Simulating the Kinetic Theory of Gases using Object-Oriented Programming

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***Abstract*— The Kinetic Theory of gases can be modelled using Object-Oriented Programming. This type of simulation where a container is filled with ball objects that, given positions and velocities, collide with one another and give rise to thermodynamical properties. This report outlines how this was achieved using Python programming and how such a simulation can effectively show how the velocity distribution of particles is a Maxwell-Boltzmann distribution, how the Van Der Waals law is accurate to the kinetic theory as well as how Brownian particles move randomly to a statistically significant degree.**

I. Introduction

In thermodynamics, the Kinetic Theory of gases is vital in our understanding of the behaviour of gases and has been for centuries. The theory, in its simplest form, states that a gas consists of very large numbers of identical microscopic molecules that exist inside a container [1]. These molecules undergo elastic collisions with the container and each other that give rise to macroscopic quantities – temperature and pressure. Despite its strong foundations, Kinetic Theory is tedious to derive mathematically. It is only recently with the option of computational methods such as Python programming that Kinetic Theory can be modelled more rigorously. The strength of modern-day computers has allowed me to exploit such methods, specifically Object-Oriented Programming (OOP) to simulate the conditions of an ideal gas and investigate its properties and behaviour. Properties such as the Maxwell-Boltzmann velocity distribution, the Van der Waals' law and Brownian motion were all aspects explored in my investigation.

II. Theoretical Background

My model allowed me to test three major thermodynamical principles of the kinetic the gases. The first being the Maxwell-Boltzmann distribution. The distribution states that (in 2 dimensions) the distribution of velocities obeys the probability density function shown in (1) with a single variance parameter σ [2]. This parameter can be rewritten in terms of the temperature of the gas, *T*, the mass of the particles, *m*, and the Boltzmann constant, k_B.

$$P(v:\sigma) = \frac{v}{\sigma^2}\exp\Big(-\frac{v^2}{2\sigma^2}\Big) \qquad \sigma = \Big(\frac{k_B T}{m}\Big)^{\frac{1}{2}} \quad (1)$$

Where the temperature of the simulated gas can be simply determined by calculating the total energy of the balls in the container (that is the total kinetic energy of the particles as we assume a zero potential) divided by the Boltzmann constant, k_B – for two degrees of freedom (in 2D). The second law investigated was the Van der Waals Law that is shown below in (2).

$$\Big(P + a\Big(\frac{N^2}{V^2}\Big)\Big)\Big(V - Nb\Big) = Nk_B T \quad (2)$$

In (2), *P* and *V* represent our pressure and volume respectively, *a* is a measure of the attraction between the particles and b is the 'excluded volume' – defined as being four times the total particle volume of the ideal gas. However, for my simulation, we ignore possible intermolecular forces which sets *a* to zero. Finally, I investigated the idea of Brownian motion. Einstein proposed in one of his earlier theories if *N* particles are constantly diffusing (with diffusivity constant *D*) that the particles (called Brownian particles) must obey a probability distribution (3) [3].

$$\rho(x,t) = \Big(\frac{N^2}{4\pi Dt}\Big)^{\frac{1}{2}}\exp\Big(-\frac{x^2}{4Dt}\Big) \quad (3)$$

Noticeably, this distribution is a gaussian, therefore it can be concluded that Brownian particles in an ideal gas have an equal probability of being displaced in any given direction. This random motion is what we refer to as Brownian motion.

III. Methodology

The concept of simulation in physics involves writing code that solves an equation or multiple sets of equations. In my simulation, this equation is a quadratic equation shown in (4) that calculates the time δ*t* until two balls collide [4].

$$((\mathbf{r_1} - \mathbf{r_2}) + (\mathbf{v_1} - \mathbf{v_2})\delta t)^2 = (R_1 \pm R_2)^2 \quad (4)$$

Where *R* denotes the ball radii and **r** and **v** denote the position and velocity of either ball, respectively. The plus and minus differentiate between the two types of collisions – collisions when two separated balls collide and collisions when one ball is inside the other collide. Hence, we define a collision to occur at the intersection of two ball boundaries. Using a ball and simulation class object, I could initiate a simulation, in which I initiated a larger ball of radius 10 m (that would be my container) with many smaller balls inside. By solving (1) for every combination of balls, my simulation could deduce when the next collision was as the smallest value of δt. When a collision all balls were moved to this time and the colliding ball velocities needed to be changed. This was done by reversing the velocities along the line of centres (the line that passes through both ball centres) and keeping the perpendicular components the same. All whilst keeping momentum along the line of centres conserved. However, it was important to consider the condition when multiple collisions occur at once where multiple velocities needed changing.

To ensure the simulation operated at maximum efficiency, instead of recalculating every combination of times δt after every collision, only the collided ball times needed recalculation – this turns an order N^2 problem to a problem of order N. Computationally this was done by storing time to collision values in a matrix $T_{ij.}$ To avoid duplicates and balls colliding with themselves, only elements where i>j were calculated (with an extra column for container collisions). When updating the matrix for a collision between ball i and ball j, only row i and column j were recalculated.

For a more flexible simulation and to allow for more rigorous testing, the simulation allowed for a varying number of balls in the container. To do this, balls were placed on a polar spiral curve from the centre with equation $r=\alpha\theta$ (and converted to cartesian coordinates) ensuring that the balls do not overlap. This allowed for a very large number of balls that can be evenly distributed. Most simulations performed ran with α=0.1 and spaced every 0.05 radian which allowed for 300 balls. Once the ball positions were defined, the velocities v_i needed to be specified. This was done by uniformly distributing velocities between [-10,10] $m \cdot s^{-1}$ for each ball. However, to achieve the appropriate Maxwell-Boltzmann distribution, we set the average velocity to 0. This was done by subtracting $1/N$ of the sum of the velocity components to each $v_{i.}$ Finally, before performing experiments, the simulation was tested for numerous types of known pieces of physics such as energy and momentum conservation, particle separation distributions and ideal gas laws that passed successfully. These can be seen in Fig. 2-9.

IV. Results and Discussion

To study the velocity distribution, the simulation was run 200 times for 30 balls. The velocity was taken after 1000 collisions and the binned distribution (for 78 bins – the root of the number of data points) with a fitted Maxwell-Boltzmann distribution can be seen in Fig. 8. The variance of the distribution σ was calculated to 2.22 ± 0.03 $m \cdot s^{-1}$ which by our relationship in (1) gives a temperature (3.56 ± 0.06) $\times 10^{23}$ K which does not agree with my calculated temperature determined using the energy of the particles to be 3.45×10^{23} K. However, we can test the data for a null hypothesis H_0 that the data does not follow a Maxwell-Boltzmann distribution which if we test. Using $\bar{T}=3.45 \times 10^{23}$, the resulting p-value is 0.0191 which is sufficient evidence at a 2.5% significance level to reject $H_{0.}$ Hence the histogram does follow a Maxwell-Boltzmann distribution.

The Van Der Waals law was tested by determining the value of b in (2) by running through a simulation with different container radii (in the range 5 to 20 m) with 50 R=0.5 m balls. As previously stated, we can set $a=0$ by ignoring intermolecular forces which allows us to determine b graphically by plotting the volume V against the inverse pressure P^{-1}. The result is a straight-line graph with a gradient of Nk_BT and a y-intercept of Nb (Fig. 9). If we recall that b represents the excluded volume of a particle it can be deduced that for these simulations b is equal to 1.57 m^2. The value of the y-intercept using the least-squares method was calculated to be 80.01 ± 2.52 m^2 which results in b equal to 1.60 ± 0.05 m^2. The theoretical value lies within this range hence the simulation obeys the Van Der Waals law successfully.

Finally, the concept of Brownian motion was investigated by tracking the position of a central Brownian particle through the container of 100 R=0.5 m balls. It can be seen from Fig. 1 that the trajectory of the ball seems completely random as predicted by Einstein's model and appears to follow no pattern. Although this is graphically convincing, a more extensive statistical analysis can be shown by performing linear regression. By looping through different initial conditions of the simulation and determining where the Brownian particle ended up as an angle from the centre. The result was an R^2=0.036 with an associated p-value of 0.003. Therefore, we can conclude that the motion of a Brownian particle is statistically random in my model.

Despite, my simulation showing appropriate physics in the laws and principles just explained, small errors may have propagated into the results due to the limitations of the simulation. These limitations include the number of particles in the container that was limited by size and computational processing time that did not (even nearly) come close to the number of particles in a typical ideal gas ($>10^{23}$). Additionally, the balls take time to reach a true ideal gas state from their initial positions. Balls that were uniformly distributed in the container from t=0 would be more representative of an ideal gas' perpetual state.

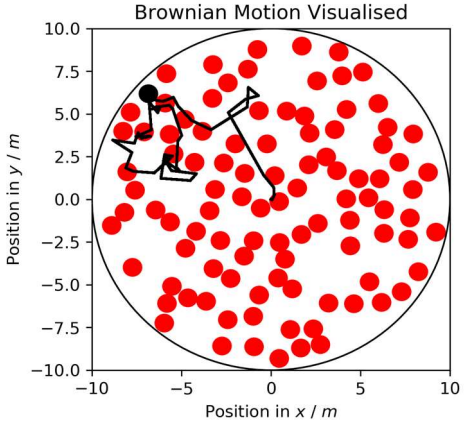

Fig. 1. The simulation graphic shows the seemingly random trajectory of a Brownian particle of radius 0.5 m in a container of 100 balls

V. Conclusion

To conclude, my simulation was able to effectively reproduce various physical thermodynamical phenomena described by the kinetic theory of gases. By modelling molecules in a gas as identical particles and the ability to simulate them and their behaviour computationally was successful in showing statistically significant results. Such results are owed to the modern computational power of simulation that only recently has been made possible.

VI. References

[1] Present, Richard D. Kinetic Theory of Gases. New York; London: McGraw-Hill, 1958. Print. International Ser. in Pure and Applied Physics.

[2] Adjodah D. Derivation of 2D Boltzmann Distribution. MAS.864 MIT; 2020.

[3] Einstein A. On the Movement of Small Particles Suspended in Stationary Liquids. Annalen der Physik, March 1905.

[4] Kingham R, MacKinnon A. Project B Thermodynamics Snookered: Lab Script, Imperial College London, 2020

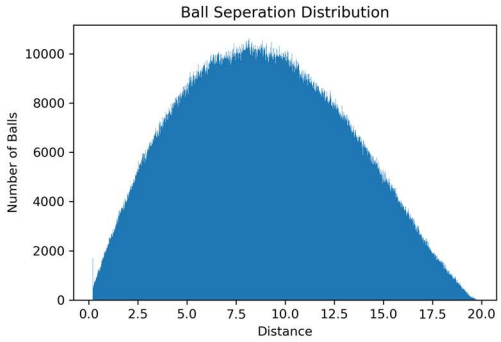

Fig. 2. The distribution of distances between balls for 100,000 balls of radius 0.1 m where the minimum separation is 0.2 m, and the maximum is 19.8 m

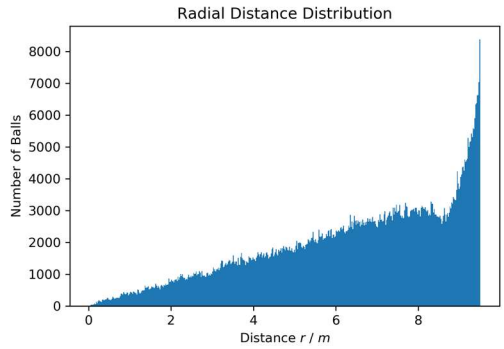

Fig. 3. The distribution of radial distances of balls from the centre of the container for 100,000 balls. The peak due to a high proportion of collisions occurring at the container border.

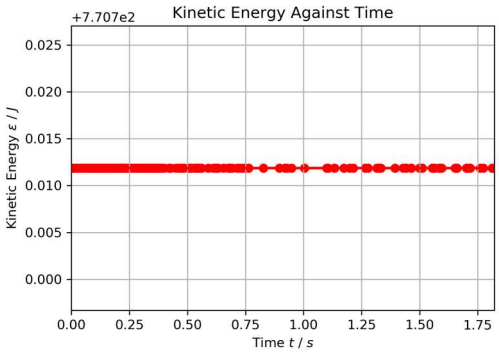

Fig. 4. The graph shows the total energy of the system, that is purely kinetic, over time. The fact that it is constant shows that the simulation conserves energy

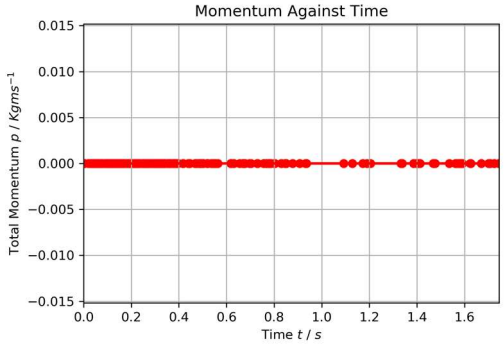

Fig. 5. The graph shows the total momentum of the system against time which is constant and zero. Zero as we set the initial average velocity to zero and constant as momentum is conserved.

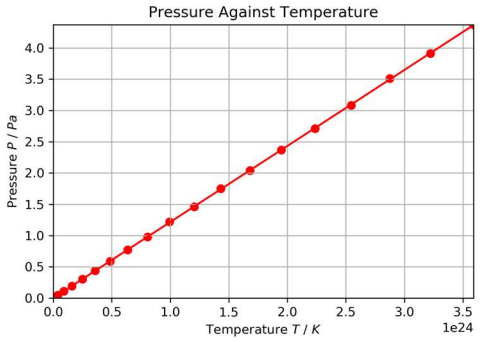

Fig. 6. Testing the ideal gas law on the simulation for linear relationship between temperature and pressure for 30 balls in the container.

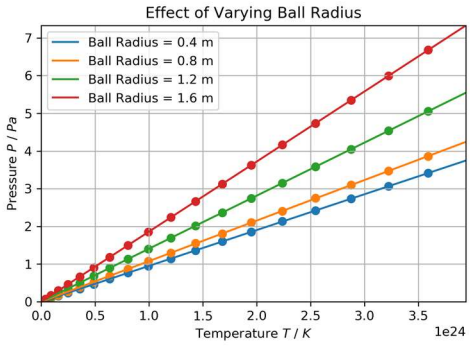

Fig. 7. The ideal gas law was tested again but for different ball radii. The graph shows how a larger ball radius yields a higher gradient on the PT graph as expected.

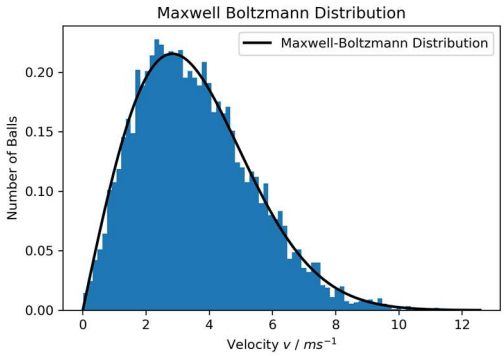

Fig. 8. The histogram shows a distribution of velocities in 78 bins for 6000 data points. The curve plotted shows how the distribution follows a Maxwell-Boltzmann distribution

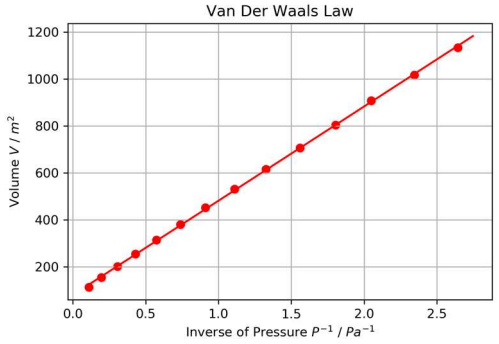

Fig. 9. The graph proves the Van Der Waals Law by showing a linear relationship between the inverse pressure and volume of the container when there are no intermolecular forces.