Project1 - FYS4460

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a) Maxwell Boltzman distribution

I simulated a $15 \times 15 \times 15$ system with face-centered-cubic packing resulting in 13500 particles. The temperature was set to $T' = 2.5[T_0]$ and I simulated for 30000 timesteps with default timestep length 0.005τ. see script a.in for more details. Then i looked at the velcity distribution for the last timestep as shown in figure 1. I calculated the inner product:

$$\frac{\sum_i h_i(t)h_i(t_n)}{\sum_i h_i(t_n)^2} \tag{1}$$

where h_i is the height of bin i in the histogram and t_n is the final time-step. This is shown in figure 2. By this we see that the distribution indeed converges towards the distribution shown in 1

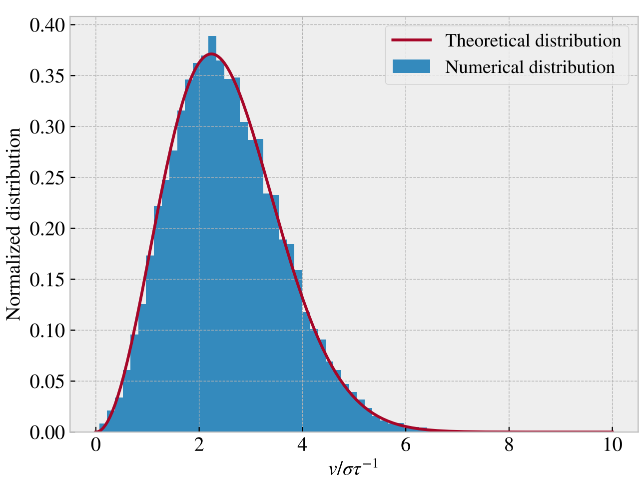

FIG. 1. Velocity distribution for the final time-step t_n in the simulation. This matches nicely with the theoretically Maxwell-Boltzman distribution.

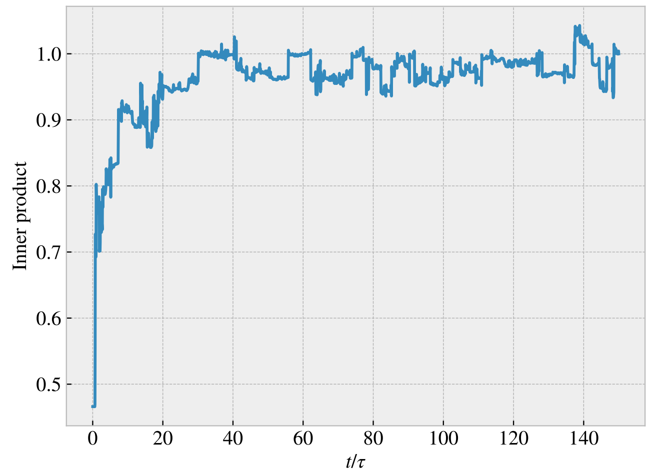

FIG. 2. Inner product as shown in equation 1. We see that it converges and stay around one quite early which shows that Maxwell-Boltzmann distribution is the steady state for this system.

b) Total energy

We user the script b.in, where we output the total energy with the fix ave/time command. We look at the development of the total energy over time for different timesteps as showed in figure 3

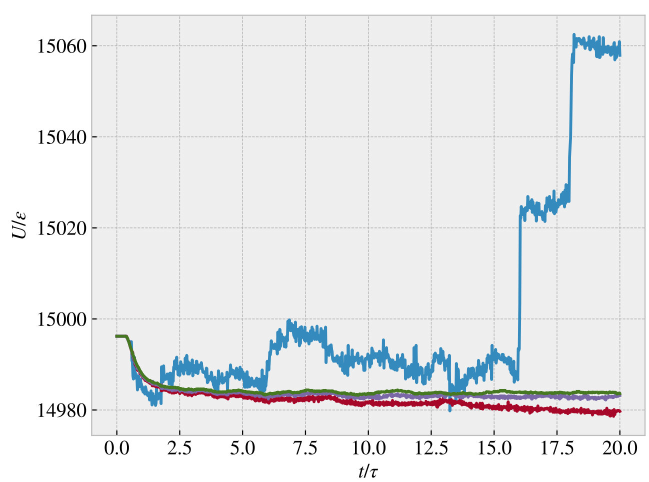

FIG. 3. Total energy over time for different timesteps dt.

We see as expected that the energy fluctuations is bigger for bigger dt.

c) Temperature

We now use the equipartition principle:

$$\langle E_k \rangle = \frac{3}{2} N k_b T \tag{2}$$

where E_k is the kinetic energy, N the number of particles, k_b Boltzmann's constant and T is the temperature. By using this relation we find the temperature in simulations as showed in figure 5

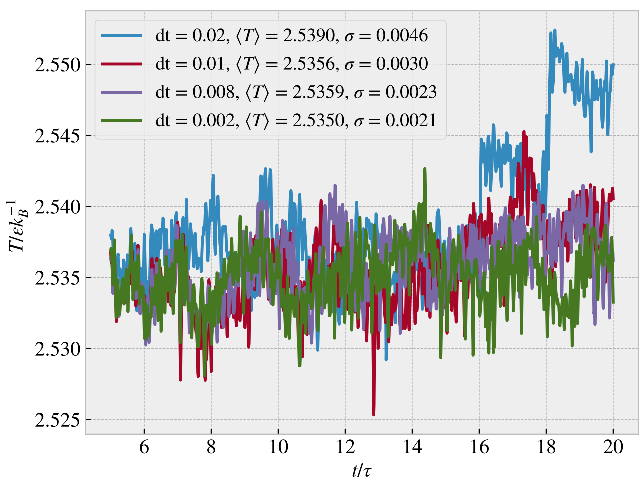

FIG. 4. Estimated temperature using equation 2 over time for different timesteps dt.

We initialized the simulations with temperature $T = 2.5$ which corresponds quite good to the mean value found here. All though we see a general ofsett of ≈ 0.035 comparied to the initialized value of 2.5. By looking at the standard deviation σ, we see that the fluctuations lower with decreasing dt

In order to see how thee fluctuations depends on the system size we also ran a series of simulations with fixed $dt = 0.002$ but increasing system size. This is shown in figure **??**

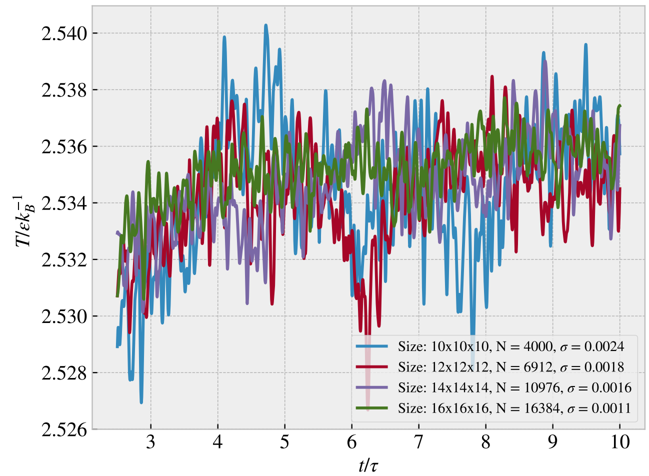

FIG. 5. Estimated temperature using equation 2 over time for different system sizes $a \times b \times c$ measured in number of unit cells. Each unit cell contains 4 atoms, which gives a total of $N = 4abc$ atoms.

We see that the fluctuations also gets smaller for bigger systems.

d) Pressure as function of temperature

I made a series of simulations at different temperature, let it stabilze and then collected the average values for the pressure and the temperature. By plotting $P(T)$ together with a linear model we get the result showed in figure 6

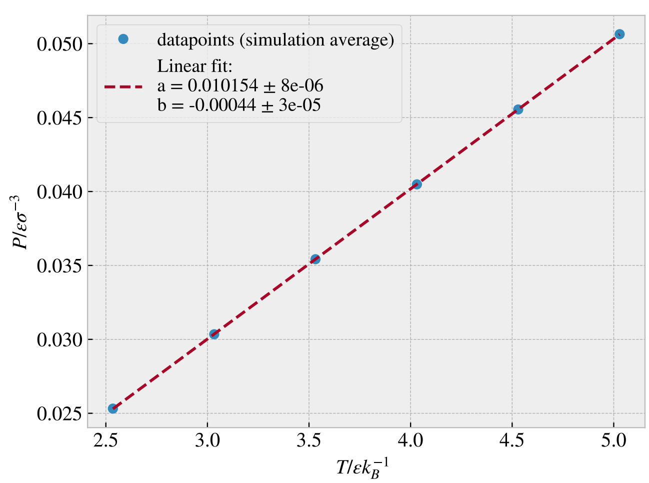

FIG. 6. Average measurements of Temperature and pressure in stabilized simulations. The linear fit confirms the proporitonality between pressure and temperature as stated by ideal gas law.

We see that the result fit nicely to a linear model. This match with the ideal gass law:

$$PV = NkT$$

where pressure and Temperature are proportional.

e) Pressure as function of both temperature and density

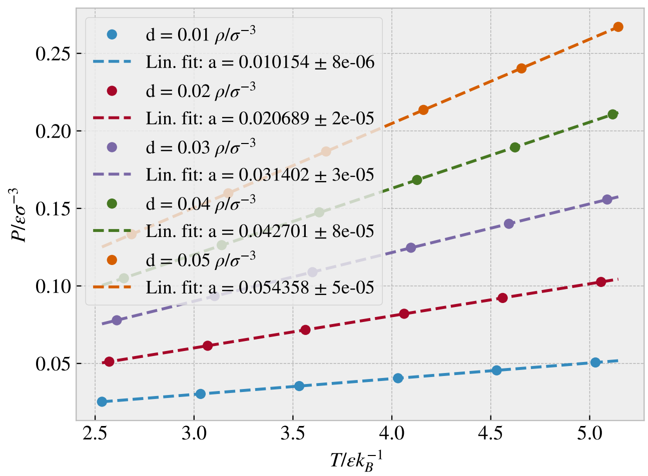

FIG. 7. Pressure as function of temperature at different densities.

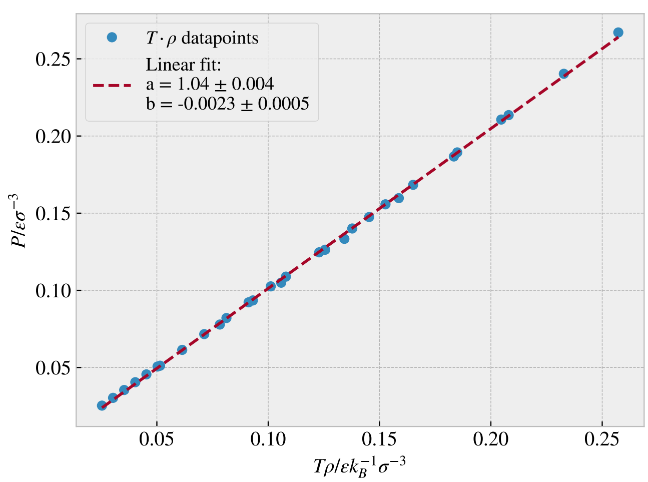

FIG. 8. Pressure as funciton of the product temperature times density.

From the figures wee see that

$$\frac{P}{T\rho k_B} \approx 1.04$$

From ideal gas law we have

$$\frac{P}{T\rho k_B} = \frac{1}{m}$$

This gives $m = 1/1.04 = 0.097 \approx 1$. This match with the settings of setting $m = 1$ in lammps. For different masses we would se the change in the slope here ...?