ASSIGMENT "Introduction to Molecular Dynamics and VMD"

Due date: 1 week 17/3/2023

Select ONE of the options

Option 1:

Modify the code for the integration of the Newton's equation of motion of the harmonic oscillator and add friction and external forcing. You can use parameters appropiate for a particular example of interest that you may like. One example is the modelling of the behaviour of the tip of an AFM microscope, which is described by these equations (you can find many places in which this is discussed but one example is here https://digital.csic.es/handle/10261/282719 , see equation 2.2)

Option 2:

Change the model! Several possible options:
- Nonlinear oscillations
- Make it 2D. For example, consider a central force (like gravity or coulomb force) or even a constant force perpendicular to the initial direction of motion and check the curvature of the motion.

Option 3: VMD

- Look at the pdb structure available at the "problema" folder of the material of the VMD session (follow the link at the campus virtual, I copy it here again: https://saco.csic.es/index.php/s/L5eB3ZaqCdq6MyX)

This pdb file has several structures inside. Identify them ! Extract the coordinates of each structure in a different pdb file and show a clear image of every one.
Guess which sort of thing is each structure (protein, nucleic acid, lipid, sugar, drug molecule, ...)