

Session 4 : Molecular Dynamics

We are interested in simulating the microcanonical behavior of a Lennard-Jones fluid. We fix the volume V , the number of particles N (mass m) and the total energy E . Particles can move in a cube of length L ($V = L^3$) and we use periodic boundary conditions. Interactions between 2 particles are described by a truncated and shifted Lennard-Jones potential

$$u(r) = \begin{cases} u_{lj}(r) - u_{lj}(r_c) & r \leq r_c \\ 0 & r > r_c \end{cases}$$

where

$$u_{lj}(r) = 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right] \quad (1)$$

1. What is the expression of the corresponding force? Is it repulsive or negative?
2. Why do we use truncated and shifted potential?
3. We express quantities in reduced units. Lengths are expressed in σ unit, energies in ϵ and masses in m . What are the reduced units for time, temperature and density ?
4. To integrate the equations of motion, we use the velocity Verlet algorithm

$$r(t + dt) = r(t) + v(t)dt + \frac{f(t)}{2m}dt^2 \quad (2)$$

$$v(t + dt) = v(t) + \frac{f(t + dt) + f(t)}{2m}dt \quad (3)$$

Show that this scheme is equivalent to the original Verlet algorithm.

5. Complete the subroutine *force.f90* to compute the forces and the potential energy of the system.
6. Complete the subroutine *integrate.f90* to implement the velocity Verlet algorithm and compute the kinetic energy.
7. Complete the subroutine *init.f90* to initialize the MD program (positions and velocities). Why do we impose that the velocity of the center of mass is zero? Why do we put initial positions on a lattice and not randomly?
8. Compute the total energy and plot its evolution in time for different values of dt . Any comments?
9. How can one compute the temperature? Add some lines in the code to implement it.
10. For different values of temperature T and density ρ , visualize the system with *xmakemol*.