How to prepare for the Advanced GROMACS Workshop 1-3 February 2021

Flash talks

All participants **must** provide a one slide presentation of themselves before the Workshop. The slides will be used in 3 minute (max, strict) informal flash talks on Monday to facilitate networking among participants. You are free to create the slide any way you like, but here are templates for (pptx) and (odp), and an example (odp). Send your slide to atte.sillanpaa (ät) csc.fi named *firstname_lastname.[pptx|odt|pdf]*. I'll show the slides to minimize zoom-hassle.

Basic Gromacs understanding

The advanced workshop requires you're familiar with Gromacs. Unless you feel like an expert, please brush up your skills by consulting the online tutorials made by Justin Lemkul and others *before* the event.

- http://www.gromacs.org/Documentation_of_outdated_versions/Tutorials
- http://www.mdtutorials.com/gmx/
- https://www3.mpibpc.mpg.de/groups/de_groot/compbio/index.html

Basic Python understanding

The BioBB is built with Python and we're also looking at Python in-memory toolchains. Basic understanding of the Python language will enable focusing to the scientific content in the tutorials instead of the Python syntax. To get started, we recommend the following interactive tool for trying out Python:

- https://www.learnpython.org/

Basic Linux command line skills

The workshop will include hands on using the Linux command line, so to maximally benefit from your time, it will be important to know the basics *before* you come the course.

In the course, you'll mostly need to be able to move around in the directory hierarchy (`cd, ls, pwd`), create directories, copy, rename, delete files (`mkdir, cp, mv, rm`), uncompress files (`tar, unzip`), edit files (any text editor, e.g. `gedit, nano, emacs`), look at file contents (`more, less, grep`), use some environment variables (`$HOME`, ...), download files (`wget, curl`).

Here are some links for easy self-study:

- https://linuxsurvival.com/ (Linux command line and tutorials that you can do in your browser)
- http://www.ee.surrey.ac.uk/Teaching/Unix/ (the first two topics are a good start, try also some editor)
- https://www.youtube.com/watch?v=uFPly_nGBMg (sit back and watch)
- [CSC Linux Cheat Sheet](#) (one page summary of most important Linux commands and then some

Q & A – help on your own systems

If you have questions related to your own systems, zip up some data and keep it available.

A temporary discussion forum will be set up in here, https://ask.bioexcel.eu/c/workshop-tutorials which will be hopefully useful also for remote participants.