CHEM-E4115 Molecular Dynamics Exercise 2:
Continuation of molecular dynamics simulation tutorial by Gromacs

In the 2nd exercise, continue the tutorial of 1st exercise. The approximate starting point is production run but please continue where you got with the tutorial last time.
To get exercise points for exercise 2, 1) self-evaluate your performance in MyCourses and 2) submit a graph showing either potential energy, box volume, or box density vs simulation time of the production run either to the MyCourses folder or the Mylly2 folder */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 tutorial by Dr. Justin Lemkul is available at
http://www.mdtutorials.com/gmx/lysozyme/index.html

1) **See exercise 1 for basic instructions**
2) **Complete the tutorial and analysis requested there**
3) When you have completed the tutorial, the following analyses are useful for moving to simulations and analysis beyond the tutorial (really doing something yourself without ready commands). Choose your favorites below. Remember that help for each command is obtained via *–h* . If you need an index file (.ndx), it is created with command *gmx make_ndx*
   a. Calculation of a protein contact map to see which residues are in contact with each other. Tip: use *gmx mdmat*
   b. Assess the diffusion of 1) a water molecule, 2) an ion and 3) the protein in your simulation. The command is *gmx msd* . Discuss with Maria about whether the numbers make sense. Why or Why not? Would you expect them to make sense?
   c. You did an analysis of radius of gyration of the protein in the tutorial. The same command *gmx gyrate* enables calculating also the moments of inertia which tell how spherical, elongated or pancake-like the protein is. Is your protein a sphere? Does your analysis match with what you see in VMD?
   d. Additionally, you can take a look at the listing of analyses available at http://manual.gromacs.org/documentation/2018/user-guide/cmdline.html
   See anything useful?

- **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**.**