

# 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

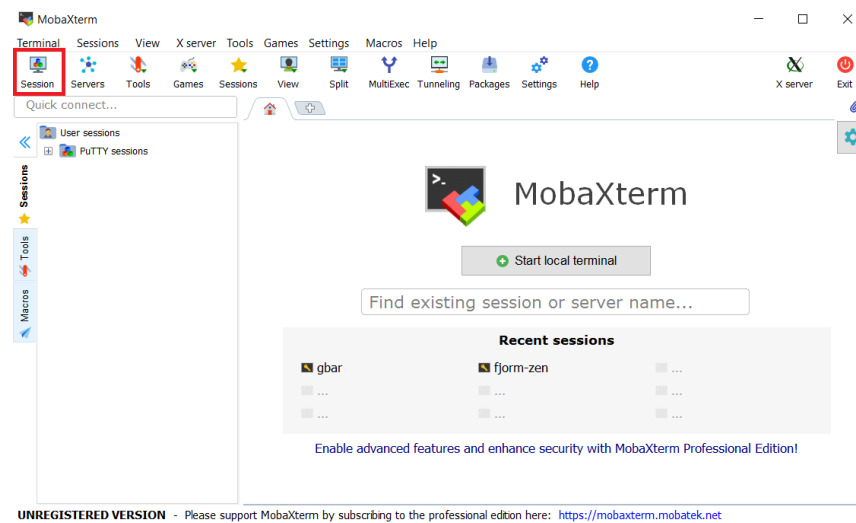
- Select the "installer" version

# 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

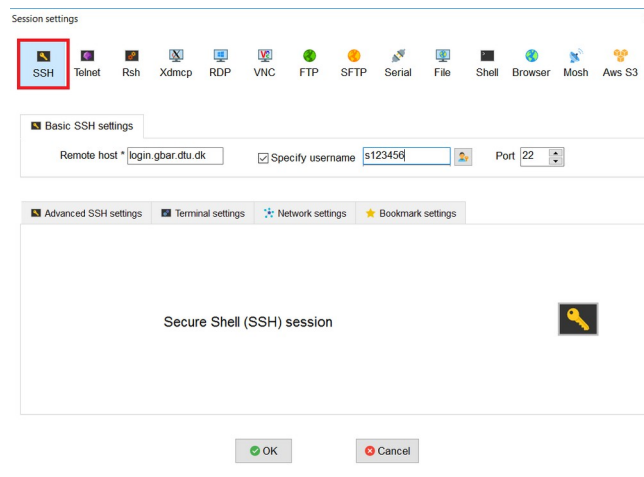
# Windows: Logging in to the cluster

- 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



```
4. login.gbar.dtu.dk (alexty)
[alexty@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
[alexty@n-62-30-3 ~]$
```

# 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-CLEAVE/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/cleave_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 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:

`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).
```

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

# Opening Jupyter (Mac & Linux)

```
(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).
```

•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
```

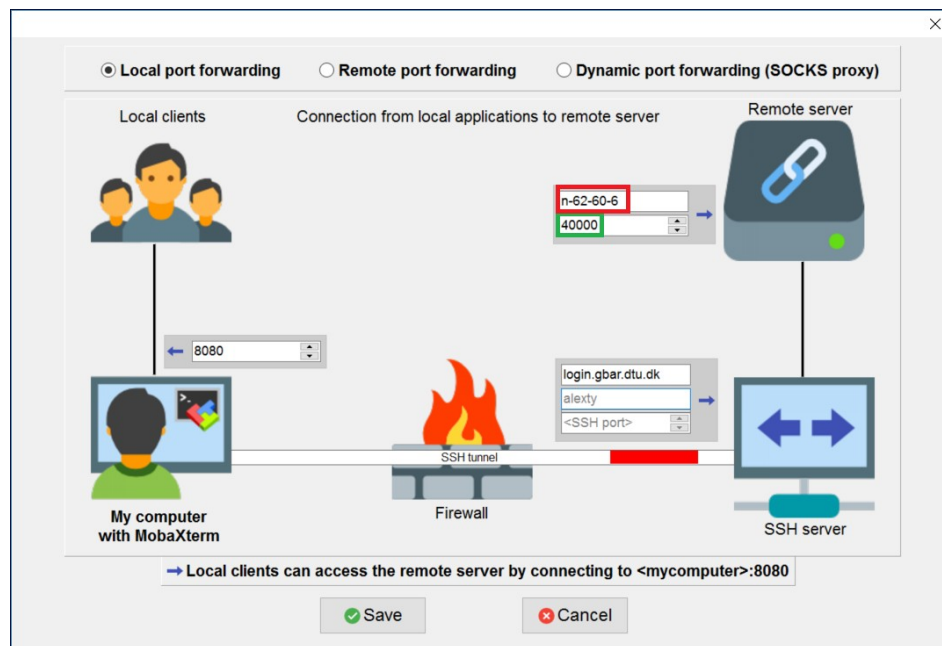
- Replace USERNAME with your username
- Replace HOSTNAME with what is in the red box above
  - In this case: n-62-27-22
- Replace PORT with the green box
  - In this case: 40000
- This may change each time you log in!**
  - So remember to double check every time! (Unfortunately)
- Go to your local browser, and in the address bar type:  
localhost:8080



# Opening Jupyter (Windows) - Part 1

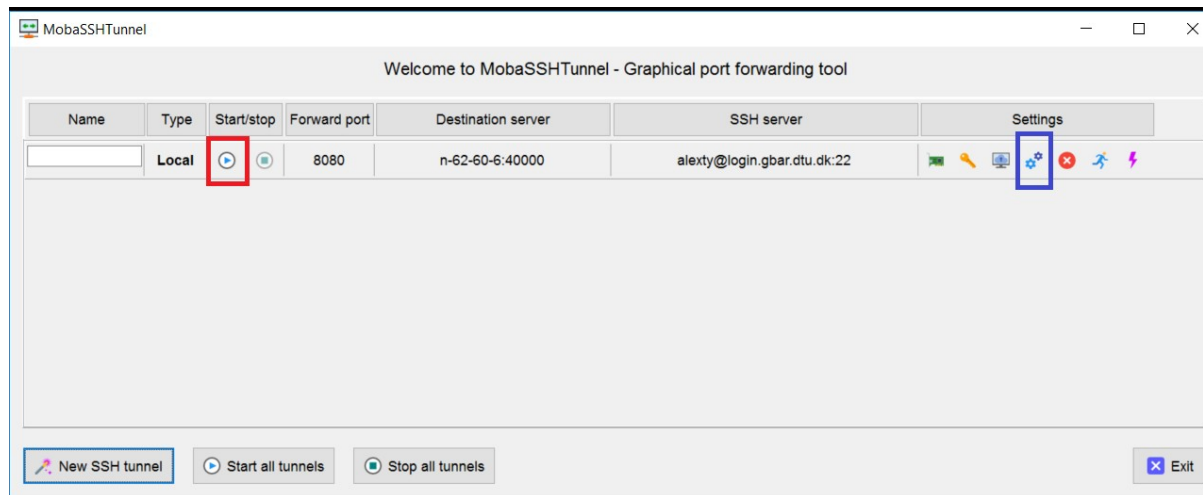
```
(online18-env) ~  
n-62-27-22(stlstud) $ notebook  
[I 10:43:16.226 NotebookApp] Writing notebook server cookie secret to /zhome/lc/4/1000167416/.local/share/jupyter/runtime/notebook_cookie_secret  
[I 10:43:17.513 NotebookApp] Serving notebooks from local directory: /zhome/lc/4/1000167416  
[I 10:43:17.513 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).
```

- 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 out your own username
- **This may change each time you log in!**
- So remember to double check every time! (Unfortunately)



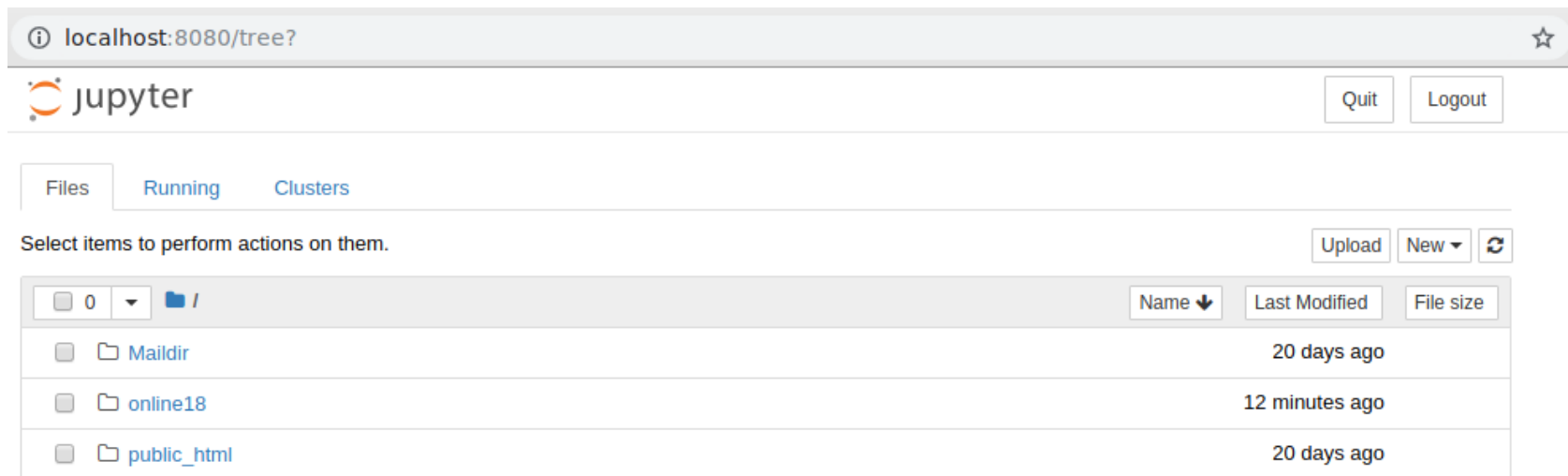
# Opening Jupyter (Windows) - Part 2

- 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)



The screenshot shows the JupyterLab interface in a browser window. The address bar displays 'localhost:8080/tree?'. The Jupyter logo is on the left, and 'Quit' and 'Logout' buttons are on the right. Below the header, there are tabs for 'Files', 'Running', and 'Clusters', with 'Files' being the active tab. A message says 'Select items to perform actions on them.' To the right of this message are 'Upload', 'New', and a refresh icon. The main area shows a file browser with a table of files and folders. The table has columns for 'Name', 'Last Modified', and 'File size'. The files listed are 'Maildir', 'online18', and 'public\_html', each with a checkbox on the left and a timestamp on the right.

	Name	Last Modified	File size
<input type="checkbox"/>	0		
<input type="checkbox"/>	Maildir	20 days ago	
<input type="checkbox"/>	online18	12 minutes ago	
<input type="checkbox"/>	public_html	20 days ago	