Particle Methods
Spring Semester 2025

Homework 3

Due date: 16.04.2025

Write a program using language of your choice (C, C++, Matlab, python, ..) implementing Lennard-Jones simulations in 2D with the following conditions:

- Assume the simulation domain is a 2D square, $L = 30$ units in size, periodic in all directions.
- Use non-dimensional (reduced) units in your simulations ($\sigma = 1$, $\epsilon = 1$) with truncated Lennard-Jones potential given as

$$U_{trunc}(r) = \begin{cases} U(r) - U(r_c), & r \leq r_c \\ 0, & r > r_c \end{cases} \quad \text{, with} \quad U(r) = 4\left[\left(\frac{1}{r}\right)^{12} - \left(\frac{1}{r}\right)^{6}\right],$$

  with the χ-component (here χ is x or y) of the Lennard-Jones force given as

$$F_\chi(r) = \frac{48\chi}{r^2}\left[\left(\frac{1}{r}\right)^{12} - 0.5\left(\frac{1}{r}\right)^{6}\right].$$

  Set $r_c = 2.5$. Assume that all particles have the same mass $m = 1$.
- Use velocity-Verlet scheme to integrate equations of motion in time.
- Use uniform distribution of N particles on the square lattice as your initial conditions. You can prescribe the initial particle velocities to be random, with the total momentum of the system equal to zero. Think about reasonable distribution of the velocities to be used if your initial temperature T should be close to some value (something between 0.1 and 1.0 may be a good value to start with). Note that the temperature can be estimated from the kinetic energy of the particles (note, that since we are using non-dimensional units in simulations, Boltzmann constant k_B should be taken equal to 1).
- Implement and use cell list to speed up your simulations.
- Use conservation of total momentum as one of the checks of correct implementation.
- Implement calculation of potential, kinetic and total energy. You can use conservation of total energy in NVE simulations as one of the checks of correct implementation.
- Implement calculation of radial distribution function. You can use the bin size of 0.05. If you decide to compute the radial distribution function for distances greater than cut-off radius r_c, make sure that your link list can accommodate this (in case you combine computation of the radial distribution function with computation of pair-wise interactions).
- Implement Berendsen thermostat with relaxation time τ set as $dt/\tau = 0.0025$.

a) Perform initial simulations with different number of particles N in the domain. Try few values of N between 100 and 900. Try different initial velocities of the particles. Try different values of the time steps dt and see which values work ($dt = 0.01$ may be a good value to start with). Don't use thermostat in these simulations. Check that the total momentum is conserved. In each case, you will be modeling NVE ensemble, with constant number of particles, constant volume, and (in theory) constant energy. However, the integration scheme does not conserve energy exactly. Plot the total energy as a function of time, see if you get reasonable results. How does the size of energy fluctuations depends on the time step used? Each time you start your simulations, the system is not at equilibrium. Look at evolution of potential and kinetic energies in time. Use it to get an estimate of how many time steps are needed to reach equilibrium.

b) Perform simulations with specified number of particles N and at specified temperature T (NVT ensemble). Use Berendsen thermostat to control the temperature of the system. Look the evolution of temperature and see how many time steps are needed for system equilibration. Look at the motion and distribution of particles in the domain. Compute radial distribution function and see if it agrees with your observations of particle motion (remember to allow the system to equilibrate before computing radial distribution function).

Consider the following cases:

- $N = 100$, $T = 0.1$
- $N = 100$, $T = 1.0$
- $N = 625$, $T = 1.0$
- $N = 900$, $T = 1.0$

Please submit your code together with the report.