Links to materials for preparing to the Spring School hands on tutorials

Flash talks

All participants **must** provide a one slide presentation of themselves before the School. The slides will be used in 3 minute (max, strict) informal flash talks on Tuesday and Wednesday evenings to faciliate networking among participants. You are free to create the slide any way you like, but the result should be one slide with aspect ratio 16:9. 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]*.

Python

Machine Learning in Chemistry will utilize iPython Notebooks. 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/

You can also have a look at the 2018 Notebooks in here (select Introduction to Machine Learning in Chemistry Notebook)

Basic Linux command line skills

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

In the course, you'll only 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`**), use some environment variables **(`$HOME`**, ...).

Here are some links for easy self-study:

https://linuxsurvival.com/ (Linux command line and tutorials that you can do in your browser)

https://www.csc.fi/web/training/-/linux1_spring2018 (check the materials links)

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)

Gromacs

If you are new to Gromacs, but would like to participate in the Intermediate or Advanced tutorials, you can either work through the Basic tutorial from 2018 (pdf) (tgz), but this will require having access to Gromacs. Participating in the Basic tutorial in 2019 does not require prior knowledge of Gromacs.

Turbomole (QC intermediate hands-on tutorial)

Please install the TmoleX 4.4 GUI on your laptop if you plan to take the intermediate QC tutorial.
http://www.cosmologic.de/support-download/downloads/tmolex-client.html

NoMachine Remote graphics access to CSC servers

Please install the NoMachine Enterprise *Client* (**not** the *Desktop*):
https://www.nomachine.com/download-enterprise