GROMACS - Workshop - 9 and 10 September 2021

Zoom Instructions:

Please

- use **your full name in zoom**, that allows us to recognize you.
- login 5 min before the meeting starts.
- keep yourself mute
- for questions use the living-document for questions or zoom chat.

  Note all the lectures will be recorded.

Link September 9th:

https://videoconf-colibri.zoom.us/j/84876831914?pwd=NjFwSnNGdzVhWnFqOUtlUDVtZm5DQT09

Meeting ID: 848 7683 1914

Password: 466836

Link September 10th:

https://videoconf-colibri.zoom.us/j/82271970301?pwd=VGZ3ckNoMnEzRFdmSHYzcHBLdFJSUT09

Meeting ID: 822 7197 0301

Password: 517354

Pre-Lecture Material:

Here some useful recorded lectures

- Basis of molecular dynamics simulation part I and partII
- Webinar: What's new in GROMACS 2021
- Webinar: Accelerating sampling in GROMACS with the AWH method

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Tutorials information:

The tutorials are provided as an interactive Jupyter notebook based on GROMACS.
See for a brief introduction to Jupyter Notebook pdf file .
You can run the tutorial online in your browser without installing anything, or download it to run locally with your own installed software.

To run the tutorial locally (suggested option): Instructions

Note: this step requires some actions and installations before the workshop. If you face problems, join support meeting on Wednesday

To run the tutorial offline you will need to install some software on the terminal command line to be able to run the tutorial offline. Jupyter notebooks are built on Python, and the GROMACS tutorial content needs various other Python packages as well. Please follow the instructions below for your operating system to get a suitable terminal.

For MacOS users

You can use the standard Terminal app. You can launch a terminal via spotlight search, either click the magnifying glass icon in the top-left corner or press the Command-space key combination. Then type “Terminal” and press Return, and a terminal window will appear for you to use.

For Windows users

We strongly recommend using (and install if necessary) the Windows Subsystem for Linux, WSL. Inside it, you will need Python 3 and the conda Python environment manager. A useful guide to doing this is found at https://github.com/kapsakcj/win10-linux-conda-how-to.

For Linux users

You can use the standard terminal. Press the ‘Ctrl-Alt-T` key combination and a terminal window will appear for you to use.

For all users once you have a terminal

First, install miniconda for Python 3 by following https://docs.conda.io/en/latest/miniconda.html#linux-installers

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Then follow the instruction on the corresponding tutorial page (Running the tutorial offline -> For all users once you have a terminal)

- FactorXa in water - basis tutorial
- DNA base opening - AWH tutorial

NOTE. If it occurs that you have modified (by mistake) the tutorial files, just download them again.

To run the tutorial online: Instructions

Note: Due to the large number of participants accessing the tutorials at the same moment, delay in loading and running the notebook may be encountered for these reasons we suggest running the tutorials locally.

- For the `FactorXa in water` - basis tutorial. Click to run free on mybinder or in alternative on BioExcel Binder using GitHub account.
- For the `DNA base opening` - AWH tutorial, Click to run free on mybinder or in alternative on BioExcel Binder using GitHub account.

Support meeting

We will be available on Wednesday, September 8th, 03:30 PM Lisbon to help you overcome any technical difficulties. Please join us via Zoom:

https://videoconf-colibri.zoom.us/j/85319743557?pwd=ako5NUlvZEZEblYrTDN2Z1AvTGpUUT09
Password: 334539