Hands-on general info

Local workstations

Local workstations boot to Linux. Username is *cscuser* and password is behind you. These are different from the Puhti training accounts (*trainingXXX*, distributed on paper). You'll be working in the command line. In the Desktop, right-click at the background and select "terminal" (or choose it from the top left Applications menu).

In the terminal, change to the work -folder (**`cd work`**) and create all your files (**`gunzip/tar xf`**) there. Don't create content in **`$HOME`**. For example, to access the hands-on input files (which are listed in the School home page):

1) In a web browser, look for the School homepage (e.g. via www.csc.fi or google)

2) Right click and save the right file in the materials section (by default it will be saved in **`$HOME/Downloads`**). While you're in the **`work`** folder, unpack the file into it (tip: hit "tab" to autocomplete your commands):

```
tar xvzf $HOME/Downloads/<downloaded file name>
```

Set up your environment in local workstations (access gmx etc.):

```
source ~/sscc20/sscc20_setup.sh
```

Set up Notebooks in local workstations (needed on Thursday):

```
source ~/sscc20/conda_sscc20_setup.sh
cd ~/sscc20/ML-CSC-tutorial
git pull
jupyter-notebook
```

Using Puhti.csc.fi

Some hands-ons can also be done on Puhti.csc.fi. You can access it in two ways. CSC user guide is in https://docs.csc.fi

NoMachine

Click the NoMachine icon, or select it from the top left menu.

Select Puhti (if available) or create a new connection to Puhti, see https://docs.csc.fi/apps/nomachine/ for instructions. Use your training account and password. NoMachine then opens a virtual desktop in our datacenter, from where you can login to Puhti (right click on the black background, select "CSC local servers", then "Puhti").

Ssh to Puhti.csc.fi

```
ssh -X trainingXXX@puhti.csc.fi
```

replace *XXX* with the number in your training account.

Your training account is a member of this project: *project_2002722*. In Puhti, change to the scratch directory (see below) and create a subdirectory for yourself there (see below). All training accounts share the same scratch folder, so please stay in your own sandbox.

To get Gromacs and some nice tools set up for your session give:

```
module load gromacs-env
module load grace
module load vmd
export OMP_NUM_THREADS=1
cd /scratch/project_2002722
mkdir <your own name>
cd <your own name>
```

Note! Puhti does not have gmx installed, but **`gmx_mpi`**. If you run this tutorial on Puhti, please replace all **`gmx`** → **`gmx_mpi`**. The scripts take care of this automatically, but the interactive command line steps have not been edited in this text. The error will remind you…

An example batch job script for simulations that take longer (adapt as needed, note the ***reservation*** and that your input files may contain a better batch script template!):

```
#!/bin/bash -l
#SBATCH --time=00:20:00      # 60 minutes on compute time
#SBATCH --partition=small    # small partition i.e. 1-40 cores
#SBATCH --ntasks=4           # we ask for 4 mpi-tasks
#SBATCH --cpus-per-task=1    # just one thread per mpi-task
#SBATCH --job-name=GMX       #   --> 4 x 1 = 4 cores in total
#SBATCH --account=project_2002722 # cpu usage billing
#SBATCH --reservation=Spring_school_11 # for the 2020 school only

module load gromacs-env

srun gmx_mpi mdrun -s topol.tpr -dlb yes
```

If you need the input files on Puhti, get them with **`wget`** (copy the URL from your browser):

```
wget https://events.prace-ri.eu/event/942/.../some-input-files.tgz
```

On Puhti, *interactive* jobs that take longer than a minute should use the **`sinteractive`** command. It will allocate you one core in an interactive batch job. Use the project account shown above. You can have only one job in the interactive partition at a time. Note the usage policy so, don't run **`mdrun`** on the login node, but all **`mdrun`** processes via a batch script file.

Please **don't** use the **`-v`** flag for Gromacs jobs on CSC environment. It slows down your jobs and causes unnecessary file I/O.

More info on interactive jobs at CSC:

- https://docs.csc.fi/computing/running/interactive-usage/

More info on Gromacs at CSC:

- https://docs.csc.fi/apps/gromacs/