

Connecting to the cluster – programs to install

- Linux users do not have to install anything further at this point

Mac users

- You need to install a so-called "x11-server". This basically allows you to view graphics from the supercomputer cluster to your own machine
- Download and install from <https://www.xquartz.org/>
- Log out of your mac, and back in (or restart)
- Done!

Windows users

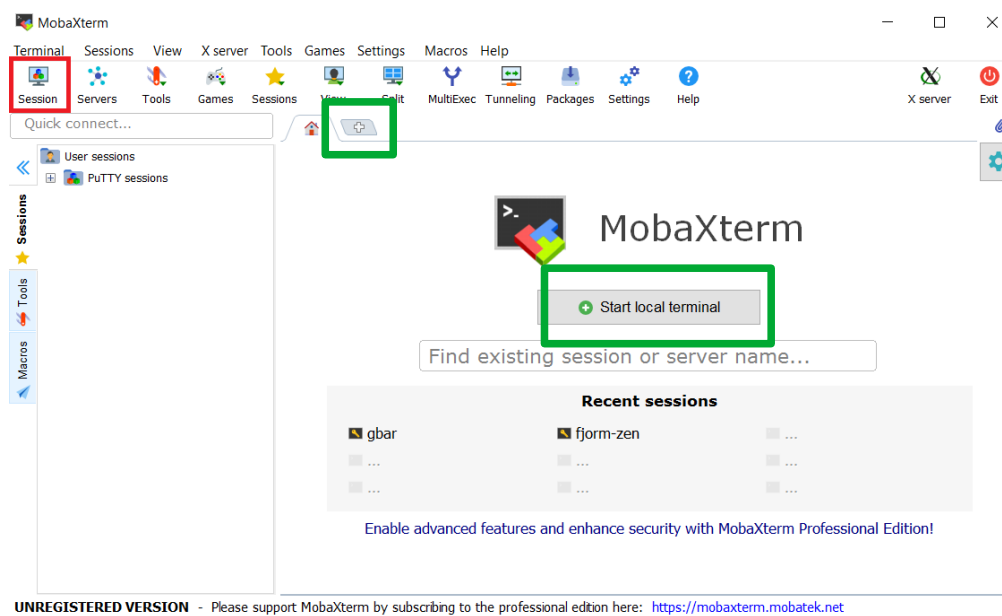
- Go to <https://mobaxterm.mobatek.net/download.html> and download the free version
- Select the "installer" version

Connecting to the cluster – information to keep handy

- DTU username
- DTU password
- ssh-key file (you have received this file zipped, so you need to unzip it and place it somewhere handy. We suggest you put it in the Desktop/ folder)
- Passphrase for ssh-key file

Open a terminal window (Windows)

- In the MobaXterm home window: Click “Start local terminal” or “+” in either of the two green squares



Logging in to the cluster: Linux, Mac & Windows

- Run the following in a terminal window:

```
ssh -i LOCATION_OF_SSH_KEY_FILE -XY USERNAME@login.gbar.dtu.dk
```

- USERNAME is your DTU user name
- LOCATION_OF_SSH_KEY_FILE is where you placed the file you unzipped
- After pressing enter, you are asked to type the passphrase for the ssh-key file (**NOTE:** the cursor will not move when you type passphrase or password)
- Then type in your DTU password
- You should now have access to the GBAR cluster

All users: After logging in

- Run the following command after logging in: *linuxsh -X*
–This transfers you to a compute node, from where you will be able to do calculations
- Your terminal should now look something like this
- Every time you log in, remember to run the *linuxsh -X* command



```
latexty@gbarlogin1 ~]$ linuxsh -X
qsub: waiting for job 381353.hnode3 to start
qsub: job 381353.hnode3 ready

*****
*                               *
*   Welcome to the G-databar at DTU   *
*   User information: See G-bar homepage http://www.gbar.dtu.dk/   *
*   User support: gbar-support@student.dtu.dk   *
*                               *
*****

The scheduled service window for the G-Bar and HPC clusters is on a Monday every
couple of months, between 17 and 07 hours. During these hours,
the G-Bar and HPC systems will be inaccessible, as most systems will be rebooted
and maintenance work will be in progress.

To subscribe to the HPC mailing list, please send an email to:

    hpc-subscribe@lists.cc.dtu.dk

*****

*** Dear OpenFoam-Users:                               *** very important ***
Please have a look here:                                http://www.hpc.dtu.dk/?page_id=1024

*** Dear Users: If you have to deal with large-datasets, please ask for a
scratch-directory: support@hpc.dtu.dk

*** Please use transfer.gbar.dtu.dk for transferring files
*** between the outside world and your home and/or SCRATCH-directory.

*****
If you run into any issues: support@hpc.dtu.dk
*****

*****
* If you have a scratch-directory under /work1 - please clean up. Thanks a lot. *
* *** this is really really important! *** *
*****

Loaded module: latex/TeXLive12
latexty@n-62-30-3 ~]$
```

All users: Getting access to the software

- Run the following command:

```
sh /zhome/43/5/58576/BATMAN-2022/setup-batman-2022.sh
```

- This will ask you to set up a password for Jupyter (which we will be using for the CLEAVE exercises)

–Choose a password

–**It is a bad idea to type your DTU password into untrusted programs, so you should probably choose a different password - *this is particularly important if you are a DTU student/employee, the security of your DTU password is critical!***

- A folder called “BATMAN2022” will be created on your user, where the exercises will be copied in to.

- For the VASP exercises you should go to the folder BATMAN2022/VASP (i.e. run:

```
cd $HOME/BATMAN2022/VASP
```

And follow the instructions from the teacher (NOTE: Calculation jobs are submitted from a folder by doing: *bsub < submit.sh* and check status of jobs with: *bstat*)

- For the CLEAVE exercises see the following pages

Opening Jupyter, and Accessing It Locally (All users)

- Jupyter is basically python in notebook style
- It is run in a browser – for our purposes, it is run on the cluster
- We need the browser on our local computer!
- In the terminal, make sure you have run

linuxsh -X

- Now run the command:

/zhome/43/5/58576/BATMAN-2022/notebook

- You should now see something like the following

```
(online18-env) ~
n-62-27-22(stlystud) $ notebook
[I 10:43:16.226 NotebookApp] Writing notebook server cookie secret to /zhome/1c/4/1000167416/.local/share/jupyter/runtime/notebook_cookie_secret
[I 10:43:17.513 NotebookApp] Serving notebooks from local directory: /zhome/1c/4/1000167416
[I 10:43:17.513 NotebookApp] The Jupyter Notebook is running at:
[I 10:43:17.513 NotebookApp] http://n-62-27-22:40000/
[I 10:43:17.513 NotebookApp] Use Control-C to stop this server and shut down all kernels (twice to skip confirmation).
```

- **Leave this terminal open** when you go to the next part
- For the next part open a new terminal window

Opening Jupyter (All users)

```
(online18-env) ~  
n-62-27-22(stlystud) $ notebook  
[I 10:43:16.226 NotebookApp] Writing notebook server cookie secret to /zhome/lc/4/1000167416/.local/share/jupyter/runtime/notebook_cookie_secret  
[I 10:43:17.513 NotebookApp] Serving notebooks from local directory: /zhome/lc/4/1000167416  
[I 10:43:17.513 NotebookApp] The Jupyter Notebook is running at:  
[I 10:43:17.513 NotebookApp] http://n-62-27-22-40000/  
[I 10:43:17.513 NotebookApp] Use Control-C to stop this server and shut down all kernels (twice to skip confirmation).
```

•In a new terminal window, on your own computer (not on the cluster) (see the second slide for how to do that on Windows in MobaXterm), run the following command

```
ssh -i LOCATION_OF_SSH_KEY_FILE USERNAME@login.gbar.dtu.dk -g -L8080:HOSTNAME:PORT -N -v
```

•Replace LOCATION_OF_SSH_KEY_FILE with the location of the file you unzipped earlier

•Replace USERNAME with your username

•Replace HOSTNAME with what is in the red box above

–In this case: n-62-27-22

•Replace PORT with the green box

–In this case: 40000

•**This may change each time you log in!** (So remember to check every time!)

•Go to your local browser, and in the URL type:

localhost:8080

Finding the exercises

- After logging in you should have a browser window with content as shown in the image below
- The exercises are the files ending with **.ipynb** (Click to open them)

[Quit](#)[Logout](#)[Files](#) [Running](#) [Clusters](#)

Select items to perform actions on them.

[Upload](#)[New](#)

<input type="checkbox"/> 0 ▾	/	Name ▾	Last Modified	File size
<input type="checkbox"/>	factorial.ipynb		36 minutes ago	262 kB
<input type="checkbox"/>	part1_clease_script.ipynb		Running 5 minutes ago	407 kB
<input type="checkbox"/>	part2_clease_gui.ipynb		Running 36 minutes ago	3.79 kB
<input type="checkbox"/>	Au1Cu1.xyz		36 minutes ago	64.1 kB
<input type="checkbox"/>	Au1Cu3.xyz		36 minutes ago	64.1 kB
<input type="checkbox"/>	Au3Cu1.xyz		36 minutes ago	64.1 kB
<input type="checkbox"/>	aucu_script.db		7 minutes ago	213 kB