Mini Project 3: Equation of state for a Lennard-Jones fluid by Monte Carlo

A Lennard-Jones fluid consists of particles interacting via the pair potential:

$$u^{lj}(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

where ϵ is the binding energy of the pair and $2^{1/6}\,\sigma$ is the equilibrium distance.

Using a series of Monte Carlo simulations on a system of *N=100* Ar atoms (*ϵ/k_B = 119.8 K, σ = 3.405 x 10^{-10} m, M = 0.03994 kg/mol*) compute an equation of state (*P vs. ρ*) of a L-J fluid at a temperature of *T=2.0 ϵ/k_B*, which is well into the critical phase of the system.

Methodology:

1. Use a truncated form of the L-J potential with cut-off radius *r_c=L/2*, where *L* is the length of the cubic simulation box. *L* is decided by the target (mass) density.
2. For calculating the pressure use the virial expression below

$$P = \frac{\rho}{\beta} + \frac{vir}{V}$$
$$vir = \frac{1}{3}\sum_i \sum_{j>i} \vec{f}(\vec{r}_{ij}) \cdot \vec{r}_{ij}$$

3. Use appropriate tail corrections for both the energy and the pressure.
4. Perform diagnostic runs to choose an appropriate step size for MC moves using the rule that the acceptance ration should be between 20 - 50%.
5. Report all plots and numbers in simulation (L-J) units.
6. Implement a neighbour list strategy to compute interactions choosing from one of the methods mentioned in Appendix F of *Understanding Molecular Simulations* (Frenkel and Smit).

Questions:

A. For at least one combination of *T, P and ρ* plot the energy and pressure as a function of Monte Carlo steps to justify the choice of number of equilibration steps. How many MC steps are required for equilibration?

B. For the production runs, compute the cumulative averages of pressure and energy and plot along with the evolving values of the same. Cumulative averages are give by the formula below:

$$\bar{A}_t = \frac{1}{t}\sum_{t'=0}^{t} A_{t'}$$

C. Compute the speed of calculation in average time taken per MC step when using a neighbour list and when not using one. How much is the speed up and why?

D. Report the acceptance ratio for every simulation performed. Are the numbers reasonable? Why/why not?

E. Plot the equation of state as a *P vs. ρ* plot for various ρ values between 0.0 and 1.0 (excluding the limits).

F. Choosing at least 2 representative densities compute the pressure for a system with double the number of particles. Is there a difference between the numbers calculated in the previous question? Why/why not?

In at most 500 words summarise your understanding of the Ising system gained from these simulations.

Note: It is important to check the performance of your random-number generator. Provide a test for the same along with the rest of the answers.