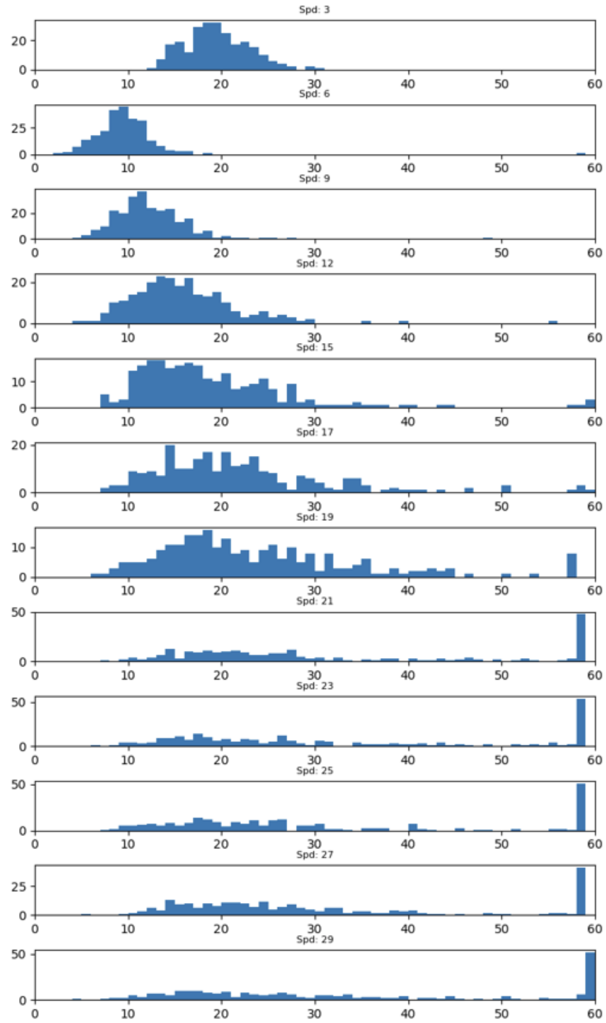

Figure 4. Trials versus the number of particles in the L region per speed boundary.

square of the speeds, but then there is a sharp trough for boundaries 15, 18. Following speed boundary 21, the root mean square begins to decrease again. This would be in direct relation to the temperature of the system as the temperature is proportional to the square or the root mean square of the speeds according to equation (3).

III. DISCUSSION

The demon certainly posed an interesting problem for physicists in the classical age to dissect: does the demon indeed violate the second law of thermodynamics? According figure 6, the second law of thermodynamics is violated at the boundaries where the particle root mean square speeds begin to decrease for steeper speed boundaries, which corresponds to a decrease in temperature. As the number of speed boundaries increases, there potentially will be a decrease in root mean square speed of the

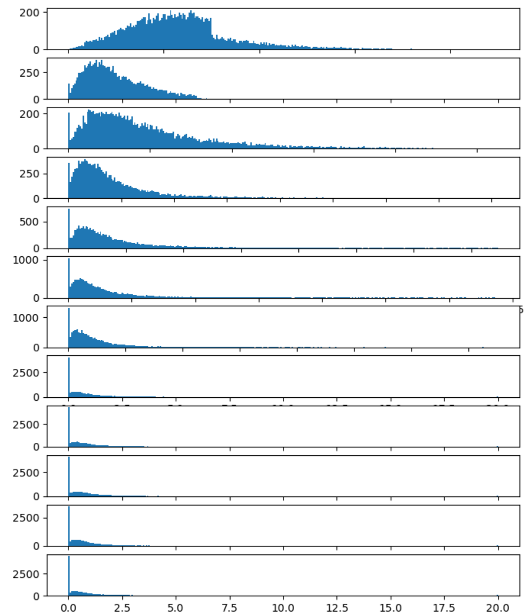

Figure 5. Distribution of Maxwell-Boltzmann speeds for the different speed boundaries.

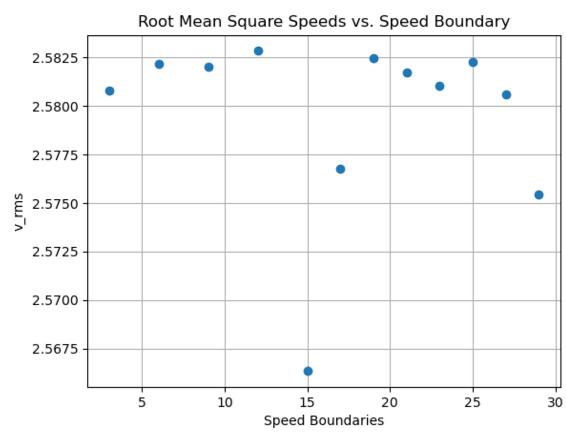

Figure 6. root mean square speeds versus speed boundaries. Notice the rise and fall in the speeds at the ends of the plot with the dips at boundary 15 and 18 pixels per second.

particles. However, what may explain the relative leveling of the root mean square speed for each of the speed boundaries is the total time of each trial, which is 4500 frames. Physically as time increases in a system, the average speed of the particles levels and so the temperature levels as well. If say the total frames per trial was around 1000 the temperature would not level but the speeds of the particles will be distributed in a bunched manner on a Maxwell-Boltzmann plot. The more selective the demon is about which particles may pass through the speed boundary the more the temperature will change. If this experiment were to be run again, a temperature versus frame graph would need to be implemented. That would be a more costly simulation in terms of computational time which would be worth investigating.

What is interesting to note is the dip in speed boundaries 15 and 18 of the simulations. A possible explanation for these dips in figure 6 is due to the collision parameters of the code. For 60 particles to be simulated at a time which take up a great deal of screen space, there may be possible collisions that are not possible such as collision at the demon boundary in which an escapee particle passes through the barrier. By enabling animations one may be able to see this. This would be due to a limitation of python as an interpreting language is not optimal for graphics, such as a compiling language like C or C++. Another possibility is that the initial particle set of in motion likely does not have enough kinetic energy at the end of thousands of frames. Where for each speed boundary the average speed of the particles decreases the root mean square of the speeds does not. Improvements would need to made to the code that simulates the physics such as improving collision parameters. The total amount of time for the simulations to finish the 12 different speed boundaries was around 36 hours of computational time.

IV. APPENDIX A: ELASTIC COLLISION IN TWO DIMENSIONS

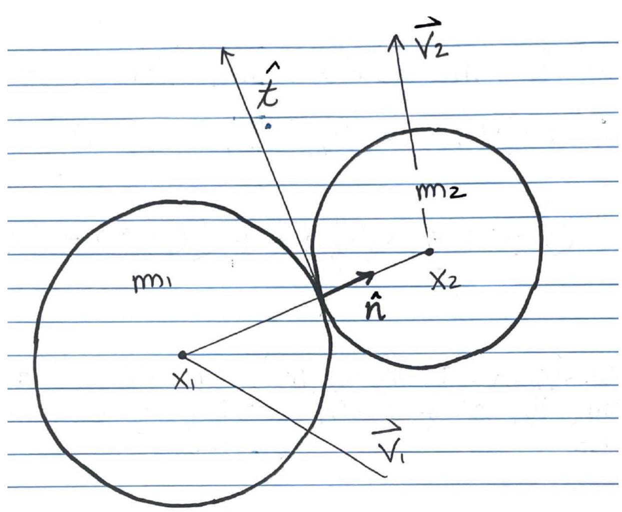

Figure 7. Two balls the instant before they collide elastically.

The mathematics of the elastic collision between two balls of different masses and two different initial velocities.

The distance between the centers of the balls is given by

$$\left\|\vec{\Delta x}\right\| = \|\vec{x_1} - \vec{x_2}\| \tag{6}$$

whose normal vector is

$$\hat{n} = \frac{\vec{x_1} - \vec{x_2}}{\|\vec{x_1} - \vec{x_2}\|} \tag{7}$$

The conservation of momentum and the conservation of energy leave no forces in the tangential component of the velocity after collision, that is

$$\vec{v_1} \cdot \hat{t} = \vec{v_1'} \cdot \hat{t} \tag{8}$$

$$\vec{v_2} \cdot \hat{t} = \vec{v_2'} \cdot \hat{t} \tag{9}$$

For the normal component of the velocity, conservation of momentum and energy say

$$m_1(\vec{v_1} \cdot \hat{n}) + m_2(\vec{v_2} \cdot \hat{n}) = m_1(\vec{v_1'} \cdot \hat{n}) + m_2(\vec{v_2'} \cdot \hat{n}) \tag{10}$$

$$m_1(\vec{v_1} \cdot \hat{n})^2 + m_2(\vec{v_2} \cdot \hat{n})^2 = m_1(\vec{v_1'} \cdot \hat{n})^2 + m_2(\vec{v_2'} \cdot \hat{n})^2 \tag{11}$$

Rearrange equation (11), factor out m_1 and m_2 on two different sides...

$$m_1(\vec{v_1} \cdot \hat{n})^2 - m_1(\vec{v_1'} \cdot \hat{n})^2 = m_2(\vec{v_2'} \cdot \hat{n})^2 - m_2(\vec{v_2} \cdot \hat{n})^2 \tag{12}$$

and undo the difference of squares yields

$$m_1[(\vec{v_1} \cdot \hat{n}) - (\vec{v_1'} \cdot \hat{n})][(\vec{v_1} \cdot \hat{n}) + (\vec{v_1'} \cdot \hat{n})] = m_2[(\vec{v_2'} \cdot \hat{n}) - (\vec{v_2} \cdot \hat{n})][(\vec{v_2'} \cdot \hat{n}) + (\vec{v_2} \cdot \hat{n}) \tag{13}$$

Recognizing that $m_1[(\vec{v_1} \cdot \hat{n}) - (\vec{v_1'} \cdot \hat{n})]$ and $m_2[(\vec{v_2'} \cdot \hat{n}) - (\vec{v_2} \cdot \hat{n})]$ in equation (13) are equal due to the conservation of momentum so equation (13) may be simplified to

$$(\vec{v_1} \cdot \hat{n}) + (\vec{v_1'} \cdot \hat{n}) = (\vec{v_2'} \cdot \hat{n}) + (\vec{v_2} \cdot \hat{n}) \tag{14}$$

By solving for $(\vec{v_2'} \cdot \hat{n})$ in equation (14), then substituting it into equation (10), and finally solving for $(\vec{v_1'} \cdot \hat{n})$ in equation (10) yields the normal component of particle 1's final velocity

$$(\vec{v_1'} \cdot \hat{n}) = \frac{(m_1 - m_2)(\vec{v_1} \cdot \hat{n}) + 2m_2(\vec{v_2} \cdot \hat{n})}{m_1 + m_2} \tag{15}$$

which may be simplified to

$$(\vec{v_1'} \cdot \hat{n}) = (\vec{v_1} \cdot \hat{n}) - \frac{2m_2(\vec{v_1} \cdot \hat{n} - \vec{v_2} \cdot \hat{n})}{m_1 + m_2} \tag{16}$$

Finally, the resulting velocity for particle 1 is the sum of the normal and tangential components

$$v_1' = (\vec{v_1'} \cdot \hat{n})\hat{n} + (\vec{v_1'} \cdot \hat{t})\hat{t} \tag{17}$$

and substituting equation (7) for the normal vector into the expression above

$$\vec{v_1'} = \vec{v_1} - \frac{2m_2[(\vec{v_1} - \vec{v_2}) \cdot (\vec{x_1} - \vec{x_2})](\vec{x_1} - \vec{x_2})}{(m_1 + m_2) \left\| x_1 - x_2 \right\|^2} \tag{18}$$

The same procedure may be followed to find the final velocity for the second particle.

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[3] Daniel Schroeder. *Introduction to Thermal Physics*. Addision Wesley Longman, 2000, p. 15.