

Exercise week 36: FYS2160, Thermodynamics and statistical physics

1 Install Lammmps and run first simulation

Follow the instructions in [the lecture notes](#) to install Lammmps and start your first simulation. All the necessary files can be found on the same page.

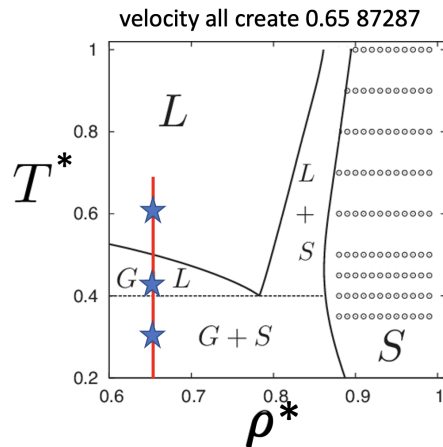


Figure 1: The phase diagram of the 2 dimensional Lennard-Jones model. L = liquid, G = gas and S = solid. The Lammmps input line "velocity all create 0.65 87287" creates a system with reduced LJ density $\rho^* = N\sigma^3/V = 0.65$ which is indicated by the red line. The stars indicate where in the phase diagram simulations at $T^* = k_B T/\epsilon = 0.3, 0.45$ and 0.6 are situated, that is, in the gas-solid, gas-liquid and supercritical liquid regions, respectively.

In the input file `in.myfirstmd` comment the line with "nve" and uncomment the line with "nvt" to make Lammmps run the simulation at constant temperature:

```
# Define thermodynamic ensemble
fix 1 all nvt temp 0.3 0.3 0.3
# fix 1 all nve
```

1. Run the simulation and visualise the output with Ovito.
2. Change the temperature to 0.45:

```
fix 1 all nvt temp 0.45 0.45 0.45
```

rerun and visualise

3. Change the temperature to 0.6 and repeat.
4. Relate your observations from the visualisations to the phase diagram in Figure 1.
5. If your computer is fast enough, increase the system size to 100 times 100 unit cells

```
region simbox block 0 100 0 100 -0.1 0.1
```

and repeat the simulation.

2 Dimensionless Lennard-Jones units

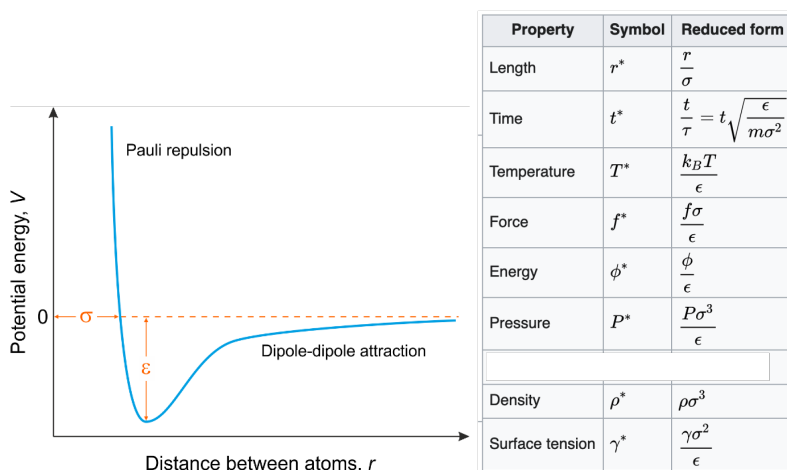


Figure 2: The Lennard-Jones potential and reduced (dimensionless) LJ units.

The Lennard-Jones potential expresses the interatomic potential energy U as function of distance r between the atom centres:

$$U(r) = 4\epsilon \left(\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right), \quad (1)$$

where σ is the atomic diameter and ϵ is the strength of the interatomic attraction. It is practical to use dimensionless units when working with simulations on the LJ model. The dimensionless units, often called "reduced" or "LJ" units are obtained by dividing by the pertinent combination of the LJ parameters m , σ and ϵ and are indicated by an asterisk subscript. For example length $r^* = r/\sigma$,

energy $U^* = U/\epsilon$, temperature $T^* = k_B T/\epsilon$, number density $\rho^* = N\sigma^3/V$ and pressure $P^* = P\sigma^3/\epsilon$.

Argon can be modelled using Lennard-Jones units with the following parameters: $m = 6.6 \cdot 10^{-26}$ kg, $\sigma = 3.4$ Å and $\epsilon/k_B = 120$ K

1. Argon has critical temperature $T_c = 150$ K, pressure $P_c = 4.9$ MPa and (mass) density $\rho_c = 536$ kg/m³. What are the reduced critical temperature T_c^* , pressure p_c^* and number density ρ_c^* of the critical point when using the LJ parameters for argon?
2. How does that compare to the critical point of the LJ model $T_c^* = 1.32$, $p_c^* = 0.13$ and $\rho_c^* = 0.32$?
3. If you wish to do a simulation of Argon at ambient conditions, $T = 293$ K, $P = 10^5$ Pa, which reduced pressure and temperature do you have to choose for your simulation?