Computing Project: Thermodynamics Snookered

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I. Creating an Animation

A. The class Ball (Task 1-Task 3)

A class *Ball* was created to create balls and a container. The container was considered to be the same type of object as the balls but had a negative radius. To perform collisions, the time to collision δt of a ball with another ball was calculated by

$$\delta t = \frac{-\vec{r}\cdot\vec{v} \pm \sqrt{(\vec{r}\cdot\vec{v})^2 - |\vec{v}|^2(|\vec{r}|^2 - R^2)}}{v^2} \tag{1}$$

, where $\vec{r}$ is $\vec{r_1} - \vec{r_2}$, $\vec{v}$ is $\vec{v_1} - \vec{v_2}$ and R is $R_1 \pm R_2$.

There are some possibilities of the solutions for δt. Two solutions are both real numbers in most of the cases. In real number solutions, one of them might sometimes be negative, which corresponds to the time the balls that have collided in the past. However, there is also another extreme case. If two balls have the same velocity, the collision of two balls would not happen, which gives the complex solutions. In the method *time_to_collision*, both of the solutions were calculated, but only the smallest positive value was recorded.

Sometimes, Python would return a positive value but smaller than 10^{10}. This is due to the limitation of the computer calculating the number in a binary system, and thus the solutions that were less than 10^{10} were set to be zero. With the obtained time to collision, the velocity and the position after a collision can be calculated.

The method *collide* calculated the new velocity by

$$v_1' = \frac{m_1 - m_2}{m_1 + m_2}v_1 + \frac{2m_2}{m_1 + m_2}v_2 \tag{2}$$

All balls performed elastic collisions were assumed.

B. The class Simulation (Task 4-Task 6)

A class *Simulation* was created to perform a simulation of balls moving inside a container. The class has an attribute of a list of balls, which saved all the information of balls and the container in one simulation. The container was always saved in the last item of the list. The method *next_collision* updated the new position of the balls and moved the patch of the balls with regards to the position. The new velocity was also updated after a collision. The unit vector of the change in position was found to move the patch of the ball repeatedly to the new position.

C. A group of balls (Task 7-Task 9)

The time to collision of the ball to every other ball was appended in a list. The time interval until the next collision was found by finding the minimum value in the list. The balls were initialised with random velocities and arranged spirally following the equation r= a θ in polar coordinates as shown in Fig. 1.

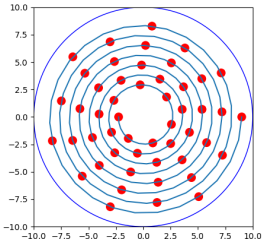

Fig. 1: The arrangement of the balls inside the container. 50 balls were placed inside the container.

The balls were assigned at the same angle separation with a different radius. As the radius increases, the number of balls decreases, which corresponds to the histogram shown in Fig. 2 (LHS).

The histogram in Fig. 2 (RHS) shows the separation between each pair of balls. The distribution is an approximation to a normal distribution.

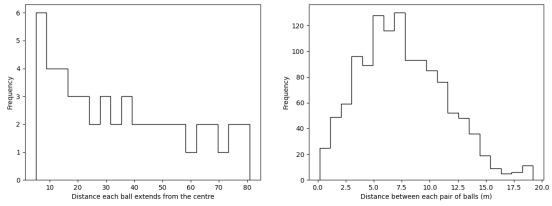

Fig. 2: The histogram of ball distance from container centre (LHS) and the histogram of inter-ball separation (RHS).

II. Thermodynamics Investigation

A. Kinetic energy and Momentum (Task 10)

Particles colliding in a closed system obey the law of conservation of energy. In the simulation, the particles were assigned to perform elastic collision during each collision. An elastic collision occurs when the total kinetic energy between two balls before and after a collision are the same. Therefore, kinetic energy is expected to remain constant over time.

Fig. 3 (LHS) shows the graph of system kinetic energy versus time for an ideal gas from the simulation. The system kinetic energy was calculated by summing the kinetic energy of every molecule and the container. To ensure the gas was an ideal gas, the radius of the molecules was set to be 0.1, which is 100 times smaller than the container.

Apart from the conservation of energy, momentum is also conserved as there is no external force exerted in the system.

The graph of momentum over time is plotted out in Fig. 3 (RHS). Momentum was obtained from summing momentum of each particle.

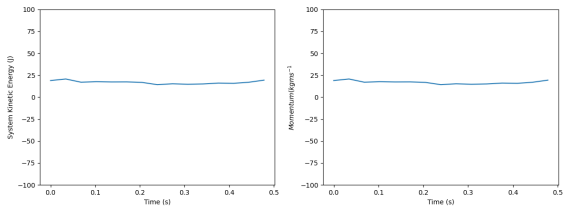

Fig. 3: System kinetic energy (LHS) and momentum (RHS) over time

B. Pressure (Task 11-Task 12)

The pressure on the wall of the container can be determined from the force exerted on the container over the circumference of the container. The force was measured by the change of momentum of a ball colliding with the container over a collision time.

The graph of Pressure P against Temperature T is a linear function with the gradient $\frac{Nk_B}{A}$ as shown in eq. 3.

$$P = \frac{Nk_B}{A}T \tag{3}$$

, where k_B is the Boltzmann constant. The number of particles and the area of the container are associated with the value of the gradient. The slope is flatter as A becomes smaller whereas the slope is steeper as N increases. Fig. 4 displays how P and T change when the radius of the container is changing.

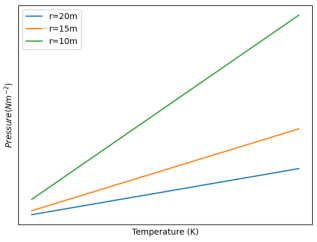

Fig. 4: The expected graph of pressure against Temperature varying with the radius of the container

C. Maxwell-Boltzmann distribution (Task 13)

The distribution is used to determine if the system is in an equilibrium state. Most of the systems do not initialise with an equilibrium state. However, the system is expected to evolve towards its equilibrium state following Maxwell distribution. Fig. 5 (LHS) shows our simulation of the speed of two-dimensional gases. In the plot, 200 hard spheres with a radius of 0.1m moving in a circular container were simulated. Fig. 5 (RHS) is the expected distribution of the speed approximating to Maxwell-Boltzmann distribution.

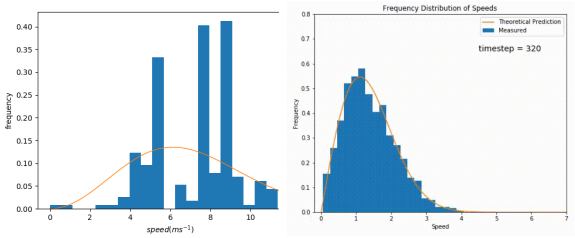

Fig. 5: Histogram of ball speeds approximating to Maxwell-Boltzmann distribution. LHS graph is generated by our simulation and RHS graph is taken from a source [1].

D. Van Der Waals' Equation (Task 14)

The ideal gas law only holds when particles are assumed to be dimensionless points and do not interact with each other. However, particles can participate in electrostatic interaction in the reality. When gas is pressurised or at a low temperature, the behaviours of the gas can no longer approximate to an ideal gas. The Non-ideal gas law can be described by van der Waals' equation (eq. 4).

$$(P + a(\frac{N^2}{v^2})(V - Nb) = Nk_BT \tag{4}$$

, where a is the correct factor for the inter-molecular attractive force and b is to adjust the total volume occupied by molecules.

However, there are no inter-molecular attractive forces in our simulation, which means a is zero. The equation can be rewritten as

$$P = \frac{Nk_BT}{V - Nb}N \tag{5}$$

Fig. 6 shows the expected graph of P against N obtained from the simulation. The measured pressure for non-ideal gases is expected to increase quicker than ideal gases as the number of molecules increases.

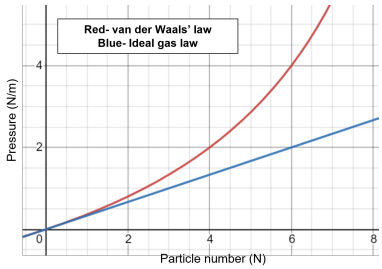

Fig. 6: The expected graph of P against T for ideal and non-ideal cases.

REFERENCES

[1] Wikipedia. *Maxwell–Boltzmann distribution*. Available from: https://en.wikipedia.org/wiki/Maxwell