CSC Spring School in Computational Chemistry 26-28.4.2023

Links for preparing for the hands-on exercises

Python

Some exercises of the spring school will utilize Jupyter Notebooks. Basic understanding of the Python language will enable focusing on the scientific content in the tutorials instead of the Python syntax. To get started, we recommend the following interactive exercises for trying out Python:

- https://learn-python.adamemery.dev/

You can also have a look at other Notebooks available at https://notebooks.rahtiapp.fi which you can access with your CSC account or Haka/Virtu. E.g. this https://github.com/csc-training/python-introduction Notebook is available directly to be used in a browser.

Basic Linux and command-line skills

The school will include hands-ons using the Linux command-line, so to maximally benefit from the school, it will be important to learn the very basics **before** you attend the course.

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

Here are some links for easy self-study:

- https://docs.csc.fi/support/tutorials/env-guide/ (all basic commands explained)
- https://aaltoscicomp.github.io/linux-shell/ (detailed instructions on how to get started)
- https://docs.csc.fi/img/csc-quick-reference/csc-quick-reference.pdf (a one-page summary of the most important Linux commands and other CSC-specific commands/concepts/resources)
- https://csc-training.github.io/csc-env-eff/ (comprehensive self-learning materials for working in CSC's computing environment)

GROMACS

If you are new to GROMACS, but would like to participate in the intermediate or advanced classical molecular dynamics hands-ons, you can either work through this tutorial https://tutorials.gromacs.org/md-intro-tutorial.html or the first one at http://www.mdtutorials.com/gmx/. Participation in the basic exercise does not require any prior knowledge of GROMACS.

CHARMM-GUI

The classical MD hands-ons will utilize CHARMM-GUI. This requires you to register in advance at https://charmm-gui.org/?doc=register. Processing the request takes about 24 hours. **Please use your institutional email address** (Gmail etc. will not work).

TURBOMOLE

Please install the TmoleX GUI on your laptop if you plan to participate in the basic or advanced quantum chemistry exercise tracks. Download links for Linux, Windows and MacOS systems are found on the page:

- https://www.3ds.com/products-services/biovia/products/molecular-modeling-simulation/solvation-chemistry/turbomoler/

Note that TmoleX comes bundled with a demo version of TURBOMOLE and the program will warn that it only works for input structures containing a certain number of atoms. This warning can be safely ignored, since we will be submitting the calculations to be run on CSC supercomputers where a license has been configured.

VMD

The visualization hands-on will be performed using the VMD software and some of the MD exercises will utilize VMD as well. We recommend that you install VMD locally from the link below:

- https://www.ks.uiuc.edu/Research/vmd/

TBA

We may add more info depending on the details of the hands-on exercises.

Posters

If you agreed to present a poster, thanks! The school will be a great opportunity to tell others about your research and get new ideas on how to approach your subject – and a poster helps explaining what you've already found out. Any typical poster size/material will do.

Questions?

Contact us at servicedesk@csc.fi.