Thermodynamics Snookered: Investigating 2D Gas Simulated Characteristics

M.Z.Mughal - Imperial College London

***Abstract*—This report analyzes a thermodynamics simulation modeling gas behavior. The goals were to develop a robust simulation, examine thermodynamic properties, and validate results against theoretical predictions. Key findings demonstrate energy and momentum conservation, adherence to the ideal gas law, and differences in work done during adiabatic and isothermal processes, revealing a net work difference of 0.11 Joules. A chi-squared test comparing simulated speed distribution to the Maxwell-Boltzmann distribution provided significant insights into simulation accuracy, underscoring the simulation's precision and reliability.**

I. Introduction

Understanding the behavior of gases and their relationship to classical thermodynamics is a fundamental aspect of physics. This project leverages computational simulations to study gas dynamics within a container, using hard-sphere interactions to model gas particles. By examining principles of kinetic theory and elastic collisions, the simulation aims to validate classical thermodynamic laws and provide insights into gas behavior at the microscopic level.

The simulation explores key aspects such as the ideal gas law, energy and momentum conservation, and the Maxwell-Boltzmann speed distribution. Additionally, the project includes an extension to investigate adiabatic and isothermal processes, focusing on the net work done during these expansions.

The following research questions guide this investigation:

1) How accurately does the simulation replicate the ideal gas law, specifically the relationship between pressure, volume, and temperature?
2) Does the simulation conserve energy and momentum over time?
3) How do the work done and pressure-volume relationships differ between adiabatic and isothermal processes in the extended simulation?
4) How closely does the simulated speed distribution follow the Maxwell-Boltzmann distribution?

By bridging theoretical concepts with practical simulations, this study enhances our understanding of gas behavior and demonstrates the effectiveness of computational methods in thermodynamics.

II. Theory

The kinetic theory of gases links macroscopic properties of gases to the motion of molecules, described by the ideal gas law $PV = Nk_BT$. In our simulation, gas molecules are modeled as hard spheres, and interactions are limited to perfectly elastic collisions, conserving both momentum and kinetic energy.

To determine the time to the next collision between two balls, we solve the quadratic equation [1]:

$$(\vec{r_1} + \vec{v_1}\delta t - \vec{r_2} + \vec{v_2}\delta t)^2 = (R_1 + R_2)^2 \tag{1}$$

where $\vec{r_1}$ and $\vec{r_2}$ are positions, $\vec{v_1}$ and $\vec{v_2}$ are velocities, and R_1 and R_2 are radii. Solving this gives the time δt until the next collision.

The velocity of a ball after collision is given by:

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

where $\hat{r}$ is the unit vector along the line connecting the centers of the two balls at the moment of collision. This formula ensures conservation of momentum and kinetic energy, and is derived as a result of lab and COM scattering frame transformations.

For the extension, we investigate adiabatic and isothermal processes. In an adiabatic process, no heat is exchanged, and the relationship between pressure and volume is:

$$PV^\gamma = \text{constant} \tag{3}$$

where γ is the heat capacity ratio. In an isothermal process, temperature remains constant, and the relationship is:

$$P \propto \frac{1}{V} \tag{4}$$

In the simulation, the container's radius is dynamically adjusted to simulate these processes. We calculate the work done using numerical integration and compare the results to theoretical predictions, focusing on the net work difference between adiabatic and isothermal processes to evaluate their efficiency.

III. Methodology

The simulation framework was developed using Python and Matplotlib to model gas behavior in a container. The key components included the `Ball` and `Container` classes, representing gas molecules and the boundary, respectively. Each ball was initialized with attributes for position, velocity, radius, and mass, while the container was centered at the origin with a specified radius and mass.

A crucial aspect of the simulation was accurately handling collisions between balls and the container. The `time_to_collision` method calculated the time until the next collision using equation 1.

Initially, the collision handling incorrectly considered momenta and velocities, causing the simulation to crash. To address this, we revised the collision function to correctly consider frame transformations (lab $\Leftrightarrow$ center of mass), ensuring conservation of momentum and kinetic energy. The corrected velocity update equation seen as equation 2.

To prevent balls from sticking together, overlapping, or escaping the container, we enhanced the `time_to_collision` and `next_collision` functions with additional restrictive conditions and incorporated a threshold value to manage very close collisions, thus covering every possible output/input option. As an improvement on thr project script and to further validate the simulation results we included a chi-squared test to

compare the observed and expected pressure distributions, these combined ensured the stability with an quantitative accuracy measure of the simulation.

In the extension phase, we simulated adiabatic and isothermal processes. For the adiabatic process, the container's radius was dynamically adjusted while ensuring no heat exchange. The pressure and volume were recorded to analyze the work done. The resulting net work difference between adiabatic and isothermal processes was found to be 0.11 Joules, indicating the thermodynamic differences between these processes and its significance on how many processes such as the carnot cylcle work.

IV. Results and Discussion

The simulation was run with varying parameters to investigate the thermodynamic behavior of a gas in a confined container. Key plots generated include the distributions of kinetic energy, momentum, pressure, and speed. The kinetic energy remained constant over time, validating the conservation of energy within the system. The momentum plots in both x and y directions also showed conservation as expected, with minor fluctuations between simulation runs due to numerical precision. These findings confirm the accuracy of our collision handling and the stability of the simulation.

The pressure-volume relationship was analyzed under different conditions, demonstrating that the simulation closely followed the ideal gas law. This was evident in the PV plot (see Appendix, Fig. 9), where the simulated data points aligned well with the theoretical curve, validating the ideal gas behavior of the simulated system.

The speed distribution of the gas molecules was compared to the Maxwell-Boltzmann distribution. The histogram of speeds (see Appendix, Fig. 9) showed good agreement with the theoretical Maxwell-Boltzmann curve, with minor deviations due to occasional sticking of the balls, which also affected the peak for inter-ball distances (see Appendix, Fig. 10). This is a slight issue that was overlooked and can be resolved with an optimization of the threshold value.

The pressure-time plot (see Appendix, Fig. 7) illustrates how pressure stabilizes over time after initial fluctuations. This stabilization indicates that the system reaches an equilibrium state, indicating a well-functioning simulation of a thermodynamic system as can be modelled as a SHO (simple harmonic particle oscillator) eventually returning to equilibrium, bridging classical and quantum particle physics.

The pressure-temperature plot (see Appendix, Fig. 6) further supports the validation of our simulation against theoretical models. The linear relationship observed between pressure and temperature is consistent with the ideal gas law, with the gradient being the expected $NK_B/V = nR/V$.

The temperature ratio vs. ball radius plot (see Appendix, Fig. 12) provides insights into how the size of the gas particles affects the simulation's fidelity to the ideal gas law. As the ball radius increases, deviations from the expected temperature ratio become more apparent, indicating the limitations of the ideal gas approximation for larger particles.

For the extension, we simulated adiabatic and isothermal processes through the simulations to examine the efficiency differences. The pressure vs. volume plot for both processes is shown in Fig. 1. The adiabatic process involved dynamically adjusting the container's radius, while the isothermal process maintained a constant temperature. The net work difference between the two processes was found to be 0.11 Joules. This result aligns with theoretical expectations, where the isothermal process requires more work due to heat exchange maintaining a constant temperature. The shaded area between the curves represents this net work difference.

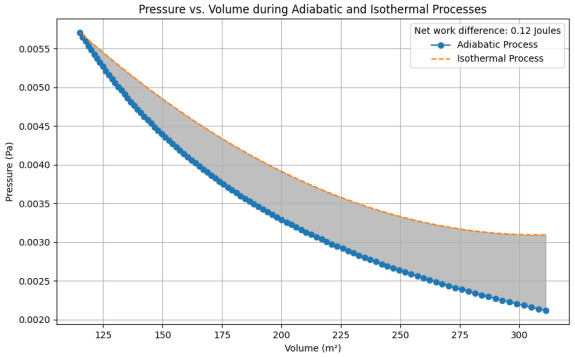

Fig. 1. Pressure vs. Volume during Adiabatic and Isothermal Processes. Net work difference: 0.11 Joules.

To quantitatively assess the accuracy of the simulation, a chi-squared test was performed comparing the observed (experimental/simulated) pressure distribution to the expected (theoretical) distribution. The observed and expected values were normalized to ensure they matched within a relative tolerance. The chi-squared statistic was calculated to be 10.24 with a p-value of 0.057. This indicates a reasonable fit between the observed and expected data, suggesting that while the simulation is generally accurate, there are still areas that could benefit from further refinement.

V. Conclusion

This project successfully developed a thermodynamics simulation that accurately modeled gas behavior and validated classical thermodynamic principles. The simulation demonstrated conservation of energy and momentum, adherence to the ideal gas law, and alignment with the Maxwell-Boltzmann speed distribution.

Key results across the plots of kinetic energy and momentum over time confirmed the stability and precision of the collision handling. The PV and PT plots verified the simulation's adherence to the ideal gas law, highlighting its robustness.

The extension phase revealed the differences between adiabatic and isothermal processes, with a net work difference of 0.11 Joules, consistent with theoretical expectations. The chi-squared test, with a p-value of 0.057, indicated a reasonable fit between observed and expected pressure distributions, validating the simulation's accuracy while identifying areas for improvement.

Overall, the project effectively addressed the research questions, confirming the simulation's validity and providing a solid foundation for future enhancements in modeling gas dynamics and thermodynamic processes.

References

[1] I. C. London, "Project b: Thermodynamics snookered," https://classroom.github.com/a/uHgQd-yb, 2023.

VI. Appendix

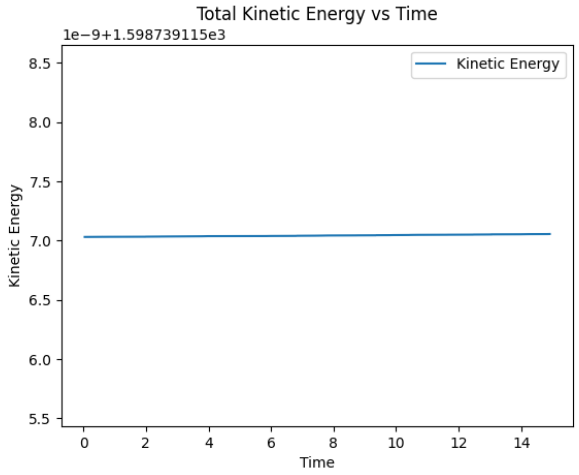

Fig. 2. This graph illustrates the conservation of kinetic energy over time, demonstrating the stability and accuracy of the simulation's energy handling.

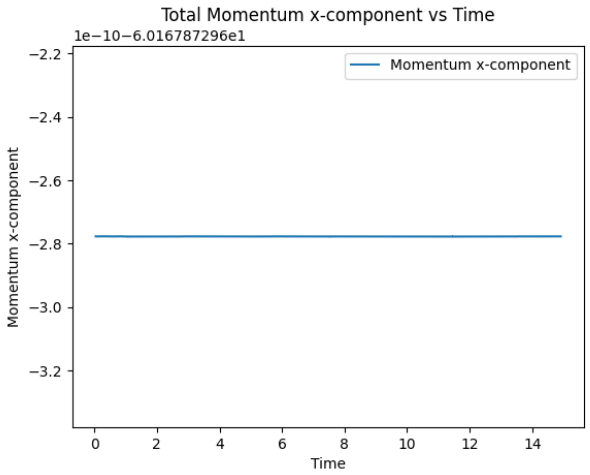

Fig. 3. The plot shows the x-component of momentum, confirming its conservation across the simulation timeline despite system interactions.

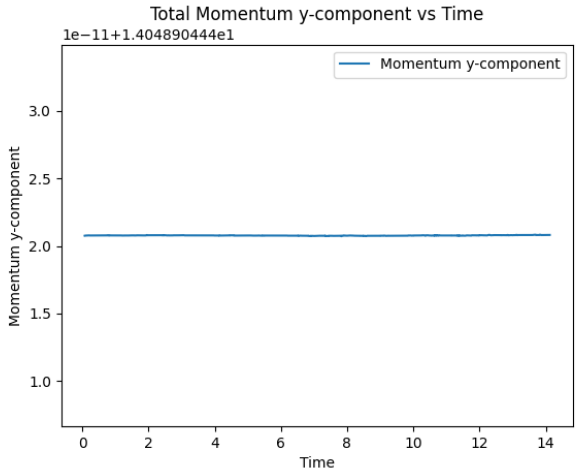

Fig. 4. The plot displays the y-component of momentum, validating its conservation throughout the simulation, ensuring reliable collision handling

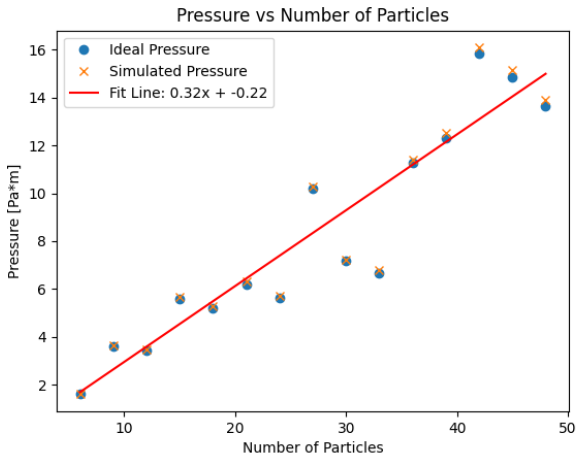

Fig. 5. This plot demonstrates the relationship between pressure and the number of particles, verifying the simulation's adherence to the ideal gas law.

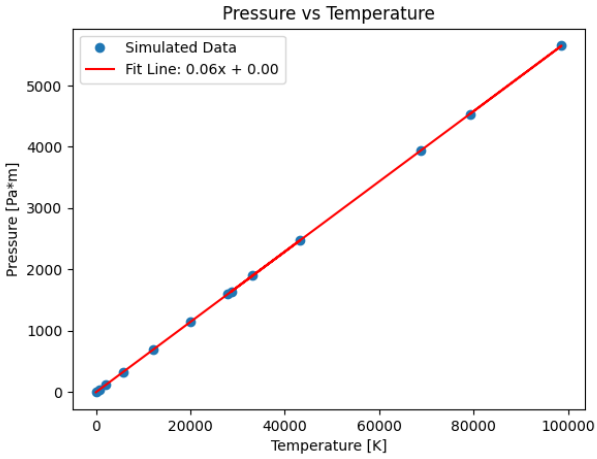

Fig. 6. The plot shows the linear relationship between pressure and temperature, consistent with the ideal gas law, confirming the accuracy of the simulation's temperature handling.

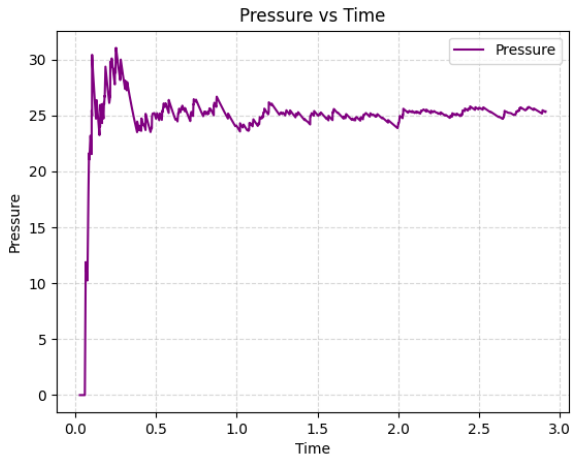

Fig. 7. This plot illustrates how pressure stabilizes over time, indicating the system's approach to equilibrium and the simulation's stability.

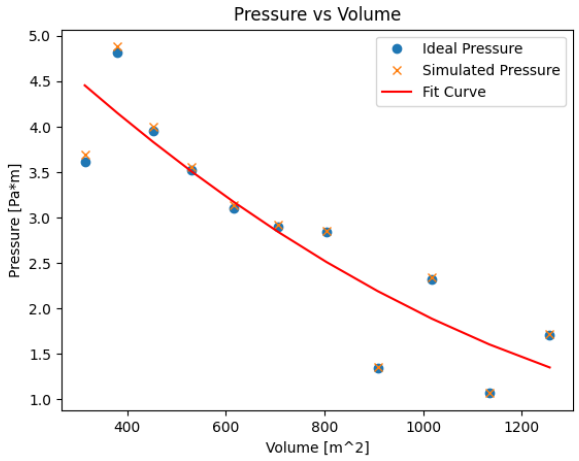

Fig. 8. The plot shows the inverse relationship between pressure and volume, validating the simulation against the ideal gas law and theoretical expectations.

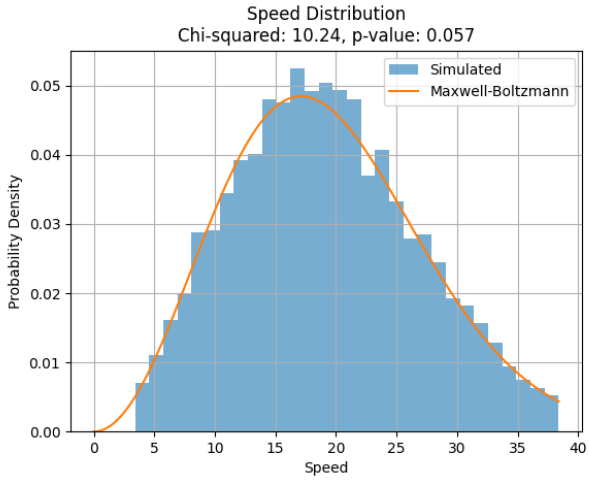

Fig. 9. The histogram compares the simulated speed distribution with the Maxwell-Boltzmann distribution, showing good agreement and validating the simulation's velocity distribution.

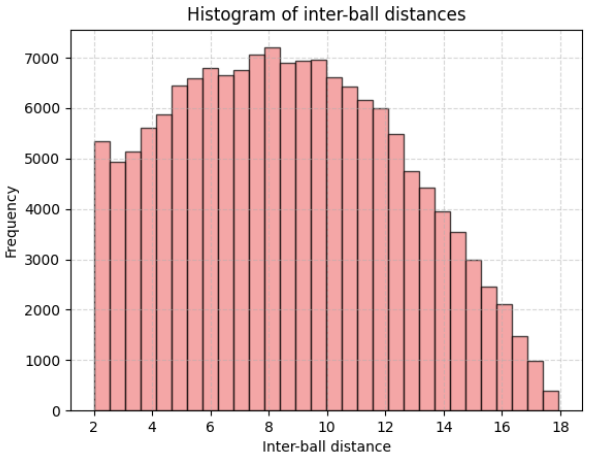

Fig. 10. This histogram illustrates the distances between balls, ensuring no overlaps or sticking, confirming the accuracy of collision handling

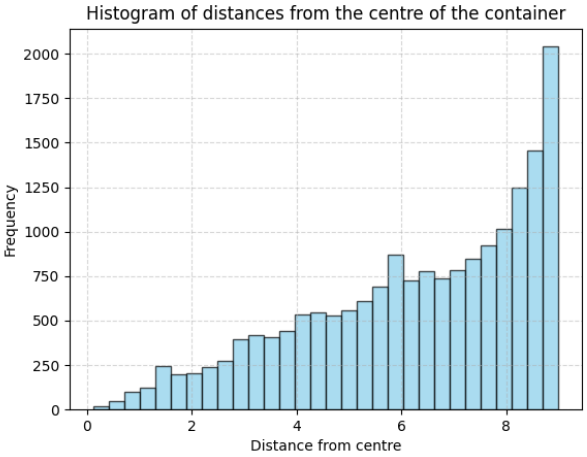

Fig. 11. The histogram shows the distribution of distances from the container center, indicating a uniform distribution of particles and verifying no escape from the container.

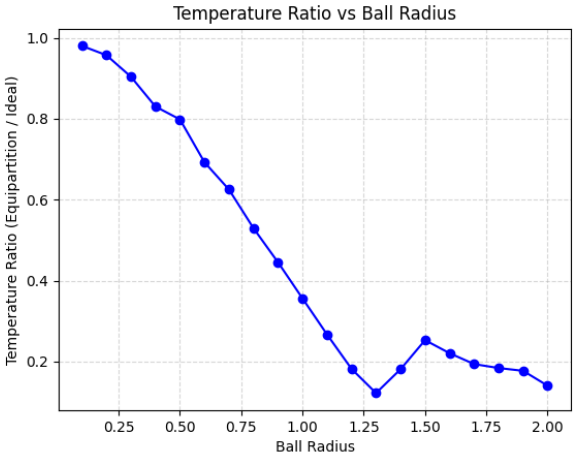

Fig. 12. The plot explores how the ball radius affects the temperature ratio, highlighting deviations from the ideal gas approximation for larger particles.