1   Install Lammps and run first simulation

Follow the instructions in the lecture notes to install Lammps and start your first simulation. All the necessary files can be found on the same page.
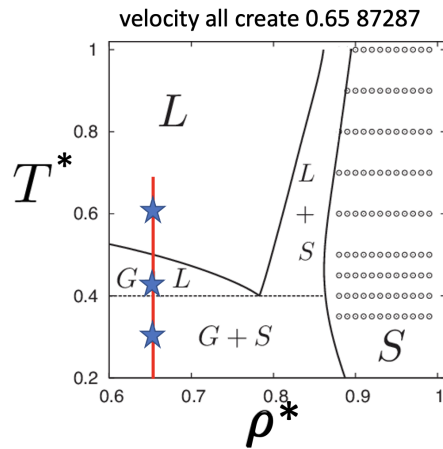

Figure 1: The phase diagram of the 2 dimensional Lennard-Jones model. L = liquid, G = gas and S = solid. The Lammps input line "velocity all create 0.65 87287" creates a system with reduced LJ density $\rho^* = N\sigma^3/V = 0.65$ which is indicated by the red line. The stars indicate where in the phase 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 Lammps 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
```
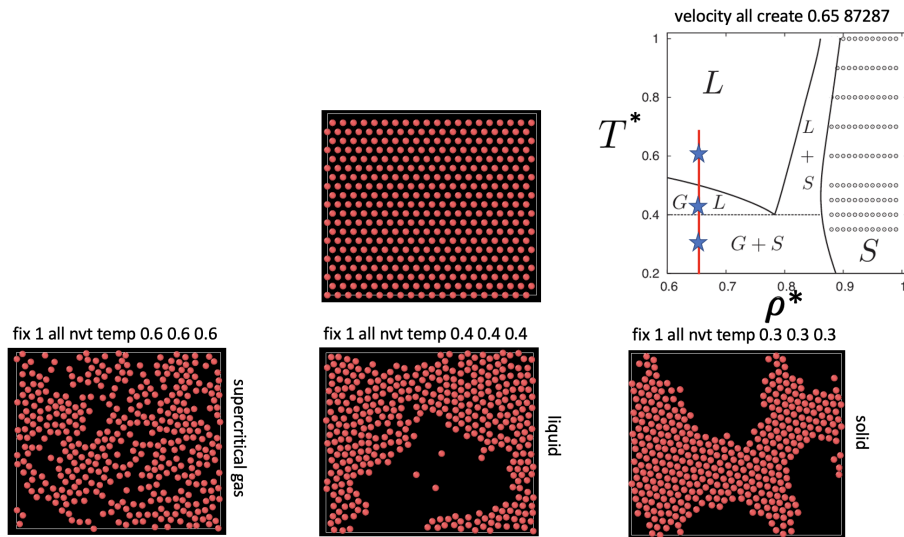
and repeat the simulation.

Solution:

Figure 2: Initial configuration (crystalline structure) and output of simulations at $T^* = 0.3$, 0.4 and 0.6. The blue stars along the red line ($\rho^* = 0.65$) At the lowest temperature the state is in the gas + solid (G+S) part of the phase diagram and the output shows a crystalline solid with voids with gas (a particle from time to time). At the intermediate temperature the solid has melted to a liquid (the atoms are disordered and move around each other) and the system is in the liquid + gas (L+G) state. At the highest temperature the atoms are not as closely bound together and there is only one state that we call the supercritical gas state.

2 Dimensionless Lennard-Jones units

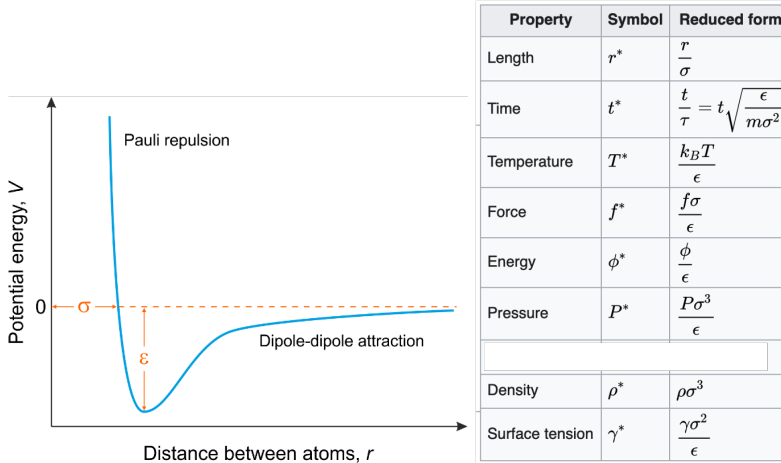| Property	Symbol	Reduced form
Length	r^*	$\dfrac{r}{\sigma}$
Time	t^*	$\dfrac{t}{\tau} = t\sqrt{\dfrac{\epsilon}{m\sigma^2}}$
Temperature	T^*	$\dfrac{k_B T}{\epsilon}$
Force	f^*	$\dfrac{f\sigma}{\epsilon}$
Energy	ϕ^*	$\dfrac{\phi}{\epsilon}$
Pressure	P^*	$\dfrac{P\sigma^3}{\epsilon}$
Density	ρ^*	$\rho\sigma^3$
Surface tension	γ^*	$\dfrac{\gamma\sigma^2}{\epsilon}$

Figure 3: 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:

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

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 asterix 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/m^3. 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?

   Solution:

   $$T_c^* = \frac{k_B T_c}{\epsilon} = \frac{150}{120} = 1.25$$

   $$p_c^* = \frac{P_c\sigma^3}{\epsilon} \approx \frac{(4.9 \times 10^6) \times (3.4 \times 10^{-10})^3}{120 \times 1.3 \times 10^{-23}} \approx \frac{4.9 \times 39.3}{12 \times 13}10^{-1} \approx 0.12$$
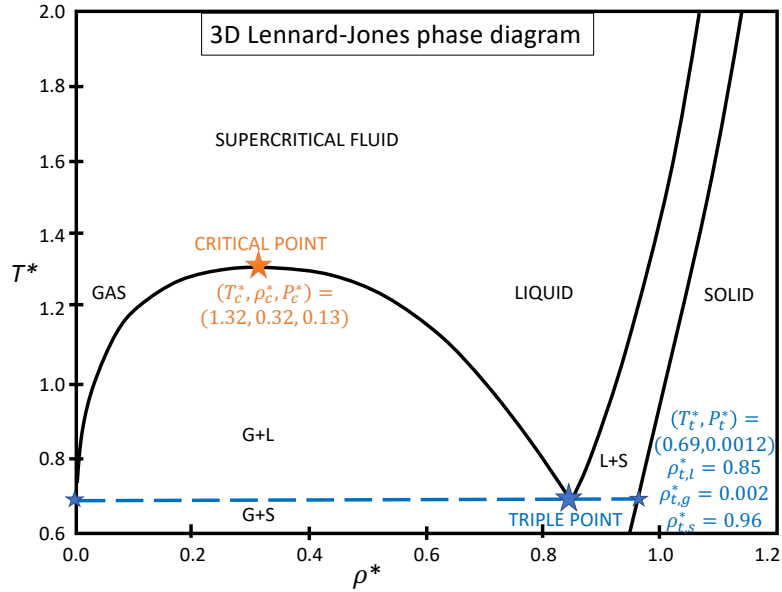
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Figure 4: 3D phase diagram of LJ model.

$$\rho_c^* = \frac{\rho_c \sigma^3}{m} = \frac{536 \times (3.4 \times 10^{-10})^3}{6.6 \times 10^{-26}} = \frac{536 \times 39.3}{6.6} 10^{-4} \approx 0.32$$

2. How does that compare to the critical point of the LJ model $T_c^* = 1.32$, $p_c^* = 0.13$ and $\rho_c^* = 0.32$?

   Solution:
   It is closely comparable in value to the critical point of the LJ model.

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?

   Solution:
   We would have to rescale this T and P by the same units as in sub problem 1 above. Thus, we have that

   $$T^* = \frac{k_B T}{\epsilon} = \frac{293}{120} \approx 2.4$$

   $$p^* = \frac{P \sigma^3}{\epsilon} = \frac{10^5 \times (3.4 \times 10^{-10})^3}{120 \times 1.3 \times 10^{-23}} \approx \frac{39.3}{12 \times 13} 10^{-2} \approx 0.25 \times 10^{-2}$$

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One observes from the LJ phase diagram in Figure 4 that this is clearly in the supercritical fluid region.