8. Übungsblatt

(1) Analysis of the data produced by molecular dynamic simulation with NAMD.

You can use the trajectories (*.dcd files) calculated in the previous exercise at 50 K and 350 K for the myoglobin protein. Now we are aiming at a graphical presentation of the time dependence of various parameters.

(1a) Plot the total energy of the system during the initial minimization versus time (first 100 steps)! Are the curves different for the simulation at 50 K and at 350 K? Why?

Hints:

In the VMD program, load: (1) the structural file "myoglobin.psf", (2) the file with the initial coordinates "myoglobin.pdb", and (3) the corresponding trajectory file with extension "dcd".

From the main VMD window, choose: Extensions > Analysis > NAMD Plot.

In the new window, select: File > Select NAMD Log File, and choose the file corresponding to this calculation with extension "log" (this file might not exist if you have run NAMD without specifying an output file name).

After selecting the file, chose the parameter you want to plot (in this case "total"). Select: File > Plot Selected Data. Save the data choosing: File > Export to ASCII matrix, and plot them using another program, selecting only the first 100 steps (for better visualization omit also the points with very high energies).

(1b) Investigate how he total energy changes during the equilibration of the protein at 50 K and 350 K! Plot also the kinetic energy, the temperature, and the bond energy (versus time)! Discuss the differences between 50 and 350 K!

(1c) Create a plot showing the changes in the number of H-bonds during the equilibration at both temperatures! Why does the number of H-bonds change in this way at the two temperatures?

Hint: From the main VMD window, choose: Extensions > Analysis > Hydrogen Bonds. Select the molecule and press the button "Find hydrogen bonds!"

(1d) Plot the distance between the hem Fe (iron of the heme group) and the oxygen atoms from two specific neighboring water molecules, namely resid 294 and resid 239! Discuss the differences observed when comparing the behavior at 50 K and 350 K! Why the behavior of the two water molecules is different?

Hint: Proceed in a similar way as in the previous exercise when plotting the distance between hem Fe and the nitrogen from the His ligand.

To identify the two water molecules you may create new presentations (Graphics > Representations > Create Rep) and select, e.g., "resid 294", then change the color of the molecule, e.g., to yellow (Coloring Method – ColorID – 4).

In the main VMD window, choose: Mouse > Label > Bonds. Select first the Fe atom, and then the O atom from the selected water molecule. In the main VMD window, choose: Graphics > Labels.

From the drop-down menu in the new window, select "Bonds" instead of "Atoms". Mark the bond you want to investigate (water molecules are labeled as TIP3).

Select Graph and click on the button “Graph”. You should see a graphic showing the Fe-O distance during the simulation and now you can save the data in ASCII format for further analysis.

(e) In another plotting program (for example EXCEL), create histograms to visualize the distribution of the selected Fe-O distances for the two temperatures. How many semi-stable states can you identify?

(2) Maxwell-Boltzmann energy distribution

Confirm that the kinetic energy distribution of the atoms in the system corresponds to the Maxwell distribution for a given temperature, by plotting the distribution (histogram) of the kinetic energies of the atoms in one moment of simulations and comparing it to the theoretically predicted distribution. When comparing the two curves, assume a normalization (scaling) factor, which can be fitted to the “experimental” data.

Hint: The Maxwell-Boltzmann distribution for the kinetic energy can be written as:

$$f(E_k) = \frac{2}{\sqrt{\pi}} \cdot \frac{1}{(k_B T)^{3/2}} \sqrt{E_k} \cdot \exp\left(- \frac{E_k}{k_B T} \right)$$

The kinetic energies might be calculated for each atom during the simulation. For these exercises however, it is sufficient to calculate the kinetic energy for one point in time.

This can be done, e.g., with *.restart.vel or any velocity file automatically generated during the simulation. In the main VMD window, right-click on the loaded molecule (myoglobin.psf) and choose “Delete Frames”. Delete all frames. This will delete also the initial coordinates, so no molecule will be visible anymore.

Now right-click on the “myoglobin.psf” and choose “Load Data Into Molecule”. Choose a velocity file corresponding to the temperature you want to study.

In the “Determine file type:” windows choose “NAMD Binary Coordinates” and click “Load”. The displayed molecule will look very strange, as VMD program treats the velocities as atomic coordinates, but that is okay. In the main VMD window go to Extensions > TkConsole.

Go to the folder where the files for this exercise are stored (for example typing “cd D:”, or “cd Tutorials”). In this folder you should have a simple script (file called get_energy.txt), downloaded from our webpage, which calculates the kinetic energies for each atom and saves them in a file called “energy.dat”. Take a moment to look at the script and try to understand it. The script can be called from the VMD program, typing in VMD TkConsole: “source get_energy.txt”. The created file (energy.dat) contains the kinetic energies for each atom in the moment of simulation when the velocity file was created.