Exercise 05

Simulation setup with GROMACS

Deadline: Please hand in your protocol in pdf format by Thursday, the 7th of June 2018, 10 am to jan.joswig@fu-berlin.de. The protocol should contain analytical solutions, short discussions, Python-code and plots.

You can download a set of files needed for this exercise from: `https://www.dropbox.com/sh/vmqi8vl0sxj6q2k/AAAuDrZi_gRZRY82xHyr6Ygta?dl=0`.

5.1 Download a PDB file and visualise it in VMD

Download a X-ray crystal structure from the RCSB protein data bank (`www.rcsb.org`, e.g. one of langerin, PDB-ID 3p5g). Open the .pdb file in a text editor and extract the data for a protein monomer by deleting other protein chains, crystal water, ions and unnecessary information. Visualise the structure in VMD. Choose a representation in which the secondary structure is emphasised (NewCartoon, NewRibbons, ...) and highlight α-helices, β-sheets and loops/coils in different colours. Set the backround colour to white, remove the axes icon, render the image and include the output in your report.

5.2 Structure minimisation

Use `gmx pdb2gmx` to generate the files needed for a simulation with GROMACS (.top, .itp, .gro). Use a dodecahedral box and place the protein at least 1 nm away from the borders of the box. Minimise the structure in vacuum (you can use minim1.mdp). Solvate the structure with TIP3P water. Are counter ions needed? Why? If yes, add them.

Check the size of the simulation box. How many water molecules have been added? How many atoms are in your system?

Minimise the system again (now you can use minim.mdp). Check if the minimisation was successful with `gmx energy` and plot the potential, kinetic and total energy (python). Change the number of minimisation steps (1000, 5000) and the energy cutoff (10, 100) and check again the potential energy. How do the changes effect the minimisation.

5.3 *NVT* ensemble

Use your minimised structure as starting frame for a 100 ps equilibration in the *NVT* ensemble at 300 K. The output should be updated every 1 ps (you can use and modify nvt.mdp). Check the temperature, the potential, kinetic and total energy during the simulation and include the plots in your report.

5.4 *NVT* ensemble

Use your *NVT* equilibrated system for a 100 ps equilibration in the *NPT* ensemble (you can use and modify npt.mdp). Check the pressure, the potential, kinetic and total energy during the simulation and include the plots in your report. How could you improve the equilibration?

Strip the water molecules from the equilibrated structure with `gmx trjconv`. Align this structure with the initial crystal structure in VMD, colour them differently and include a figure in your report.

5.5 Production MD run

How should a .mdp file (you can use and modify md.mdp) look for a MD run over 100 ns at a time step of 2 fs in which the coordinates are written to a compressed trajectory file every 1 ps while the .log file, velocities and energies are written to output every 50 ns?

Depending on your computational resources this run can take a long time, so you don't need to actually start it (on an average CPU with four cores you can expect a performance of 10 to 20 $\mathrm{ns\,d^{-1}}$ for a system of the size of langerin).