Simulació a la nanoescala Jordi Faraudo

NAMD Simulation and Analysis **11-May-2023**

DESCRIPTION

The objective is to perform a simulation of a simple atomic system (a nanoparticle in vacuo) with the NAMD package at different temperatures, analyse the structures, correlations and atomic motions in these systems.

Do the following Activities and write a short Report (add all the images that you consider appropiate at each point).

Please download the material from my GitHub with NAMD_Examples
https://github.com/jfaraudo/Examples_NAMD
(MD_nanoparticle folder)

ANALISIS OF INITIAL STRUCTURE

1. Locate the following files in the input folder: a file with the initial coordinates of the system, a structure file, and a file with the force field. With a text Editor, open the file containing the Force Field for the simulations. What is the interaction potential between the atoms?

2. Using VMD, take a first look of the system to be simulated. Open VMD and load the psf structure file and the pdb file containing the initial conditions. In the Menu Display use Orthographic and in Graphics > Representations and try the options CPK or VDW from the Drawing methods. Looking at this image, can you tell which sort of structure do you have?

3. Using the CPK representation and the "label" command, try to obtain the distance between atoms in this initial configuration (Help: in the VMD Main Menu, select the option Mouse > Label > Bonds. Now, with the Mouse click over two neighbouring atoms of the simulation and create a label indicating the distance between them).

4. Let us now compute the g(r) (rdf, radial pair distribution) function describing the structure of this initial configuration. Go to the *Extensions > Analysis > Radial pair distribution function*

   Now we have a new panel with options for g(r). In Selection1 and 2 we have to indicate the atoms name or a certain condition (i.e. Atoms with a given mass or a protein residue name, or a coordinate interval or whatever we want). Type *all* in both boxes (we want to use everything). Be sure to tick the option to show the results in the screen (the results can be saved in data text files, or *xmgrace* or other formats). Look at the results and try to understand them. What are the positions of the peaks? Can you see here a relation with the distances seen in section 3 and with the periodicity of the structure?

SIMULATION RESULTS

We provide as an example two short simulations, at different temperatures (300K and 1500K). Take a look at the trajectories provided (in VMD, go to File > Load Data into Molecule and open the dcd file for each simulation.

5. "Play the movie" of each simulation using the triangular "play button" in the main menu. The speed of the movie can be changed using the speed tool. What happens to the initial structure in each case?

(NOTE: depending on your temperature it will be a good option to align your structure).

6. Run a simulation of your own with NAMD. You can either modify one of the .namd files provided or use one of the example NAMD input files provided in the GitHub https://github.com/jfaraudo/Running_NAMD
   Possible options: change the temperature or make a longer simulation at one the the temperatures studied here. Upload the files obtained in the simulation at your GitHUb (or at the Campus Virtual as a compressed file)

7. Let us start analyzing the results. Using NAMDPlot option, plot the evolution of the kinetic energy and potential energy as a function of time. After this, plot the temperature as a function of time. Explain the meaning of the results.

8. Obtain the radial distribution g(r) function corresponding to the final thermodynamic equilibrium state. This means averaged over the last frames (use only those for which T is stabilized). Where are the peaks of the function? Compare with the peak values in the initial configuration.

9. Now let us look directly to the simulations in order to understand the atomic motion. In the VMD Main Menu, select the option Mouse > Label > Bonds. Now, with the Mouse click over two neighbouring atoms of the simulation and create a label indicating the distance between them. Let us visualize the evolution of this “bond distance” over time. Try the following: Graphics > Representations and change the “drawing Method” to “bonds”, then play the movie. You will see only a line and a number changing over time (an indication of the bond and its length). This representation can be of course improved. Try to play a bit to see both the atoms and the bond. What do you observe?