



CSC Spring School on Computational Chemistry 17-19.4.2024

Instructions for preparing for the hands-ons

1. Python

The molecular dynamics and machine learning exercises will utilize Jupyter Notebooks. **Basic understanding of the Python language is important** as it will enable focusing on the scientific content in the tutorials instead of learning the Python syntax. We recommend the following interactive exercises for learning Python if you think you need to refresh your skills:

- <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 or Haka/Virtu account. E.g., this <https://github.com/csc-training/python-introduction> Notebook is available to be used directly in a browser.

2. Basic Linux and command-line skills

The school will also 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, vim, emacs), look at file contents (more, less, cat), and understand environment variables (\$PATH, etc.).

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)

3. 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.

4. 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!**

5. TURBOMOLE

Please install the TmoleX GUI on your laptop if you plan to participate in the basic or advanced quantum chemistry exercise tracks. TmoleX will also be available on the classroom workstations, as well as in our supercomputer web interfaces, but it is good to have it available on your own laptop as well, just in case.

Follow the steps on the site below to access download links for Linux, Windows and MacOS systems:

- <https://discover.3ds.com/free-download-biovia-turbomole-demo-version>

Note that TmoleX comes bundled with a demo version of TURBOMOLE and the program may 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.

6. VMD

The MD part of the school includes an optional visualization exercise using VMD. VMD will be installed on the local workstations and using them is recommended in case you do not have a dedicated Nvidia GPU on your laptop with OptiX ray-tracing engine available. If you'd nonetheless prefer using your laptop, please install VMD beforehand. You will also need the ffmpeg tool to generate videos. See the links below:

- <https://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=VMD>
- <https://ffmpeg.org/download.html>

7. Posters

If you agreed to present a poster, great! The school is an excellent 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.

Even if you did not sign up for bringing a poster, we would still highly encourage you to prepare a few slides about your research/studies that you can show from your laptop during the poster session.

8. Questions?

Contact us at servicedesk@csc.fi.