Molecular Dynamics

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Theory

100 particles is placed in a crystal lattice in the left side of 30 by 30 box. Calculating the Force using the Lennard jones formula:

$$F = \sigma(\frac{-6}{r^7} - \frac{-12}{r^{13}})$$

The system trajectory is obtained by velocity verlet diffrential solving method. Reduced units are used for faster simulations.

Results

The initial states is shown below:

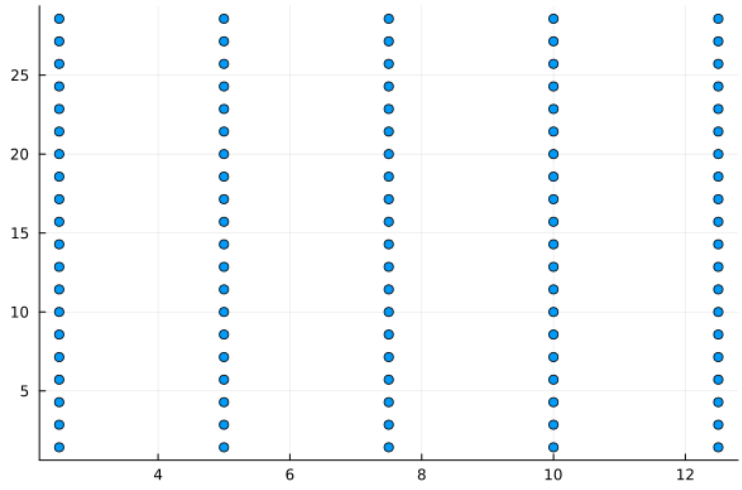

Figure 1: crystal lattice

after 3000 velocity verlet step the system would look like this:

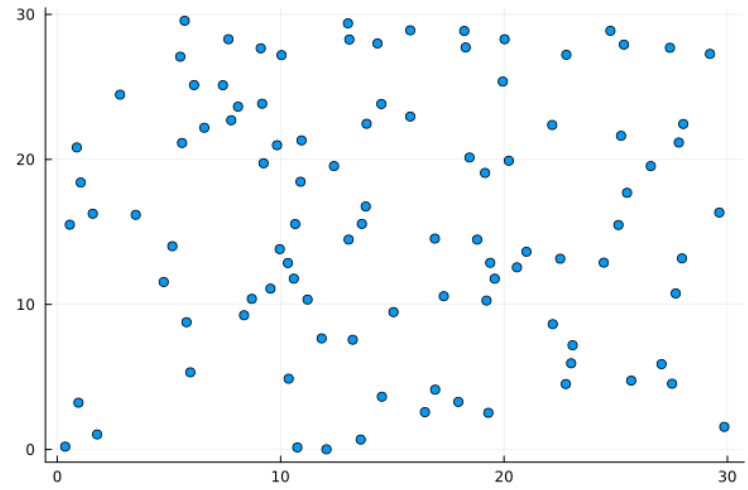

Figure 2: the state after 3000 velocity verlet steps.

The gif is also available in the attached files. The number of molecules in the left side over time is plotted.

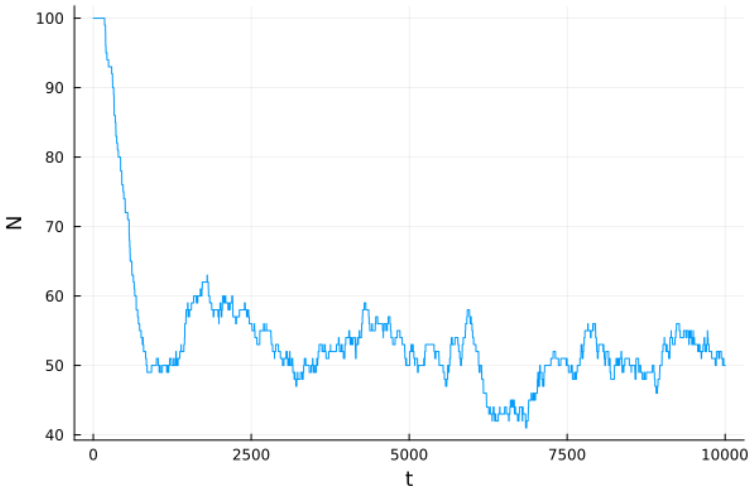

Figure 3: Number of Molecules in the left side after 10000 steps.

We analyze the energy conservation by saving the Lennard jones potential in VelVerlet function. The result is shown below:

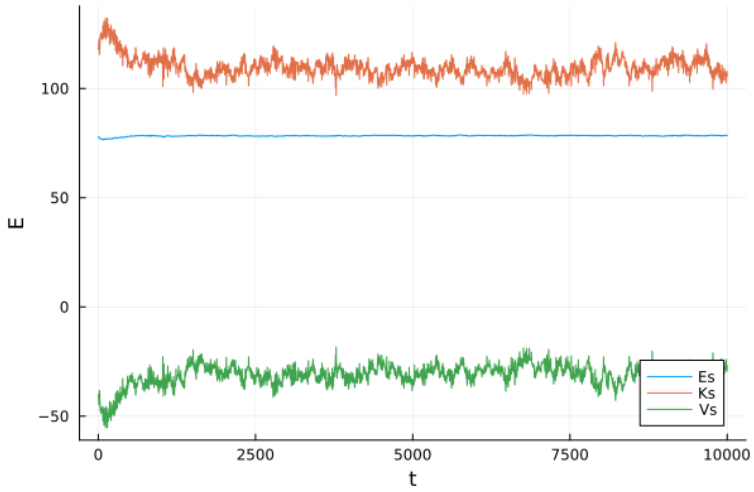

Figure 4: Energy conservation

Auto-Correlation of velocities is also calculated:

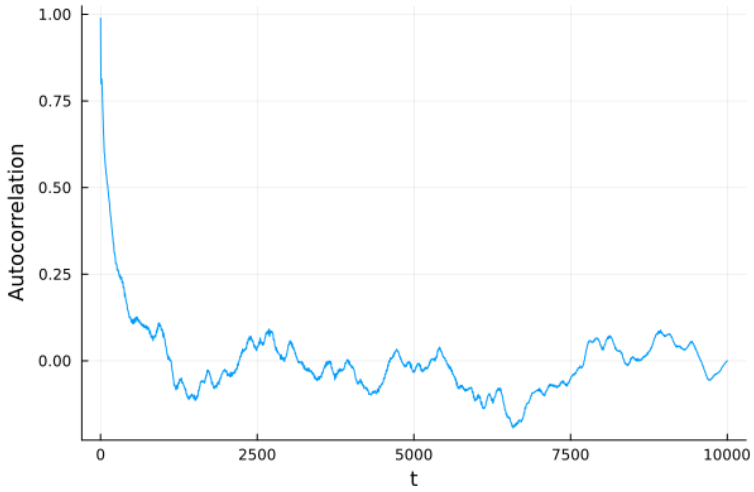

Figure 5: Auto-Correlation of velocities

Temperature is calculated useing kinetic energy:

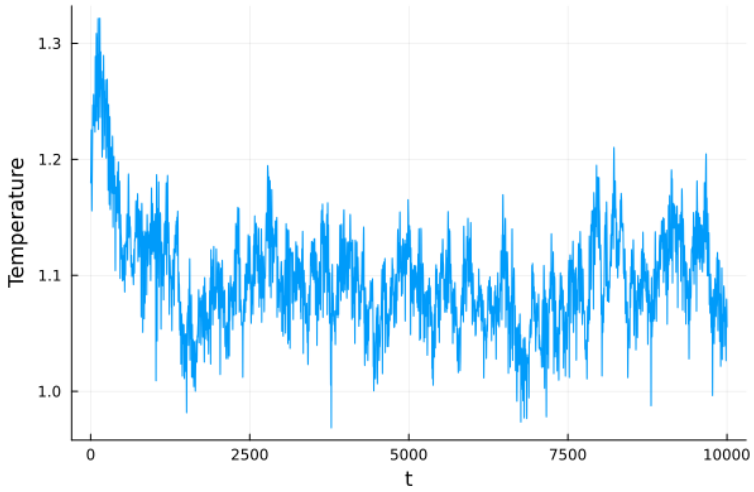

Figure 6: Temperature over time step

Pressure is calculated using virial theoream:

$$P = \frac{NkT}{V} - \frac{\sum_i F_i.r_i}{3V}$$

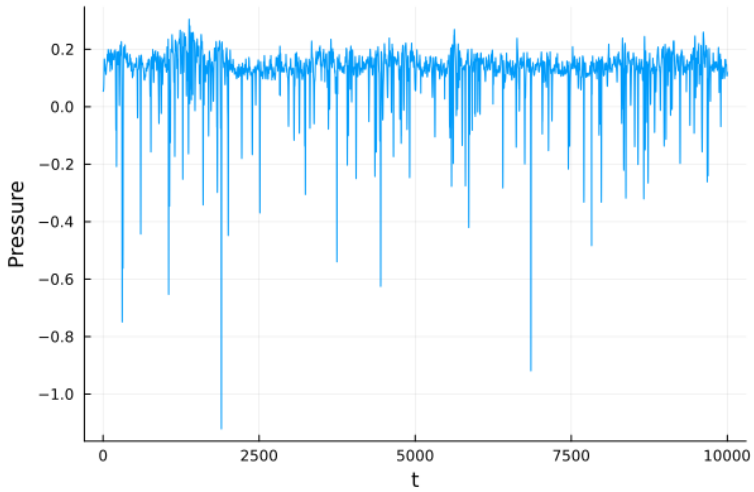

Figure 7: Pressure over time step

fiting a line to P over T graph we aim to find the Wan der Vaals coefficents.

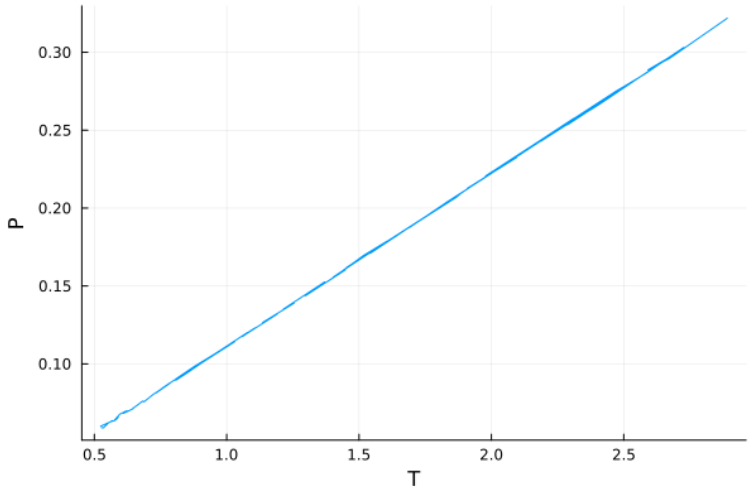

Figure 8: Pressure over Temperature after 50 millions velocity verlet steps.

$$slope = 0.11101$$
$$intercept = 0.00023$$

Phase transition is observes scaling the velocities by 0.5 coefficent every 100 steps for 10000 velocities verlet steps.

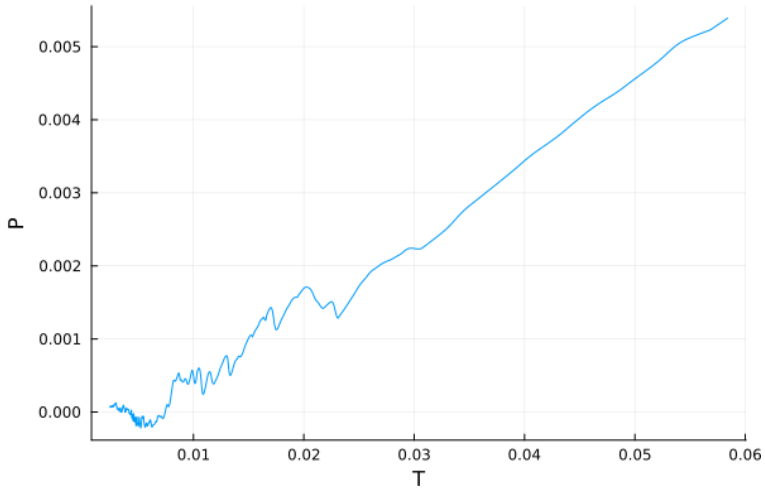

Figure 9: Phase transition in P-T diagram