1. Create an account at Metacentrum
   All students of Czech universities are eligible to use the resources of the computational center Metecantrum. First, you need to register at Metacentrum and create an account. Please visit the link:
   https://metavo.metacentrum.cz/en/application/index.html
   Then click on the “Registration form” and follow the instructions to create an account using your university credentials (the credentials from your university IT system are used to make sure that you are eligible for the Metacentrum account).

2. Install/prepare SSH and SCP in your computer
   To log into the computational resources at Metacentrum and operate Gromacs, you need to install a so-called SSH client on your computer. You need SCP client software to conveniently download files from Metacentrum to and from your computer.
   a. Linux: Everything readily available
   b. Macos: Install xquartz (https://www.xquartz.org/releases/index.htmlEverything readily available
   c. Windows:
      i. Putty and WinSCP: Download and install the free and open-source client Putty: https://www.putty.org (direct link to the current installer: putty-64bit-0.74-installer.msi). Download and install the free and open-source client WinSCP: winscp.net
      ii. MobaXterm (Preferred): *MobaXterm* X server and SSH client. *MobaXterm* is your ultimate toolbox for remote computing. In a single Windows application/

3. Install VMD on your computer
   The free and open-source VMD software package is used for visualization. Please, download and install VMD from:
   https://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=VMD
   (direct link to the recent version for Windows: Windows OpenGL (32-bit Intel x86)

4. Try to log in to Metecentrum
   After completing points 1) and 2) and after your Metacentrum account is successfully registered, use the SSH client from your computer (Putty, *MobaXterm, Console, terminal*) to test whether you can log in to Metacentrum computational resources. To log in to the metacentrum host connect to:

   tarkil.metacentrum.cz

   During the logging in, use the username and password used for the Metacentrum registration in point 1.

INSTRUCTIONS TO ENTER METACENTRUM AND TASKS TO PREPARE THE TUTORIAL MATERIAL.

1.- Using Metacentrum

Basic instruction on how to use metacentrum can be found here:
https://docs.metacentrum.cz/

1. a.- Entering to metacentrum and navigating through the files

```
$ ssh tarkil.metacentrum.cz
```

Please use **tarkil** unless you know what you are doing.

#Check localization of your home directory in which we will store the exercise files

```
$ pwd
```

The localization should look like this (the tarkil node holds home directories at /storage/praha1)
/storage/praha1/home/YOUR_USERNAME

2.- Preparing the tutorial files

The course we will follow is hosted at: https://zenodo.org/record/3569722

Go to your home directory:

```
$ cd
```

Download and extract the material of the course:

```
$ wget https://zenodo.org/record/3569722/files/task-material.tar.gz

$ tar -xzvf task-material.tar.gz
```

Don't worry about the error tar: Ignoring unknown extended header keyword 'SCHILY.fflags'

Enter the directory will the task material:

```
$ cd task-material
```

The PDF with the instructions of the course can be downloaded on your own computer.

3.- Using gromacs (Gromacs 2022) in metacentrum

!!! DO NOT RUN SIMULATIONS IN THE MAIN NODE (gmx_mpi mdrun)!!!
This is forbidden and you can be banned from metacentrum. YOU HAVE BEEN WARNED

Most of the tasks in this course can be made using interactive sessions. When this takes too long either we can use the normal queue system or simply use the precalculated files that you downloaded and extracted.

3.a - Open an interactive session

To request 1 node with 8 cores:

```
$ qsub -I -l
select=1:ncpus=8:mem=4gb:scratch_local=1gb:os=debian12:cpu_flag=avx2
-l walltime=4:00:00
```

This might take some time depending on how busy is metacentrum, so plan to issue the command before starting the course so that you can follow up the course from the very beginning

When time is unbearable try to reduce the number of cpus or the time, for example:

```
qsub -I -l select=1:ncpus=4 -l walltime=1:00:00
```

3.a.1 - Move to the folder with the files:

```
$ cd /storage/praha1/home/YOUR_USERNAME/task-material

$ cd ~/task-material
```

3.a.2 - Load gromacs

All **gromacs** programs are executed via the "**gmx** *Command*" wrapper. In metacentrum the name is changed to **gmx_mpi**. Therefore to use gromacs on the cluster, you will have to change all commands in the tutorial from **gmx** -> **gmx_mpi**

Alternatively, to be able to use the gmx command, while in the interactive mode, you may create an alias by the command:

```
$ alias gmx='gmx_mpi'
```

The gmx_mpi will only be available after you load the corresponding module. For this, run the following command:

```
$ module load gromacs/2022.5-gcc-10.2.1
```

3.a.3 - Executing Gromacs commands:

Most of the commands can be run as mentioned in the tutorial by just changing **gmx** by **gmx_mpi** (or create the alias, as mentioned above)

```
$ gmx_mpi grompp -f ...
```

3.a.4 - Running simulations

For running any simulation execute for example:

```
$ mpirun -np 8 gmx_mpi mdrun -v -s topol.tpr -deffnm md
```

This will execute the simulations using 10 processors simultaneously

THIS PART IS NOT NEEDE FOR THE EXERCISES AND MAY BE OUTDATED:

3.b Submitting simulations to the queue system (Not really needed to follow the course)

Any time that we will need **to submit a real long simulation** (i.e., gmx_mpi mdrun …), **we will need to use the queue system (PBS)**. Details about using the queue system can be found here: https://wiki.metacentrum.cz/wiki/About_scheduling_system.

We will need 3 commands:

```
# To summit simulations:
$ qsub submit_mdrun_XX.sh
```

```
# To check the status of the simulations:
$ qstat -u hseara
```

```
# To delete a running job:
$ qstat -u hseara (To find the Job ID)
meta-pbs.metacentrum.cz:
                                                                   Req'd
Req'd   Elap
Job ID                Username Queue   Jobname    SessID NDS TSK Memory
Time   S Time
-------------------- -------- -------- ---------- ------ --- ---
------ ----- - -----
6057287.meta-pbs.me* hseara   q_4h    STDIN      --    1   10 4gb 04:00
Q   --
$ qdel 6057287
```

```
# Submission Gromacs job that will use GPUs that will be faster.
```

Write the following text to the submission file(i.e., submission script) submit.dqs:

```
#!/bin/bash
#PBS -m n
module add gromacs-2020.3-gpu-mpi
cd $PBS_O_WORKDIR
gmx_mpi mdrun -v -s topol.tpr -deffnm md
```

submit job:

```
$ qsub -l walltime=0:1:0 -q gpu -l
select=1:ngpus=1:ncpus=16:mem=4gb:scratch_local=20gb submit.dqs
```

4. - Tasks to be done before the first practical session

Proceed with the tutorial until page 22 (Visualization of water box simulation)module

5.- Using xmgrace in metacentrum.

xmgrace is just an application to create 2d plots from clear text files, i.e., xvg files. When available it is trivial to use to plot gromacs files. However, you can use any other software such as excel if you do not have access to it. If you do not have access to it in your local machine you can use it from metacentrum.

You must ssh with the -Y or -X option in order to have to access to any graphical applications:

```
$ ssh -Y hseara@tarkil.metacentrum.cz
$ module load grace
$ xmgrace -nxy NAME.xvg
```

In Linux and macOS that should work without a problem. For window users, you need to install an xserver. You can for example use xlaunch that is free of charge from here http://www.straightrunning.com/XmingNotes/.
X-forwarding does not work properly in interactive sessions at Metacentrum, so while working with Gromacs, you may have to make a new ssh (or Putty) connection to create 2D plots (you can have multiple connections to Metacentrum opened).

6. Useful Linux commands

pwd – print current working directory

. current directory

.. parent directory

cd directory – Change current directory to “directory”

cd .. – Change current directory to the parent directory

~ - home directory

mkdir directory – create directory named “directory”

cp file1 file2 – Copy file1 to file2

cp -r directory1 directory2 – copy recursively “directory1” to “directory2” mv file1 file2 rename file1 to file2

mv file directory/ - move “file” into “directory”

ls – list the current directory

ll – list the current directory with details

cat file – print the file content at the screen

less file – view file

ls | less – forward the output of the “ls” command to the “less” viewer

> - redirect output to file and overwrite the file

>> - redirect output to file appending it

rm file – delete the file

rm -rf directory/ - deletes “directory” recursively

mc – text-mode file manager

mcedit – text-mode file editor

vim – text-mode file editor

emacs -nw – text-mode file editor

xmgrace data – open the “data” file in xmgrace

xmgrace -free data – run xmgrace in the scaled-window mode and open the “data” file

xmgrace -nxy data – plot multiple-column “data” file

7. VMD tutorial:

http://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/

8. Installing and using do_dssp tool for analysis of protein secondary structures at Metacentrum

1. Login to Metacentrum.
2. Follow the following steps in the command line:

```
$ cd /storage/praha1/home/YOUR_USERNAME/
$ wget https://github.com/cmbi/dssp/archive/2.3.0.tar.gz
$ tar xfz 2.3.0.tar.gz
```

```
$ cd dssp-2.3.0
$ ./autogen.sh
$ ./configure --prefix=/storage/praha1/home/YOUR_USERNAME/dssp-2.3.0/
$ make
$ make install
```

3. To use the tool, follow the steps:

a) Prepare the environment:

```
$ export DSSP=/storage/praha1/home/YOUR_USERNAME/dssp-2.3.0/bin/mkdssp
$ module load gromacs-2020.3-gpu-mpi
```

b) Use the tool:

```
$ gmx_mpi do_dssp -f YOUR_TRAJECTORY -s YOUR_TPR_FILE
```