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 initialize the positions of particles in a sc lattice.
2. Prepare a system of 216 particles in a sc lattice with reduced density $\rho' = 0.8$. Visualize and generate a snapshot of the resulting configuration (call it initconf.tga).
3. Write code (preferrably a function or subroutine) to calculate the energy of a system of N identical particles interacting through a Lennard-Jones potential.
4. For the system that you have prepared with 216 particles in a sc lattice and reduced density $\rho' = 0.8$:
   - Calculate the energy of the system (in reduced units) if no periodic boundary conditions are considered. Truncate the interactions using the following cutoff radii: $r_c/\sigma = 1.5, 2, 2.5, 3$.
   - Calculate the energy of the system (in reduced units) considering periodic boundary conditions. Truncate the interactions using the following cutoff radii: $r_c/\sigma = 1.5, 2, 2.5, 3$.
   - Do the same for a system of 256 particles in a fcc lattice with the same density ($\rho' = 0.8$).

Put your code and your results in a compressed zip file called 'P1_your_lastname.zip' and upload it to the corresponding activtiy in Campus Virtual.