Case Study 2: MC simulations of Lennard-Jones fluid

We'll simulate $N$ particles interacting with Lennard-Jones 12-6 potential in a rectangular box of size $V = L_x \times L_y \times L_z$.

$$U_{\mathrm{LJ}}(\mathbf{r}) = 4\epsilon \left[ \left( \frac{\sigma}{|\mathbf{r}|} \right)^{12} - \left( \frac{\sigma}{|\mathbf{r}|} \right)^{6} \right] \tag{1}$$

Since it's impossible to simulate an infinitely large system, we'll apply periodic boundaries to the box, $i.e.$ if any particle gets out of the box from one side, its periodic image will enter the box from the opposite side. For the same reason, we need to truncate the original potential at a certain distance $r_{\mathrm{c}}$. In order to avoid the interaction of any particle with its interacting partner's periodic image, $r_{\mathrm{c}}$ shall be smaller that the half of the box extension, $i.e.$ $r_{\mathrm{c}} < L_x/2$. The truncated potential $U_{\mathrm{LJ}}^{\mathrm{trunc}}(\mathbf{r}) = U_{\mathrm{LJ}}(\mathbf{r})$ for $|\mathbf{r}| \leq r_{\mathrm{c}}$, and 0 otherwise. The parameters $\epsilon$ and $\sigma$ of the L-J potential set the basic energy and length units of the simulated system. The units for other quantities can be easily derived, e.g. $\epsilon/k_{\mathrm{B}}$ for temperature, $\epsilon/\sigma^3$ for pressure.

## Assignment

1. Equation of state

Run simulations with temperature $T = 1.2$ and $2.0$ and number density $\rho = 0.1 - 0.9$ for each $T$, and measure the pressure $p$ of each system

Plot $p$ (with error bar) versus $\rho$, and compare with literature data (Table 2 in MOLECULAR PHYSICS, 1993, VOL. 78, No. 3, 591-618)

2. Violation of detailed balance

Modify the code such that LJ fluid particles are only allowed to translate randomly in $+x$, $+y$, $+z$ directions, and compare $p \sim \rho$ plot with previous one at $T = 2.0$.

3. Distribution of the total energy

Make a histogram of the total energy per particle, $i.e.$ $p(E)$ versus $E$

Does the distribution violate Maxwell-Boltzmann distribution?

4. Visualization

Output the trajectory file and use VMD to visualize the trajectory