Maxwell-Boltzmann Distribution and Molecular Dynamics

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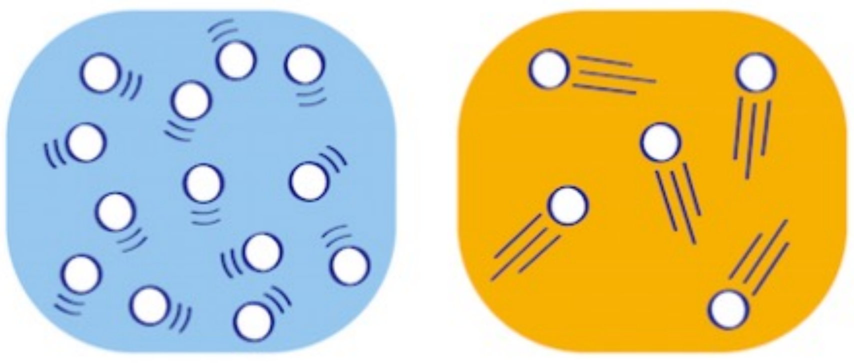
Background Information

- The air molecules surrounding us are not all traveling at the same speed, even if the air is all at a single temperature.
- Mid to late 1800s, James Clerk Maxwell & Ludwig Boltzmann discovered the **Maxwell-Boltzmann distribution** that answers the question **"What is the speed of an air molecule in a gas?"**
- In this program, I attempted to model gas molecule behaviors in a constant temperature controlled by two types of thermostat.
- **Do my gas molecules follow the Maxwell-Boltzmann distribution? How "stable" is the distribution? Which thermostat works better?**



cold air   hot air

Computational Details

Molecular Dynamics: trajectory of a system of atoms

- **Verlet Method**: integrate Newton's equations of motion
- **Lennard-Jones potential**: models soft repulsive and attractive interactions between molecules under Van der Waals forces

$$V_{\mathrm{LJ}}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

Thermostats: when modeling ideal gas behavior, it's crucial to maintain a relatively constant temperature (on average).

- **Isokinetic thermostat**: rescales all velocities with constant λ

$$\lambda = \sqrt{T/T_i}$$

- **Berendsen thermostat**: rescales all velocities with constant τ

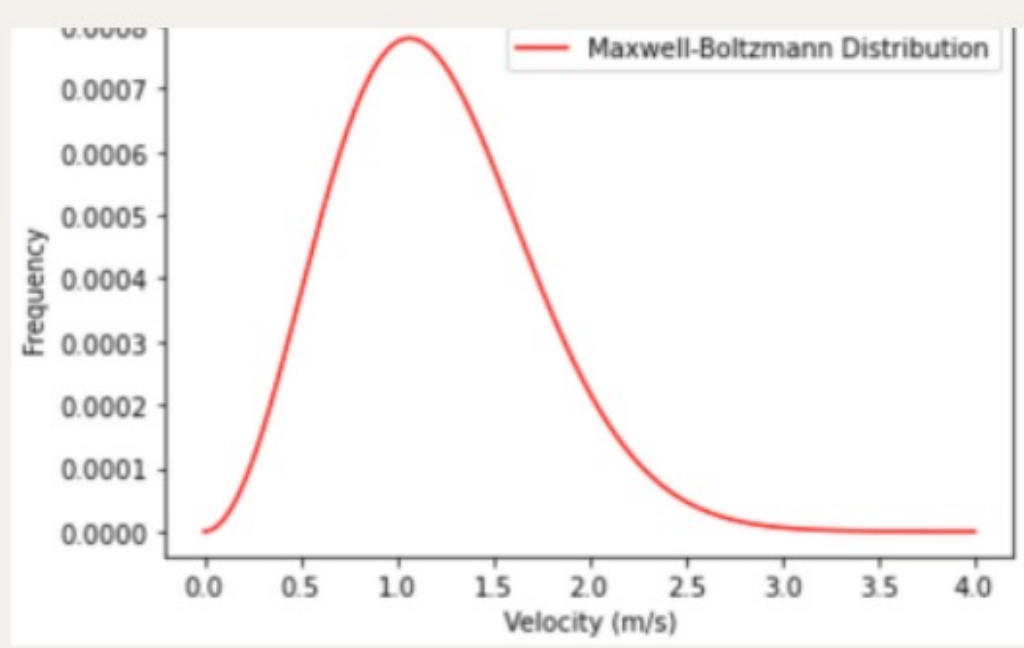
$$\frac{dT}{dt} = \frac{T_0 - T}{\tau}$$

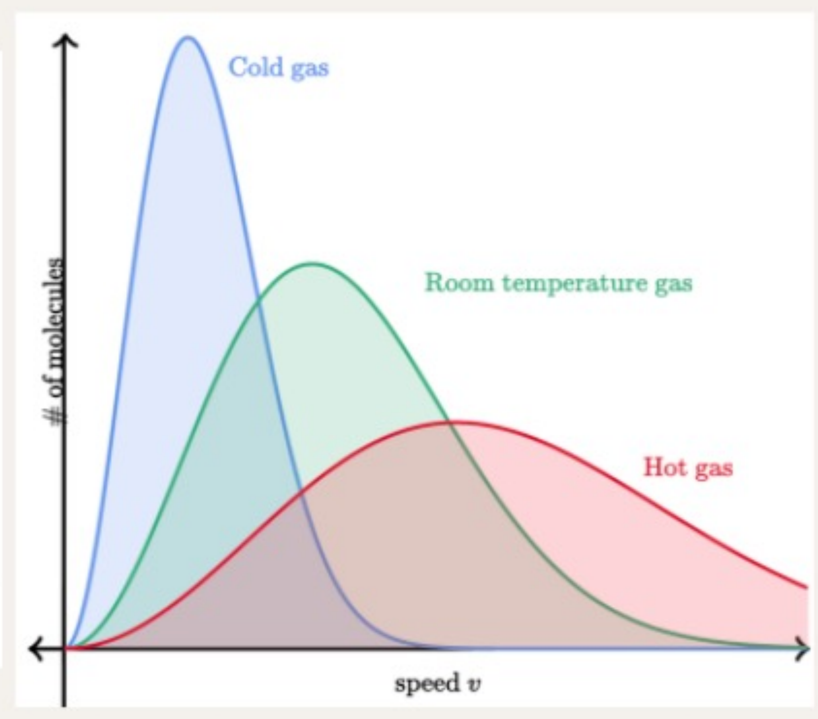
Results

$$P(s < |\vec{v}| < s + ds) = \frac{ms}{kT}\exp\left(-\frac{ms^2}{2kT}\right)ds$$

Expectation:

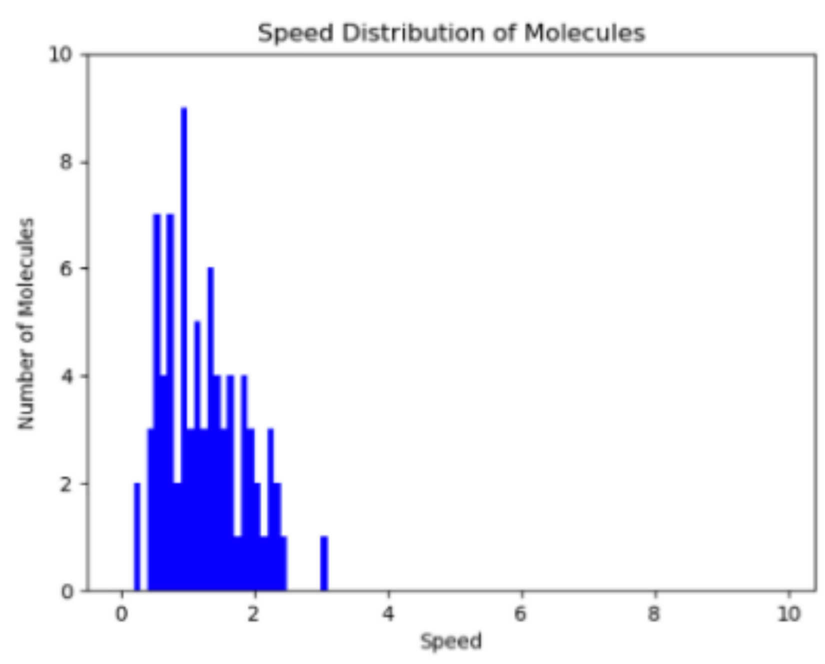
- **Maxwell-Boltzmann distribution**: a probability distribution function depicting particle speeds in idealized gases.
- Higher temperature, graph becomes shorter and wider.
- Lower temperature, graph becomes taller and narrower.



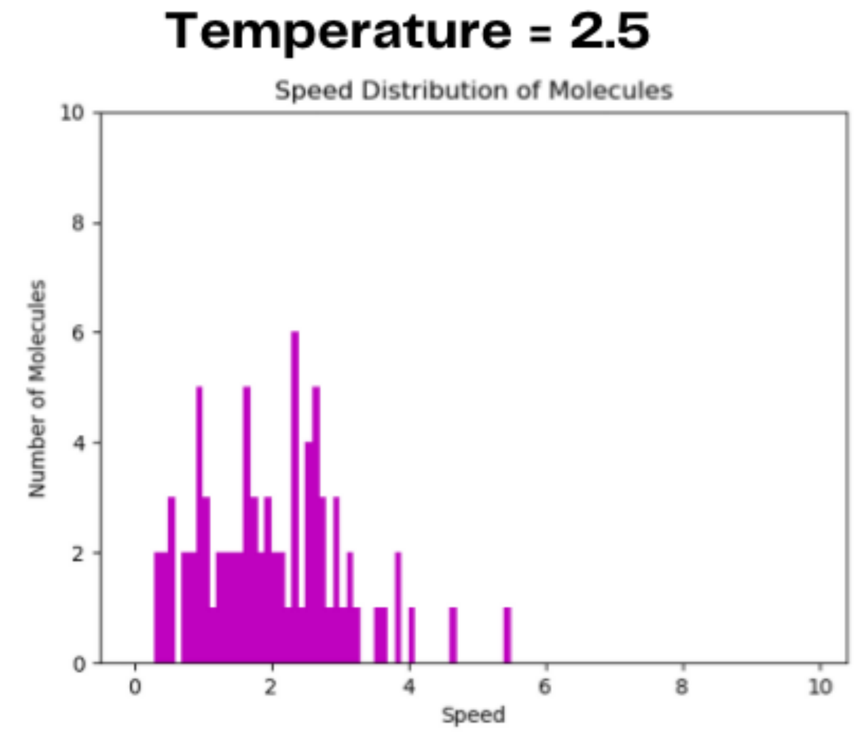


Temperature = 1.0 | **Temperature = 2.5** | **Temperature = 20.0**

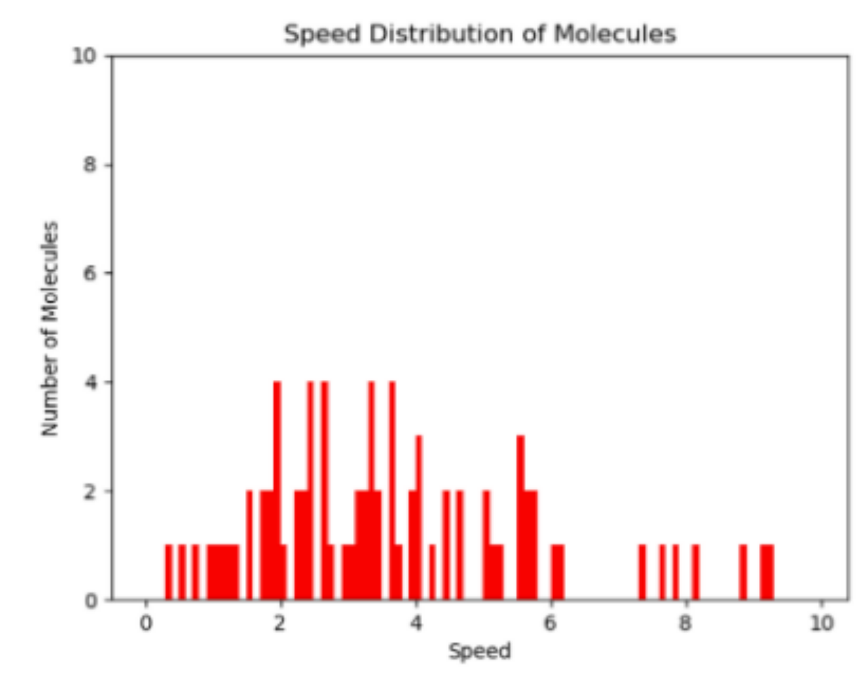
Isokinetic Thermostat



Most particle speed cluster around 0.8-1.2.

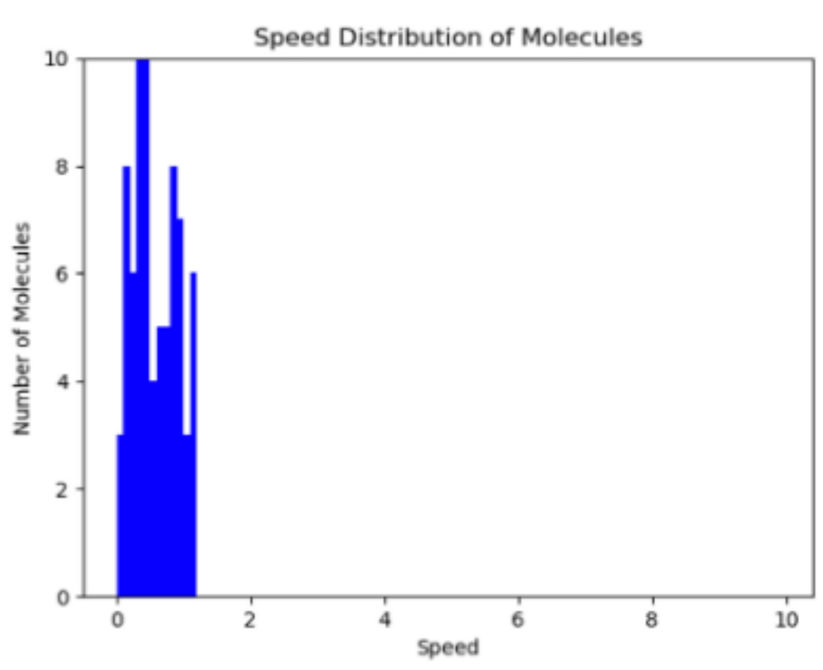


Majority particle speed cluster around 1.9-2.5, overall more spread out.

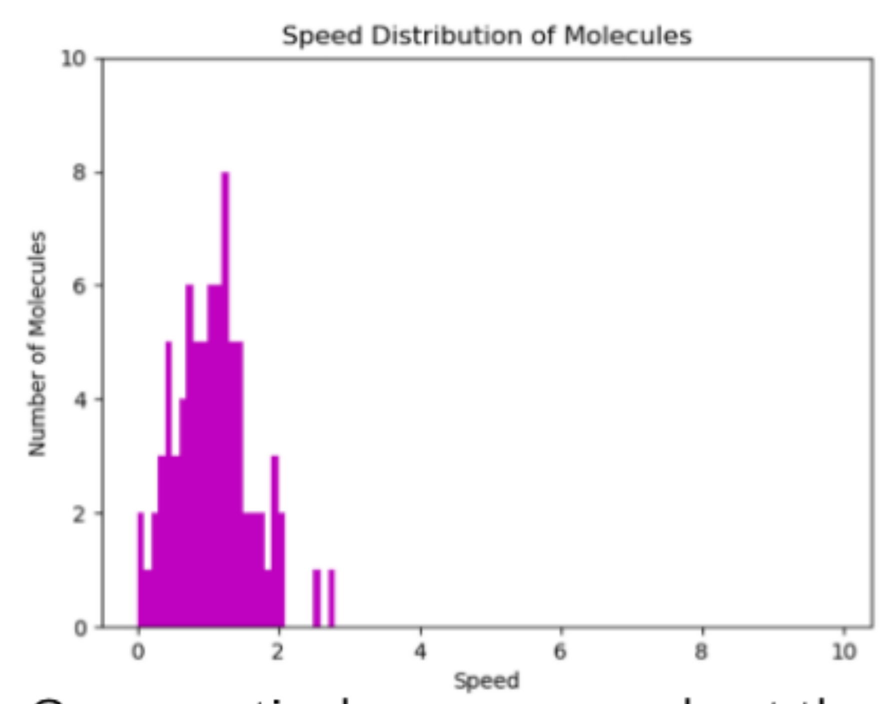


No major speed cluster; most spread out compared to other temperatures.

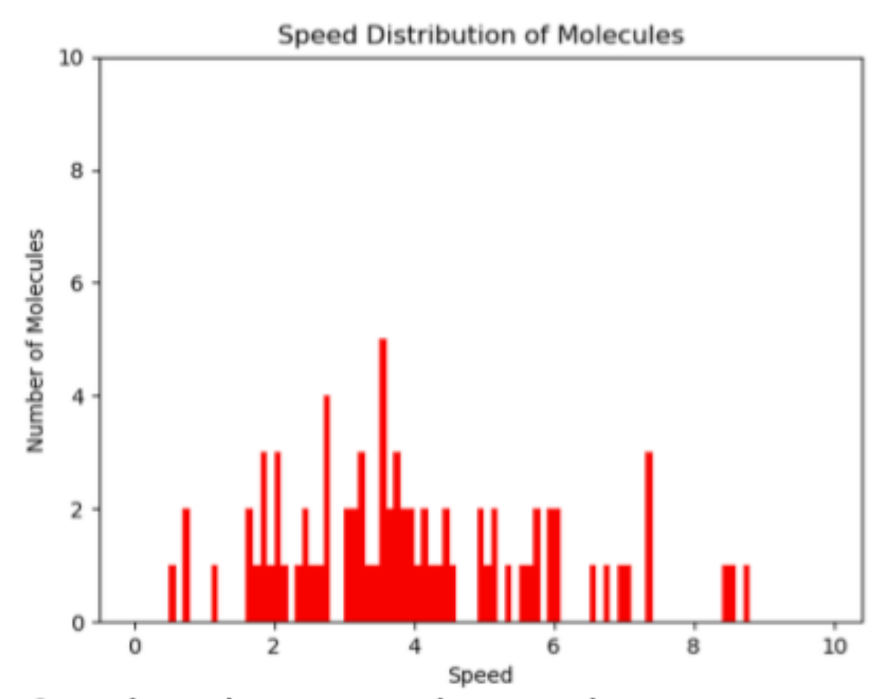
Berendsen Thermostat



Even clearer speed clustering around 0.3-0.5, no speed ever exceeds 2.



Comparatively more spread out than temp = 1.0, but more condensed than Isokinetic thermostat condition.



Similar shape to the Isokinetic thermostat condition, slightly more condensed between 3.2-3.6.

Conclusion

- Overall, the gas molecules do follow the Maxwell-Boltzmann distribution pretty closely.
- As time goes on and the gas particles keep colliding with one another, the speed distribution approximates Maxwell-Boltzmann distribution more. While the distribution never stays "stable", it does mimic the general shape that we are expecting.
- For the purpose of analyzing particle speed distribution in different constant temperature, I find the **isokinetic** thermostat to display greater changes than the Berendsen thermostat does. However, this doesn't necessarily make isokinetic thermostat "better", just that the results are easier to see by eyes.
- There are other experiments conducted that also verified the Maxwell-Boltzmann distribution via something called a "velocity selector". It consists of several spinning wheels that ensures only gas particles with a certain velocity will pass through all the holes as the wheels are spun at various rates. However, such technology is difficult and expensive to manufacture, so testing the hypothesis computationally, though permitting some small errors, will still be more optimal.