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

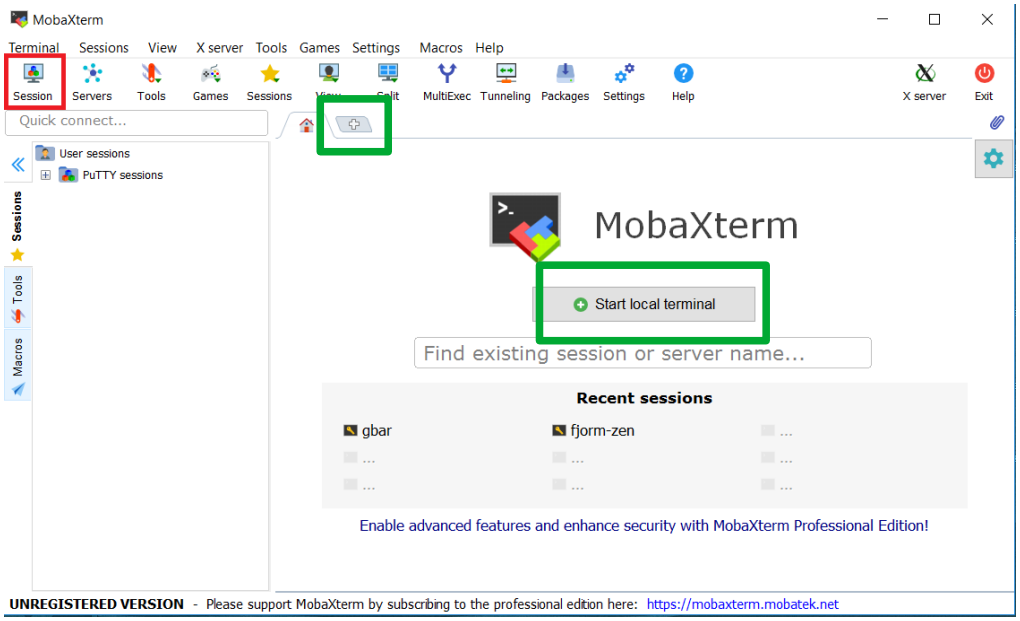
- Go to https://mobaxterm.mobatek.net/download.html and download the free version
  - Select the ”installer” version

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

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 CLEASE 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 CLEASE exercises see the following pages

Opening Jupyter, and Accessing It Locally (All users)

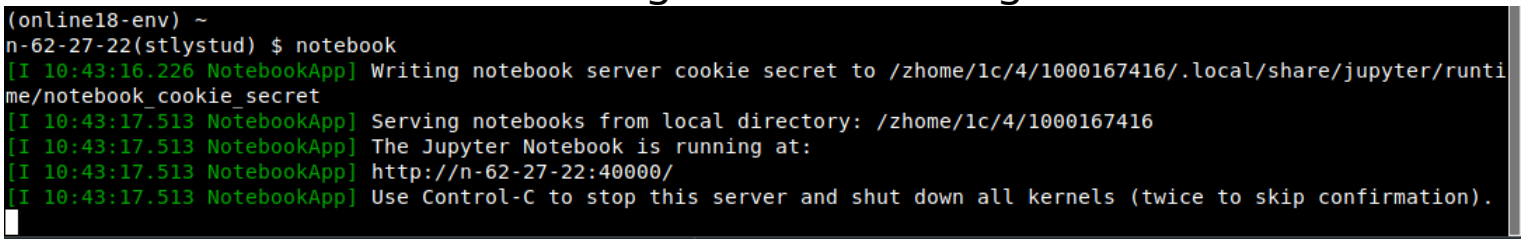
- Jupyter is basically python in notebook style
- It is run in a browser – for our purposes, it is run on the cluster
- We need the browser on our local computer!
- In the terminal, make sure you have run

  linuxsh -X

- Now run the command:

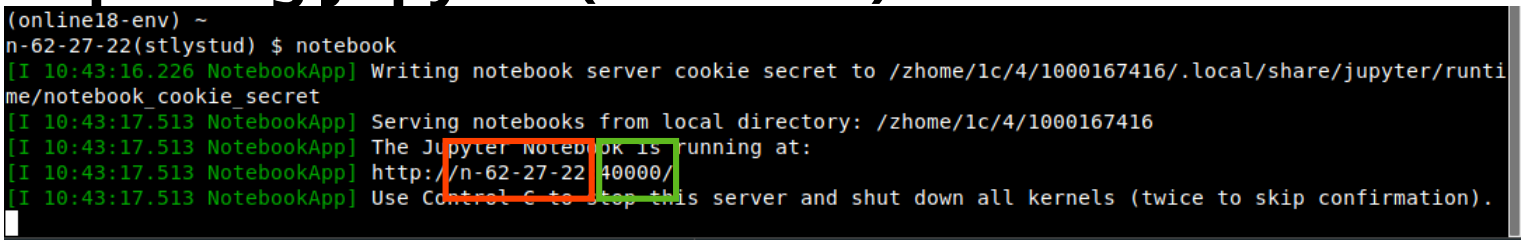
  /zhome/43/5/58576/BATMAN-2022/notebook

- You should now see something like the following



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

Opening Jupyter (All users)



- 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
- **<u>This may change each time you log in!</u>** (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)