Usage of local workstations

Login on Linux (username given on-site and password behind you), open a terminal:

- right click at the desktop background, select “terminal”

In the terminal, in $HOME, source a setup script to get the right applications in your path

```
source setup-gmx-etc.bash
```

Before you start working, create a subfolder for your files and change there:

```
mkdir <something>

cd <the same something>
```

Pymol starts simply with `pymol`, Gromacs tools are available via `gmx_mpi -h`, `gmx_mpi mdrun` etc. Start Jupyter notebooks with

```
jypyter notebook
```

Quick and dirty cheat sheet on how to run Gromacs jobs on Puhti

Complete Puhti documentation: https://docs.csc.fi

Linux/CSC Cheat sheet:

Replace XXX or anything in <quotes> with your username, project, filename etc.

Logging in:

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

Change into scratch from $HOME to have room to play with

```
cd /scratch/project_2001889
```

Make a subdirectory for yourself (everyone will be in the same scratch_2001889)

```
mkdir <mycoolstuff>

cd <mycoolstuff>
```

Initialize Gromacs default version (to see all installed versions use `module spider gromacs`):

```
module load gromacs
```

Edit your mdp etc. files and then create the tpr:

```
gmx_mpi grompp -f grompp.mdp -n index.mdp -c confout.gro -p topol.top
```

Copy paste a template batch script from https://docs.csc.fi/#apps/gromacs/ or use one of the templates below.

Edit following things:

- #SBATCH –account=project_XXXXX to match the same as in your scratch directory

- number of nodes, tasks, partition, requested time
- input and output files
- One GPGPU card is requested with #SBATCH –gres=v100:1
- …

Submit the job with

```
sbatch <your file name>
```

follow execution

```
squeue -u trainingXXX
```

check contents of log file:

```
more, less, grep ...
```

SLURM batch script template for Gromacs with GPGPUs

```
#!/bin/bash -l
#SBATCH -t 00:10:00
#SBATCH -p gputest
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=6
#SBATCH --gres=gpu:v100:1
#SBATCH --account=project_2001889
#SBATCH --reservation=YYYY

module purge
module load gcc/8.3.0  hpcx-mpi/2.4.0 gromacs/2019.4-cuda
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK
srun gmx_mpi mdrun -s topol.tpr -dlb auto -g md_try_1 -maxh .05
```

SLURM batch script template for Gromacs with CPU coress

```
#!/bin/bash -l
#SBATCH -t 00:10:00
#SBATCH -p test
#SBATCH –nodes=1
#SBATCH --ntasks-per-node=40
#SBATCH --account=project_2001889
#SBATCH --reservation=YYYY

module purge
module load gcc/9.1.0  hpcx-mpi/2.4.0 gromacs/2019.4
srun gmx_mpi mdrun -s topol.tpr -dlb auto -g md_cpu_try_1 -maxh .05
```