8 Off-lattice Monte Carlo simulations

Reduced units (pen&paper) Typical sets of parameters for Argon and Krypton are $\sigma_{Ar} = 3.41\overset{\circ}{A}$, $\sigma_{Kr} = 3.38\overset{\circ}{A}$ for their typical size and $\epsilon_{Ar}/k_B = 119.8K$ and $\epsilon_{Kr}/k_B = 164.0K$.

- At the reduced temperature $T^* = 2$, what is the temperature of Argon and Kelvin?

- A typical value of the integration time step for MD is $\Delta t = 0.001\tau$. Convert it into SI units for Argon and Krypton.

Off lattice Monte Carlo of Lennard Jones particles The Lennard-Jones interaction is a paradigmatic interaction potential, used in different contexts. It reads

$$V_{\text{LJ}}(r) = \begin{cases} 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right] & \text{for } r < \sigma_{cut} \\ 0 & \text{for } r \geq \sigma_{cut} \end{cases} \tag{1.19}$$

where $\sigma = 1$, $\epsilon = 1$ are the units of length and energy and σ_{cut} is the so-called cut-off length and is set, for this exercise, to half the box size. Beyond this cut-off, we introduce two tail corrections: one for the energy (per particle)

$$u^{tail} = \frac{8}{3}\pi\rho \left[\frac{1}{3}\left(\frac{\sigma}{\sigma_{cut}}\right)^9 - \left(\frac{\sigma}{\sigma_{cut}}\right)^3 \right] \tag{1.20}$$

and one for the pressure

$$P^{tail} = \frac{16}{3}\pi\rho^2 \left[\frac{2}{3}\left(\frac{\sigma}{\sigma_{cut}}\right)^9 - \left(\frac{\sigma}{\sigma_{cut}}\right)^3 \right] \tag{1.21}$$

Write a simple Monte Carlo code, following the scheme detailed in class. Perform two sets of simulations, one at reduced temperature $T^* = 2$ (above the critical temperature) and one at $T^* = 0.9$ (well below the critical temperature) an compute, for both cases, the equation of state in the pressure-density plane. Compare the results with the equation of state for the two temperature (data shared).