Master's in Computational Modelling in Physics, Chemistry and Biochemistry
COURSE: MOLECULAR MODELLING
DEPARTMENT: FÍSICA DE LA MATÈRIA CONDENSADA
ACADEMIC YEAR: 2022-2023

1. Write code (preferrably a function or subroutine) to calculate the force on each one of the particles of a N-particle system interacting through a Lennard-Jones potential. Consider periodic boundary conditions and truncate the interactions using a cutoff radius r_{cut} (which we assume is $r_{cut} < L/2$, being L the length of the simulation box).

2. Implement the Verlet, velocity Verlet, and Euler algorithms in different functions or subroutines.

3. Write code (preferrably a function or subroutine) to calculate the kinetic energy of a system of N particles.

4. Consider a system of two particles interacting through a Lennard-Jones potential with $\sigma = 1$ and $\epsilon = 1$. Initialize their velocities to zero and their positions so that the distance between them is $d = 1.5$.

   - Solve the dynamics of this system by performing a simulation with the velocity Verlet algorithm in a cubic simulation box of $L = 10$. As reference, use a timestep $dt = 0.001$ and run at least 10000 simulation steps. Implement the periodic boundary conditions to put back into the simulation box those particles that escape.
   - Write your trajectory in XYZ format in a file called trajectory.xyz. Visualize the trajectory using VMD (see below for instructions on the format).
   - Calculate at each timestep the potential, kinetic and total energy of the system. Produce a plot with the evolution of the energies as a function of time. Investigate what happens if you modify the value of the timestep ($dt = 0.0001, 0.001, 0.01, 0.1$). Is the total energy conserved? And the total momentum?
   - Run the same simulation with the Euler algorithm. Compare the evolution of the energies and the distance between particles for the two algorithms.

The trajectory file in XYZ format is written as a succession of configurations for each recorded frame:

```
Configuration1
Configuration2
...
ConfigurationN
```

Each configuration is written as:

```
Number of particles in simulation
Blank line
NamePart1 X1 Y1 Z1
NamePart2 X2 Y2 Z2
...
NamePartN XN YN ZN
```

Put your code and your results in a compressed file called 'P2_your_lastname.zip' and upload it to the corresponding activtiy in Campus Virtual.