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

- Implement the Andersen thermostat in a function or subroutine. Help: In Python you can use the function random.normal of the numpy package (see theory slides). In Fortran you can use the function in BoxMuller.f (which I can provide) to generate stochastic numbers distributed following a gaussian distribution.
- Our goal is to study a Lennard-Jones liquid. To generate the initial positions of our system in a random configuration we will depart from a crystalline configuration which will be disordered by running a short simulation coupled to a thermostat at high temperature so the crystal melts into a disordered liquid. To do that:
  - Create an initial configuration of 125 particles in a sc lattice which interact through a Lennard-Jones potential so that the density of the system (in reduced units) is $\rho' = 0.7$.
  - Initialize the velocities of all particles to 0
  - Run a simulation of 10000 steps and a timestep of dt = 0.0001 using the velocity Verlet algorithm coupled to an Andersen thermostat at reduced temperature T'= 100.
  - Write the final configuration resulting from that simulation in a XYZ format. Visualize it using VMD to make sure it looks disordered.
- Starting from the last configuration of the previous simulation, run a simulation at a fixed temperature (in reduced units) of $T' = 1.5$ for 500000 timesteps.
  - Save into a file called 'thermodynamics.dat' the kinetic, potential, total energy and instantaneous temperature of the system as a function of time. Plot the evolution of the energies in a file called 'energies.png' and of the temperature in a file called 'temperature.png'.
  - Based on the inspection of the evolution of the different quantities select the frames to calculate average values corresponding to equilibrium. Calculate the average values and uncertainties of the energies and temperature and add them to the file 'thermodynamics.dat'.

Put your code and your results in a compressed file called 'P3_your_lastname' and upload it to the corresponding activtiy in Campus Virtual.