CHEM-E4115 Molecular Dynamics Exercise 1:
Molecular dynamics simulation tutorial by Gromacs

The first molecular modelling computer class exercise centers on a tutorial by Dr. Justin Lemkul available at http://www.mdtutorials.com/gmx/lysozyme/index.html

It provides a stepwise walk-through of how to do a molecular dynamics simulation for a small biomolecule in water and explanations of each of the steps. The assignment uses a software package called Gromacs. Gromacs is installed in Mylly2 (mylly2.pub.chemistrylab.aalto.fi). Gromacs is mostly run from using written text commands provided in the tutorial either in the terminal window or as a queue command to Mylly2.

- Mylly2 is accessed similar to the quantum chemistry exercises using XMing and PuTTY. File transfer can be done via WinSCP in the Aalto Windows computers.
- At least the following common text editors are installed in Mylly2: *nano*, *gedit, vi*. Any one of these can be used for viewing and editing the files.
- The most important plotting software in these exercises is *xmgrace* .
- The most important molecule visualization tool in these exercises is *vmd* .
- To get exercise points, 1) self-evaluate your performance in MyCourses and 2) submit the requested graphs or snapshots.
    - For the 1st MD exercise, 1) your own VMD visualization of the lysozyme protein (modified from VMD default style or color scheme, if you are unfamiliar with the program, test a bit with the options) and 2) graph in which the simulation box volume is plotted against simulation time in the equilibration step.
    - The requested files can be copied to a Mylly2 directory */home/maria/coursefiles/* . Please make there a directory that can be identified as yours (e.g. your name) under which you copy the files.
- The 2nd MD exercise continues the analysis after the production MD.

- **Gromacs module is loaded in Mylly2 by *module load gromacs/2023*** You need to give this command to be able to run Gromacs commands in Mylly2
- Gromacs preprosessing (=preparing the files for simulation) can be done in Mylly2 head node.
- **Energy minimization, the relaxation runs and the production run etc.** should be submitted to the queue system by ***jsub -np 4 gromacs mdrun [the remainder of the command]*** or for the longer runs ***jsub -np 12 gromacs mdrun [the remainder of the command].***
- Note that the ***gmx*** of tutorial is replaced by ***gromacs*** in Mylly2 submit commands**.**

Important tips for learning from doing the tutorial

- **Throughout the tutorial, read carefully the tutorial text (instructions and explanations).** The tutorial is telling why you are doing what you are doing. The tutorial is selected as the first exercise because it tells really a lot of the background and this is necessary for understanding the next exercises.
- **Use VMD (a visualization softwares) to view coordinate files and simulation trajectories. This software are installed in the chemistry computer class computers, not in Mylly2**
    - If you are not familiar with VMD visualization options, learn with the first coordinate file how to view the system in at least ball-and-stick, space fill, or a cartoon like secondary structure visualization of the protein. Save your favorite visualization as a figure.
    - When you are preparing a configuration for a simulation or have run a simulation, VMD can and should be used to see, what happened (visualization options are useful in this).
        - To get an animation in VMD, load in with VMD the molecule and then the created .trr file. You will see the molecular dynamics (or energy minimization) time trajectory (animation of the simulation). What is going on with energy minimization? NVT? NpT? Production run?
        - Tip: writing “pbc box” in the vmd command window makes the simulation box visible
- Chemistry computer class has also OVITO installed. Feel free to use it for the visualizations if you do not like VMD. Important is that you know how to use one visualization software.
- When doing the exercise, **examine the contents of each coordinate and parameter file and think what the content means.** Ask the lecturer to explain the file contents if they are not clear.
- The NVE and NPT relaxation take ~5min using 4 cores (-np 4) in Mylly2. The production run takes ~45min using 12 cores (-np 12) in Mylly2.
- You can try the analysis and plotting, as well as, trajectory visualization already while the simulation is running although for the production run, the simulation should have progressed at least 1/3.
- Exercise 2 continues from the analysis of the production run so you can leave it running in Mylly2.