Final Project
Thermal Statistical Mechanics in Particles Simulation

Stephen Hsieh 謝至剛 (109022205)
Lab group 10(Monday) Lab partner:Sheng-Chieh Chiu(109022125)
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In our project, By simply simulated the particles trapped in free space, which follow Newton’s law, also the conservation of motion and energy. We verify the Maxwell-Boltzmann distribution and also find the interesting phenomenon in the Kinetic Theory of ideal gases, such as thermal separation, heat transfer, thermal expansion, and adiabatic expansion.

I. INTRODUCTION

A. Kinetic Theory of Ideal Gases

Microscopic motions of ideal gases molecules can derive from Newtonian mechanic, and follow the rules below:

1. The gas consists of very large number of identical molecules which are in random motion.
2. The kinetic energy is purely translational (monatomic, no rotations and vibrations).
3. No interactions between molecules except elastic collisions between molecules and with walls (no potential energy, only kinetic energy).
4. The average distance between molecules is much larger than their diameters (consider it as a point particle, ignore its size effect).

Thus, molecules’ behavior can be simply described by the elastic collision of a rigid body.

B. Maxwell-Boltzmann distribution

Maxwell-Boltzmann distribution describe the speed probability distribution of an ideal gases at thermal equilibrium. It can derive by the assume bellow:

1. At equilibrium, the probability distribution no longer changes, but collisions continue occurring. Therefore, the probability of collision occurring forwardly must be equal to the probability of collision occurring backwardly.
2. The conservation of motion and energy.

Maxwell-Boltzmann distribution can be written as:

$$f(v) = 4\pi(\frac{m}{2\pi k_B T})^{3/2} v^2 e^{-mv^2/2k_B T} \tag{1}$$

Where $f(v)$ is the speed probability distribution, m is mass of one molecule, $k_B = 1.380649\times10{-}23(J/K)$ is Boltzmann constant, T is the Kelvin temperature of this system, v is the speed of molecules.

C. Thermal Separation

There are many ways to do thermal separation, such as compressor in the refrigerator, thermoelectric cooling module, vortex tube, but in our project, we are interested in a vortex tube.

The vortex tube is a mechanical device that separates compressed gas into hot and cold streams. The gas emerging from the hot end can reach temperatures of $200°C$, and the gas emerging from the cold end can reach $-50°C$. It has no moving parts, so it is widely used in industrial applications. The vortex simply injected the pressurized gas tangentially into the chamber and accelerated to a high rate of rotation. At the end of the tube, only the outer shell of the compressed gas is allowed to escape at that end. The remainder of the gas is forced to return in an inner vortex of reduced diameter within the outer vortex.

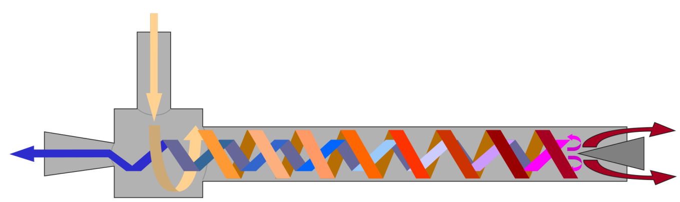

FIG. 1. Vortex tube separates hot and cold gases by injecting them tangentially into the chamber which leads to spinning.

II. METHOD

A. Reduce Operated time of Simulate

To detect whether each particle collides with another is a heavy workload to computer, so we develop an algorithm, it shortens the operating time significantly. Checking the collision of two particles far away is unnecessary, thus we cut the space in several chunks, and only judge the collision of the particles in each chunk separately; to prevent particles cannot collide at the boundary of two chunks, each chunk should overlap a little bit. It reduces the workload a lot for computers.

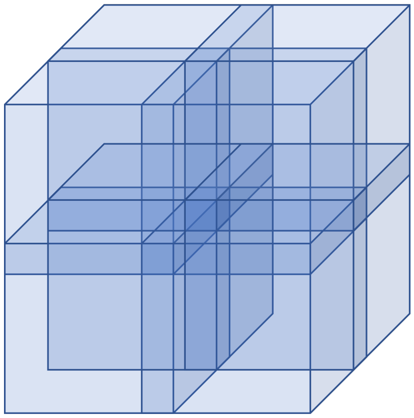

FIG. 2. Cut the space in several chunks, and only judge the collision of the particles in each chunk separately. It reduces the workload a lot for computers.

B. Check Maxwell-Boltzmann distribution

We trapped particles with initial average speed $v = 1(m/s)$ in three kinds shapes of free space, sphere, limitless long cylinder, and cube. For a limitless long cylinder, if particles pass through the upper and below boundary, there will be another particle appearing in another head with the same velocity.

Compared the speed probability distribution with theoretical Maxwell-Boltzmann distribution, and observed the speed distribution in space.

C. Change boundary effect to simulate different system.

We set up different boundary effects to make a simulation of vortex tube, a long pillar one side heats up and one side cool down, and the free space shape sphere expanding. To see thermal separation, heat transfer, thermal expansion, and adiabatic expansion.

III. RESULT AND DISCUSSION

An error will be huge in computer simulation if there is an extremely big or small value, to prevent this, we give those particles a slow speed compared to a realistic situation. However, it will lead to an extremely low temperature, so we use natural units as reference $k_B = 1(J/K)$ (so temperature T is not SI unit) and let gases molecules diameter $= 0.001(m)$.

A. Check Maxwell-Boltzmann distribution

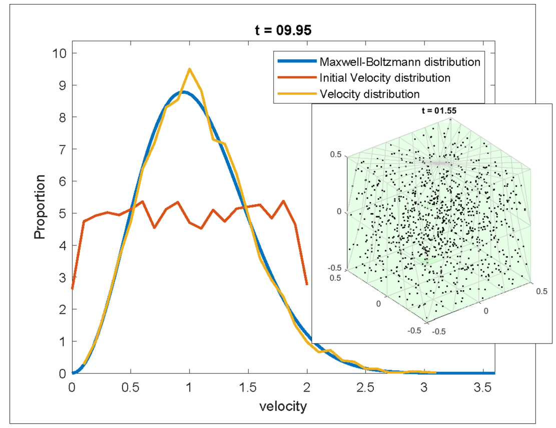

FIG. 3. 3000 particles with initial speed $v = 1(m/s)$ trapped in a cube which with length $1(m)$, will reach Maxwell-Boltzmann distribution after a while.

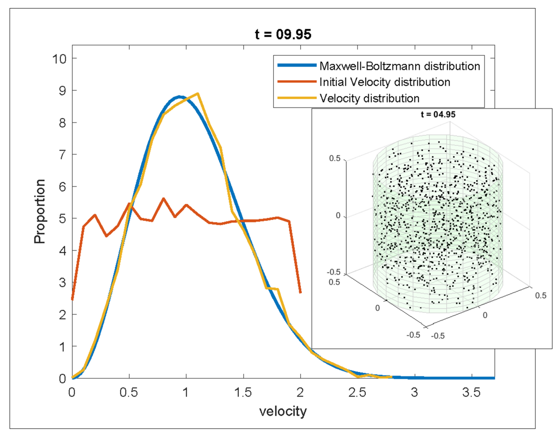

FIG. 4. 3000 particles with initial speed $v = 1(m/s)$ trapped in a limitless long pillar with radius $0.5(cm)$, will reach Maxwell-Boltzmann distribution after a while.

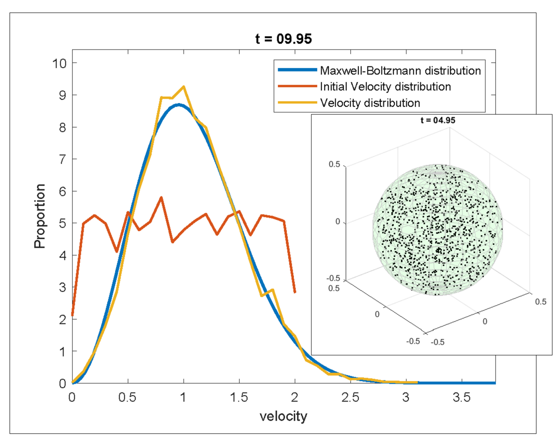

FIG. 5. 3000 particles with initial speed $v = 1(m/s)$ trapped in sphere which with radius $0.5(cm)$, will reach Maxwell-Boltzmann distribution after a while.

In this part, we show the speed probability distribution of an ideal gas with random velocity, which became close to the Maxwell-Boltzmann distribution after reaching the thermal equilibrium in three kinds of free space, and also verify that our simulation fit the theoretical expectations.

B. Simulation of Vortex Tube

We simulate the vortex tube by injecting gas tangentially into the pillar with high speed.

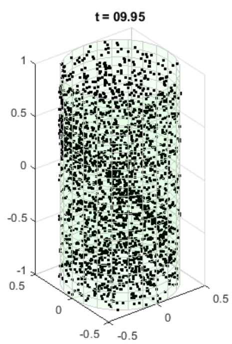

FIG. 6. Form a vortex tube in the pillar, we can see a whorl inside the tube.

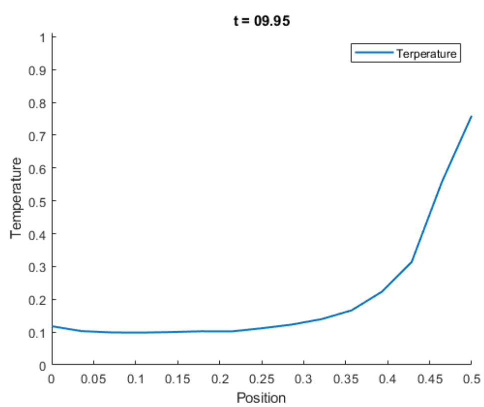

FIG. 7. Position(m) is the radius to the center of the tube, we see vortex tube can do the thermal separation.

In this part, we show the vortex tube does the thermal separation. And the inner part of the gas is colder than the outer one. It is because particles that spin faster will throw to the outer shell, they move with higher speed and higher temperature.

C. Simulation of Heater and Cooler

We simulate the heater by forming a vibrating panel as a boundary; the cooler by forming a boundary reduces the kinetic energy of particles after a collision.

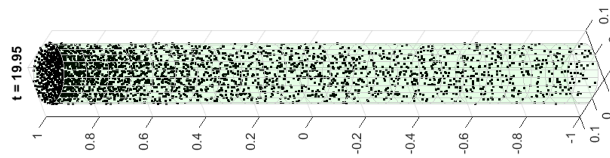

FIG. 8. A long pillar cooled from the left side and heated from the right side.

We see the particle density is high at where is cold and opposite at where is hot from the figure above. It shows the principle of thermal expansion.

Now, we turn off the heater and cooler, to see the process of heat balance.

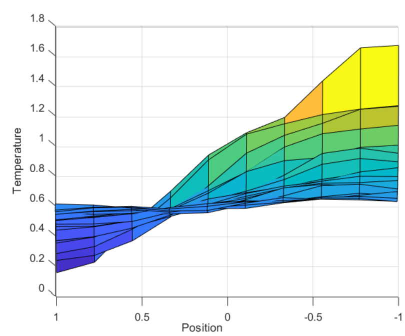

FIG. 9. It is a 3D plot of temperature to position against time, where position(m) is the length of the pillar. We choose the viewpoint to make the axis of time straight toward the reader, to see how temperature distributes in position.

We see the temperature at different positions become the same for a while from the figure above. However, in the beginning, the region, which the temperature is higher than the balance temperature, is bigger than which temperature is lower than the balance temperature. We think it is because the density is not uniform in the pillar.

We see the process of temperature balance is an exponential form to time.

In this part, we show the long pillar one side heats up, one side cool down. We can observe the phenomenon of thermal expansion. Moreover, we also see the process of heat balance is an exponential form to time. It is exactly in the theoretical expectations.

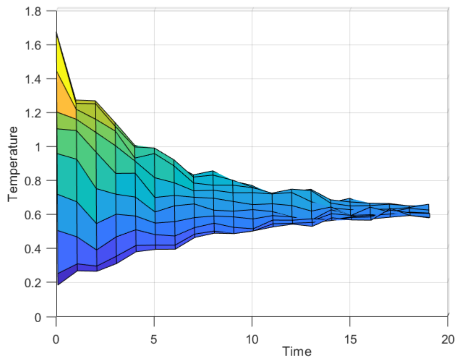

FIG. 10. It is a 3D plot of temperature to position against time, where t(s) is the time pass of the heat balance process. We choose a viewpoint to make the axis of position straight toward the reader, to see how temperature distribution goes to balance.

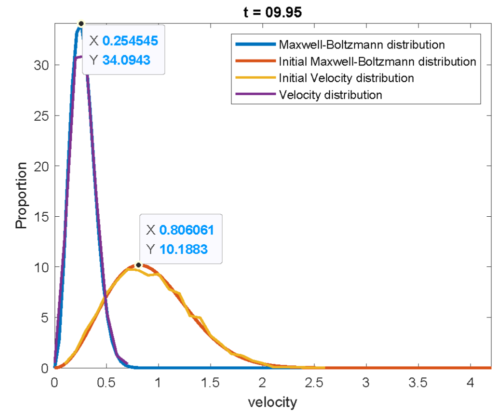

FIG. 12. The Maxwell-Boltzmann distribution of initial and final state.

D. Simulation of Adiabatic Expansion

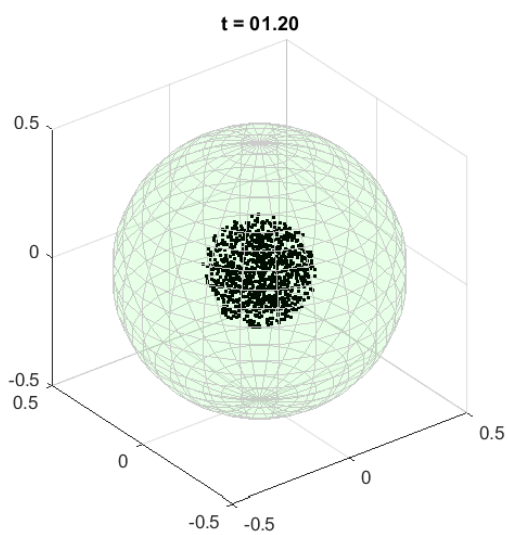

FIG. 11. The initial situation of particles. Start from a small volume and slowly expand the boundary to simulate adiabatic expansion. The area of the green sphere is the final boundary.

The radius of the boundary starts from 0.15m and ends at 0.5m. From the above graph, we know the velocity with maximum probability are 0.808(m/s) and 0.255(m/s) separately. The theory predicts that the temperature and volume in the adiabatic process will obey the equation:

$$TV^{\gamma-1} = Constant$$

where γ is the adiabatic index. In this simulation, it is 5/3. We can calculate the ratio of the constant before and after the expansion:

$$\frac{T_i V_i^{2/3}}{T_f V_f^{2/3}} = \frac{v_{imax}^2 R_i^2}{v_{fmax}^2 R_f^2} = 0.95 \approx 1$$

It is in line with the prediction, and the error of the ratio may be contributed from the volume of the particles themselves.

IV. CONCLUSION

In this simulation, we only used simple theory, Newton' s law, and the elastic collision of a rigid body, but we still observed many important phenomenon. Such as Maxwell-Boltzmann distribution, thermal separation, heat transfer, thermal expansion, and adiabatic expansion. It shows the importance of fundamental science.

On the other hand, the special algorithm we developed is also important which reduced the operating time of simulation significantly, without this algorithm, we could only waste time on endless simulation but do nothing.

If we could go further, the code in this simulation might analyze properties deeply. Such as kinetic theory of gases, which by defining the pressure on the wall, we could even build a model of a thermal engine. Or, we can add a combination reaction in the particle collision, then check the increasing or decreasing of the temperature whether obey the theory.

[1] Z.S. Spakovszky. Unified: thermodynamics and propulsion (Lecture notes), Massachusetts Institute of Technology, Cambridge, Mass. 2007. ch. 12.3.

[2] Hilsch, Rudolf (1947). "The use of the expansion of gases in a centrifugal field as cooling process". Review of Scientific Instruments.

[3] Feynman, R. P., Leighton, R. B., Sands, M. L. (1963). The Feynman lectures on physics. Reading, Mass: Addison-Wesley Pub. Co.

[4] Vortex tube. Retrieved from Wikipedia (November 28)

[5] Natural units. Retrieved from Wikipedia (November 28)