Connecting to the cluster

- A general walk-through on how to connect to the cluster for Windows, Mac and Linux users can be found on https://wiki.fysik.dtu.dk/gpaw/summerschools/summerschool18/summerschool18.html#
- 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

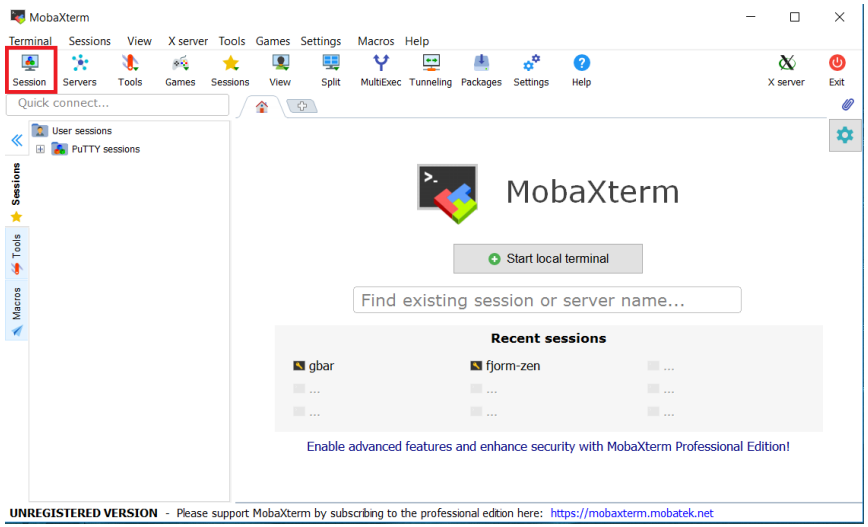
- Go to https://mobaxterm.mobatek.net/download.html and download the free version
  - Select the ”installer” version

Logging in to the cluser: Linux & Mac

- Run the following in a terminal: ssh –XY USERNAME@login.gbar.dtu.dk
  - USERNAME is your DTU user name
  - Type in your DTU password
- You should now have access to the GBAR cluster

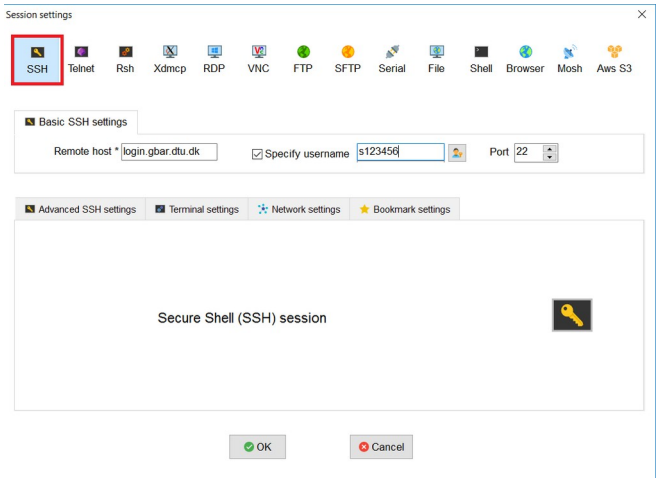
Windows: Logging in to the cluster

- Run MobaXterm, and you should now have a window that looks something like this:
  - Click the button in red



Windows: Logging in to the cluster

- In the pop-up window, click on ”SSH”, and type in the remote host ”login.gbar.dtu.dk”, and your DTU username
- Click OK, and type your DTU password
- General advice is to NOT store your password (a popup window will ask if you want to store it)
- You should now have a terminal ready to go



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 run the jupyter notebooks
- 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:

  source /zhome/43/5/58576/bike-workshop-2021/tools/setup.sh

- You should only run this command the first time you log in.
- This will ask you to set up a password for Jupyter (which we will be using for the 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 “bike-workshop-2021-hands-on” will be created on your user, where the exercises will be copied in to.

. /zhome/43/5/58576/bike-2021-venv-CLEASE/bin/activate

. /zhome/43/5/58576/bike-2021-venv-GA-AMP/bin/activate

AMP must use ASE-3.19.1

source /zhome/4b/8/70394/software/envs/clease_slab/bin/activate

Opening Jupyter, and Accessing It Locally (All users)

- Jupyter is basically python in notebook style
- It is run in a browser – for our purposses, 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:

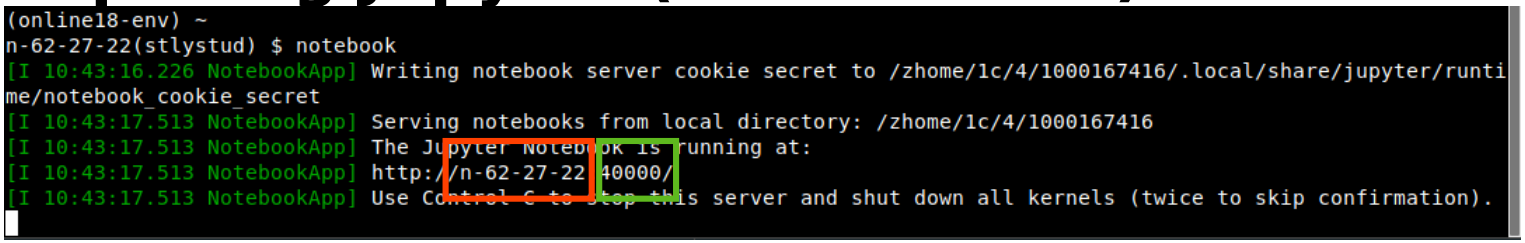
  notebook

- 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/runti
me/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).
```

- The next part depends if you are on windows, mac or linux

Opening Jupyter (Mac & Linux)



- In a new terminal, on your own computer (not on the cluster), run the following command

ssh USERNAME@login.gbar.dtu.dk –g –L8080:HOSTNAME:PORT –N

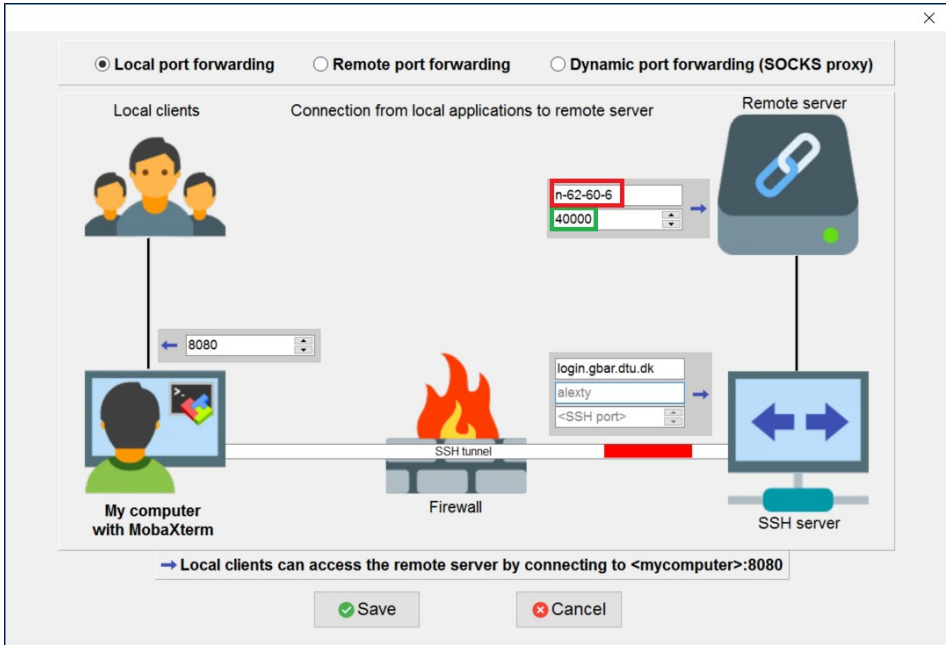
- Replace USERNAME with your username
- Replace HOSTNAME with what is in the red box above
  - In this case: n-62-27-22
- Replace PORT with the green box
  - In this case: 40000
- **<u>This may change each time you log in!</u>**
  - So remember to double check every time! (Unfortunately)
- Go to your local browser, and in the address bar type:

localhost:8080

Opening Jupyter (Windows) – Part 1

```
(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/runti
me/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).
```

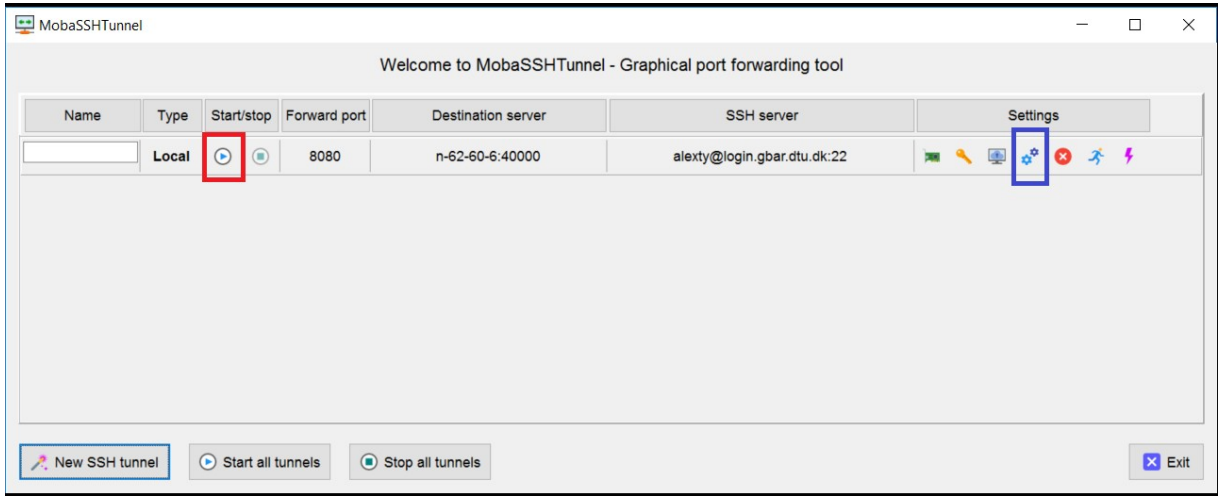
- On top of your mobaXterm window, click on the button called ”Tunneling”
- Click on ”New SSH tunnel”
- Fill out the red and green boxes
- Fill our your own username
- **<u>This may change each time you log in!</u>**
  - So remember to double check every time! (Unfortunately)



Opening Jupyter (Windows) – Part 2

- You should now have a window which looks like this
- If you need to change any settings, e.g. after a new login, use the wheels in the blue box
- Click the start button (In the red box)
- 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 exercise and introductory video notebooks are located in the **bike-workshop-2021-hands-on** folder (Click to open them)