Connecting to the Flemish Supercomputer Centre (VSC)

roadmap for UGent students

STEP 1: connecting to the Ghent University network

In order to connect to the Flemish Supercomputer Centre (VSC) it is necessary to first link your computer to the network of one of the 5 Belgian universities associated with the VSC (Ghent University, KU Leuven, VUB, University of Antwerp and UHasselt). Below, we will sometimes refer to the Flemish Supercomputer as HPC (i.e. High Performance Computer).

Note:
The information below is for student from the Ghent University only. Similar steps can be taken if you are a member of one of the other four universities associated to the VSC. However the students of the Ghent University will work on the Ghent Tier-2 clusters on which *QuantumEspresso* is already installed. If a student from one of the other four universities wishes to use *QuantumEspresso* on their local Tier-2 clusters, they will have to contact the corresponding helpdesk to help them install *QuantumEspresso,* which is freely available. Students associated to none of these five universities can use *QuantumEspresso* either on their personal computer (via the Quantum Mobile virtual machine) or on a local cluster if available and after installing *QuantumEspresso* on it.

As we will work on the Ghent Tier-2 clusters we will have to connect to the Ghent University network. The method to do this depends on your location. If you are inside one of the buildings of the Ghent University and you have a Ghent University account, simply connecting to the internet (by eduroam, by a network cable or by a UGent Wi-Fi access) is sufficient. However, if you wish work remotely from your home, you will have to set up a VPN connection.

a) Connecting from within one of the Ghent University buildings with a UGent account (eduroam)

The instructions are well explained on the website of the Ghent University:
http://helpdesk.ugent.be/eduroam/en/

b) From outside the Ghent University buildings using a VPN connections

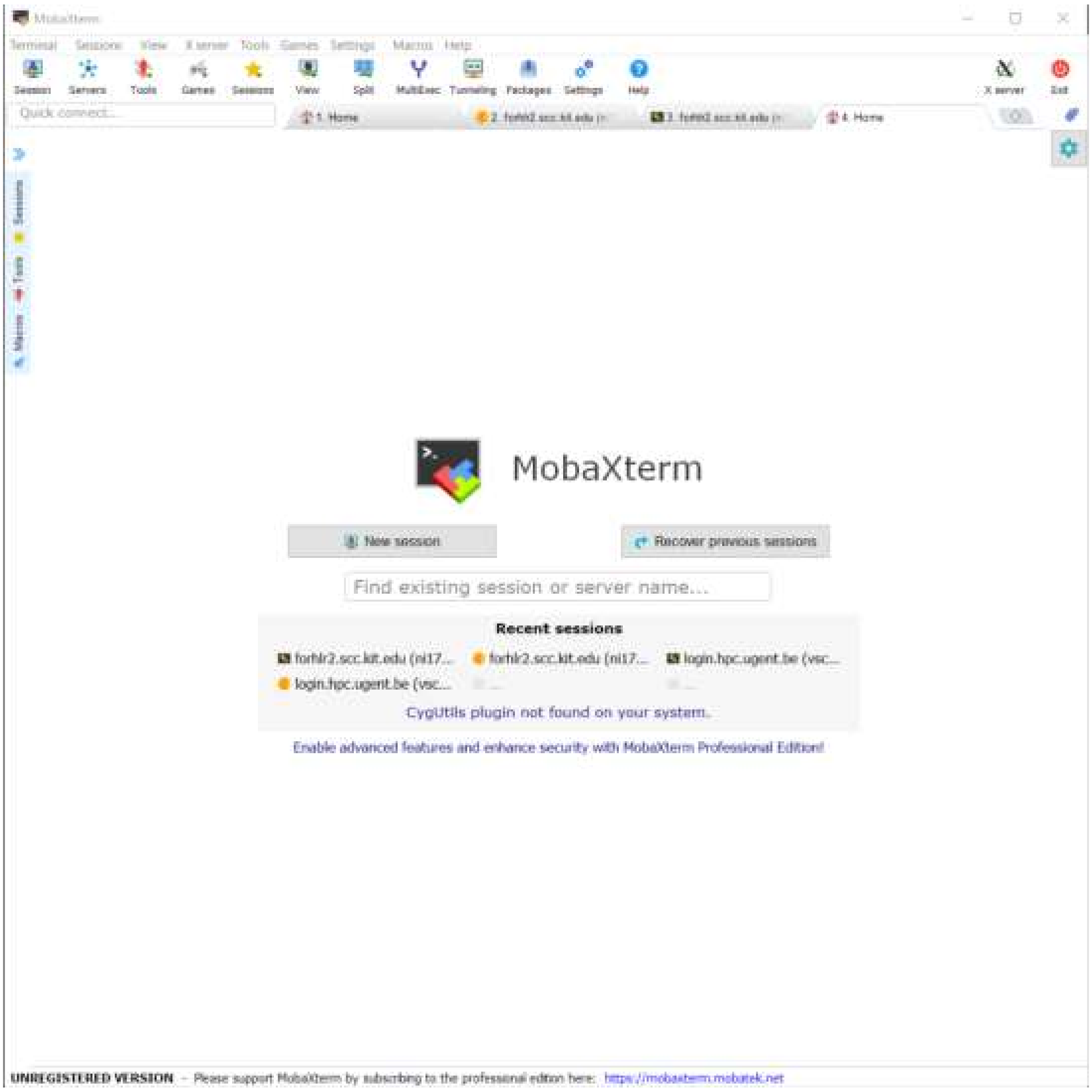
This is a connection that links your remote personal computer to the network of an institution (e.g. Ghent University)

For Ghent University students, more information can be found here:
http://helpdesk.ugent.be/vpn/en/

STEP 2: requesting a VSC account and connecting to the HPC

Instructions for Windows users

1) Start by downloading the free version of MobaXterm: https://mobaxterm.mobatek.net/download.html
2) Install MobaXterm
3) Start MobaXterm, you will get the window below:


MobaXterm
Terminal Sessions View X server Tools Games Settings Macros Help
Session
Servers
Tools
Games
Sessions
View
Split
MultiExec
Tunneling
Packages
Settings
Help
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Quick connect...
1. Home
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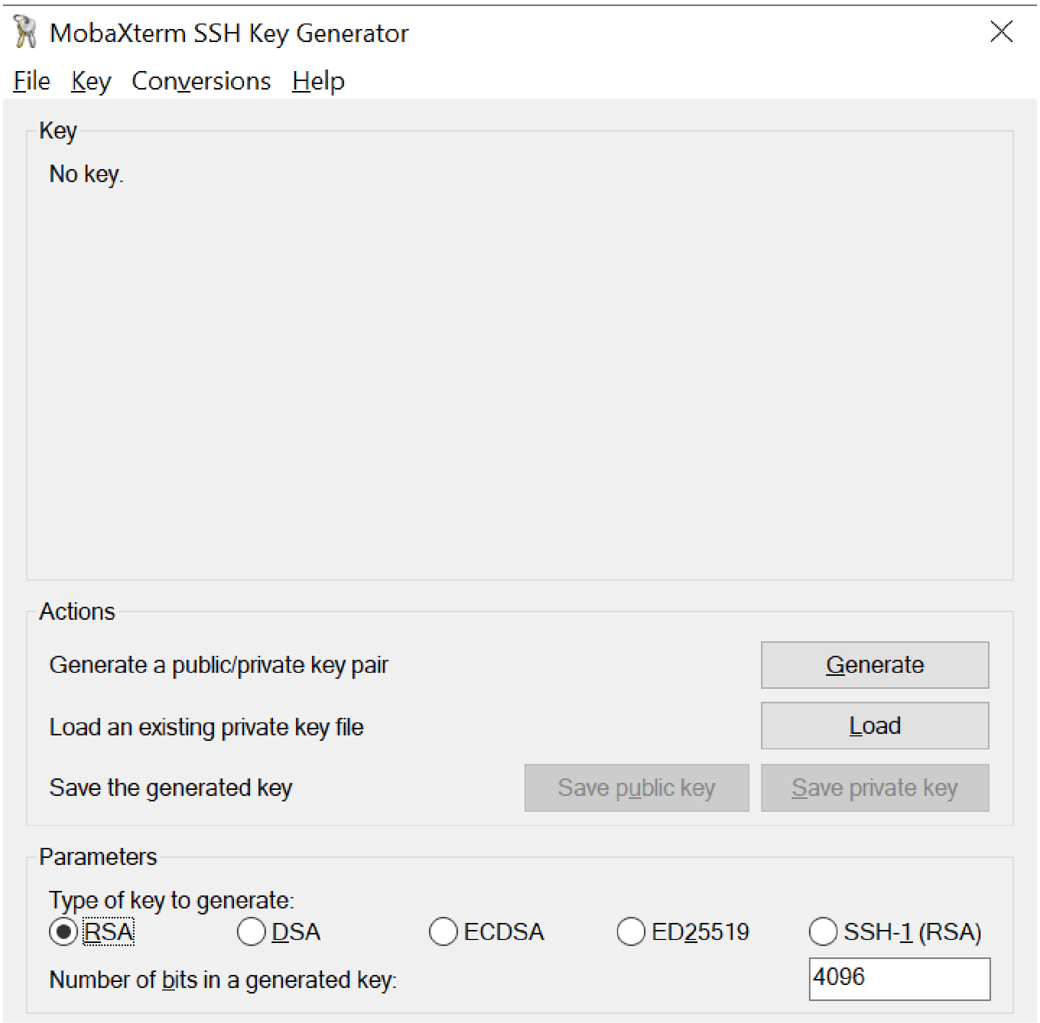
3. forhlr2.scc.kit.edu (n
4. Home
Sessions
Tools
Macros
MobaXterm
New session
Recover previous sessions
Find existing session or server name...
Recent sessions
forhlr2.scc.kit.edu (nl17...
forhlr2.scc.kit.edu (nl17...
login.hpc.ugent.be (vsc...
login.hpc.ugent.be (vsc...

CygUtils plugin not found on your system.

Enable advanced features and enhance security with MobaXterm Professional Edition!

UNREGISTERED VERSION - Please support MobaXterm by subscribing to the professional edition here: https://mobaxterm.mobatek.net

4) First we will need to generate a public-private key pair. This consists of a public key which will be uploaded to your account on the HPC and a private key which you will keep safe on your personal computer and which will allow to connect to your VSC-account.
   - Click on ‘Tools’ in the upper ribbon
   - Select ‘MobaKeyGen (SSH key generator)’ in the drop-down menu. The window below will appear:



MobaXterm SSH Key Generator

Key

No key.

Actions

Generate a public/private key pair

Load an existing private key file

Save the generated key

Parameters

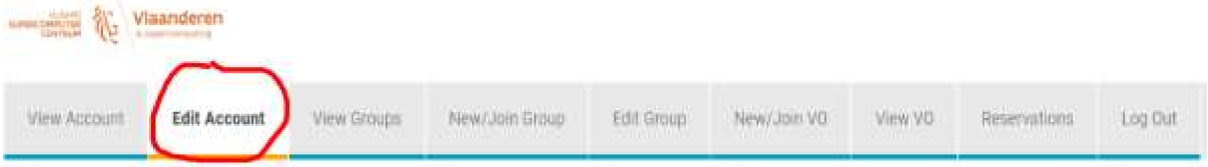
Type of key to generate:

● RSA ○ DSA ○ ECDSA ○ ED25519 ○ SSH-1 (RSA)

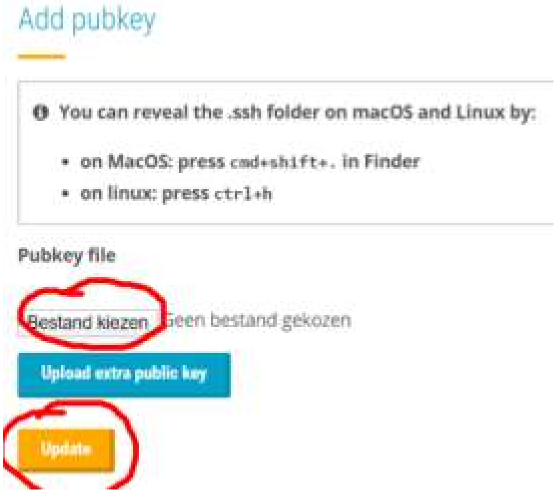
Number of bits in a generated key: 4096

- From 2020 onwards, the number of bits in a key needs to be at least 4096. If the bottom line of the window reads a smaller number, change it to 4096 (rule imposed by VSC).
- Click on the ‘Generate’ button
- Move your mouse cursor over the blank area to generate a random pattern that will be used to create your key pair.
- Now save BOTH the public key and private key to a directory of choice on your personal computer. Save the public key as ‘id_rsa.pub’ and the private key as ‘id_rsa.ppk’.
-

5) The next step is to request and account and upload the created PUBLIC key to the HPC.
   - Go to the following website: https://account.vscentrum.be
   - Accept the certificate
   - Choose ‘UGent’ as Home Institution (for UGent users).
   - Log in using your UGent credentials.
   - Select ‘Edit account’ from the top bar:



- Upload your public ssh key (which you have previously saved as ‘id_rsa.pub’) via ‘chose file’ and then click ‘update’. To upload more than one key, use the button ‘upload extra public key’ before you press ‘update’.



Add pubkey

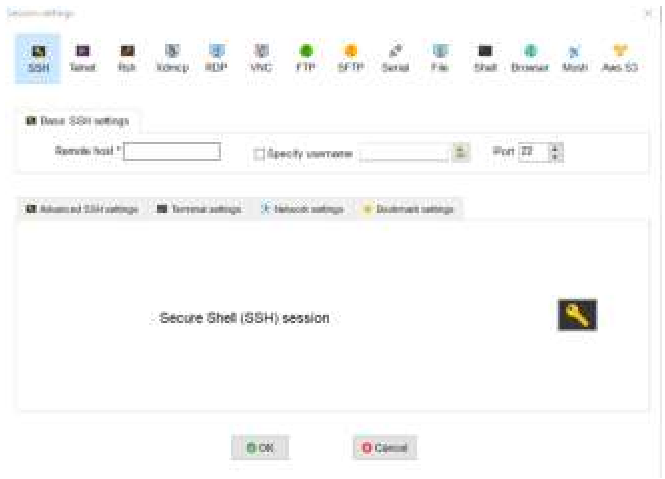
You can reveal the .ssh folder on macOS and Linux by:

- on MacOS: press `cmd+shift+.` in Finder
- on linux: press `ctrl+h`

Pubkey file

- Once the key is uploaded, you will receive an e-mail.
- Click on the link in the e-mail to confirm your VSC-id request.
- You will receive another e-mail once your request has been processed and your VSC-id is created.
- Detailed information can be found here: https://docs.vscentrum.be/ and/or https://www.ugent.be/hpc/en/access/policy/access
- If you wish to access the HPC from multiple computers, it is a good idea to use a different public-private key pair for each computer. You can create a public-private key pair on each of the computers using the instructions above and you can upload the additional public keys via the account management page: https://account.vscentrum.be. To do this, scroll down to the ‘Add pubkey’ section on this page and upload the new public key. You can check whether your public key was successfully uploaded by checking the ‘View account’ tab. Using this strategy, if one of your computers is stolen, you only need to delete the corresponding public key on your account to prevent the thief of having access to your account.

6) Once you have the e-mail confirming the activation of your vsc-account, it is time to define the parameters to successfully start your session on the HPC. The goal is to save these settings so that you don’t have to enter them each time we want to connect to the HPC. Go back to MobaXterm and click on the ‘New session’ button (in the centre of the window). This gives you the window below:



Remote host *

□ Specify username

Port 22

7) Fill out the following:
    - Remote host: login.hpc.ugent.be
    - Check the ‘specify username’ box
    - Username: vscXXXXX with XXXXX being the account number you received.
    - Port: 22

8) Go to the ‘Advanced SSH settings’ tab and fill out the following:
    - Check the ‘X11-Forwarding’ box
    - Check the use private key box
    - Browse to the correct private key file which you have saved on your pc (rsa_id.ppk).
    - Press ‘OK’.

9) Your session will now start. Depending on whether or not you chose to also protect your account by a password, you will be asked to enter it. If so, simply enter the password you chose earlier.

10) You are now connected to one of the *log in nodes* of the Flemish Supercomputer. From these *log in* nodes, you can submit scripts defining the tasks to be performed on the *compute* nodes. Performing calculations on the *log in* nodes themselves should be avoided at all times, as this can inhibit a proper connection to the HPC for other users!

All information on requesting a VSC account can be found here:
https://docs.vscentrum.be/

A stepwise roadmap can be found here:
https://www.ugent.be/hpc/en/access/faq/access

Instructions for Mac Os or Linux users

The information at https://docs.vscentrum.be/access/index.html distinguishes at the relevant places between Windows, Mac or Linux.

STEP 4: Create an SFTP session to transfer files between you computer and the HPC

- Click on the 'Session' button at the left in the upper ribbon of MobaXterm.
- Select 'SFTP' in the window that appears
- Fill out the Remote host, your username and the Port as before.
- Also add your private key in the Advanced Sftp section.
- Click 'OK'. A window will appear that allows transferring files between your computer and the HPC.

STEP 5: getting used to the LINUX environment

The VSC clusters use Linux as their main operating system. For some of you this will be a totally new environment. You do not need to know everything about this operation system to be able to complete your work, the most often used commands will do. You work here using what is called a 'command line'. Instead of clicking pictograms in Windows or Mac OS you will literally tell the computer what you want to do. A list of the most used Linux commands can be found here: http://www.dummies.com/computers/operating-systems/linux/common-linux-commands/

Additionally an unlimited amount of guides and tutorials on the Linux operating system can be found on the internet e.g. a very basic guide can be found here: https://docs.vscentrum.be/jobs/basic_linux_usage.html

If you want to have more information on a specific aspect of Linux or on a command, simply google it. http://stackoverflow.com will often answer your questions!

If a certain command is not clear, you can request the manual page for it within the Linux command line itself by typing:

`man <command>` (e.g. `man ls`)

Most used commands for you will be:

`cd <foldername>` → CHANGE DIRECTORY: to go to another directory (e.g. cd map1).

`ls` or `ls <foldername>` → LIST: to list all files and folders within given folder.

`cp <source> <destination>` → COPY: to copy a file to another directory.

`mv <source> <destination>` → MOVE: to move or rename a file.

`rm <filename>` → REMOVE: remove file (remove directory using `rm -r <directory>`).

`mkdir <directory>` → MAKE DIRECTORY: to make a new directory.

`pwd` → PRINT WORKING DIRECTORY: display the pathname for the directory you are working in.

`touch` <filename> → create an empty file with the specified filename.

`vi` <filename> →VIM editor: to start the VIM editor to make or edit text files.

`cat` <filename> → display content of file in the terminal.

`echo` <variable> → prints the variable in your terminal.

`grep` 'STRING' <filename> → to search for a given string in a file.

`>` → write to file (e.g. echo $VARIABLE > variable.txt), if the file already exists, it will be overwritten.

`>>` → append to an (existing) file (e.g. echo $VARIABLE >> variable.txt), text will be added to file.

Special directory shortcuts

`.` Current directory

`..` Parent directory (e.g. use 'cd ..' to go up 1 directory, cd ../.. to go up 2 directories, …)

`/` Root directory (directory at the highest level of a hierarchy)

`~` Home directory (often the highest level of your personal directories)

`$VSC_SCRATCH` your scratch directory (for temporary data, no back-up, fast data transfer)

`$VSC_HOME` your home directory (same as ~ unless changed by user)

`$VSC_DATA` your data directory (for long term storage of results, a back-up exists)

More information on where to store what data can be found here:
https://docs.vscentrum.be/access/where_can_i_store_what_kind_of_data.html

Check what cluster you are working on

`echo $VSC_INSTITUTE_CLUSTER`: print variable that shows which cluster you are working on

Module system on the VSC

In order to use a certain programs e.g. QuantumEspresso, the corresponding module has to be loaded. Below a few useful commands concerning this module system can be found:

`module av` : to check which modules are available on the cluster you are working on

`module list`: to list the modules that are currently loaded in your session

`module load <modulename>`: to load a given module in your current session

Submit, check, delete jobs

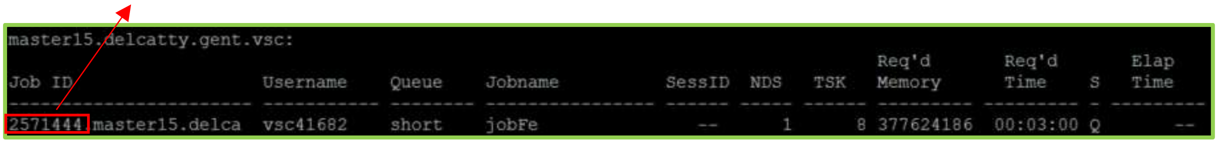
As mentioned before, our calculation jobs will be submitted to compute nodes. As there are many people using the hpc, calculations are submitted to a queue before they are started. When your calculation will eventually start depends on your 'priority'. This parameters depends on your statute (student/PhD-student/…), on how often you used the hpc the past month, on how long your calculations have been queueing, on what resources you request, … If your calculation doesn't start immediately, don't worry, they should eventually start after some time (seconds to days).

The commands used here to submit, check and delete jobs are:

`qsub <jobscript>`: to submit a jobscript to the queue

`qstat`: check the queue, see if your calculations have started and find out what their jobnumber is

`qdel <jobnumber>`: to delete a queueing or running job with a certain jobnumber



```
master15.delcatty.gent.vsc:
                                                                                   Req'd     Req'd       Elap
Job ID                  Username    Queue    Jobname          SessID NDS   TSK    Memory    Time      S  Time
----------------------- ----------- -------- ---------------- ------ ----- ------ --------- --------- - ---------
2571444.master15.delca  vsc41682    short    jobFe                --     1      8 377624186  00:03:00 Q        --
```

STEP 6: using QuantumEspresso on the VSC

Using QuantumEspresso on the VSC is very similar to using it on your personal computer. There are two main differences:

- Before you can use QuantumEspresso on the VSC the corresponding module needs to be loaded.
- It should be avoided to run calculations on the login nodes of the hpc as this can block access to the hpc for other users. Instead a *job script* has to be created which is then submitted to one of the compute nodes of the cluster. How to do this will be explained below.

When you log in to the hpc, you will experience that you are connected to the 'victini' cluster (you can check this by typing '`echo $VSC_INSTITUTE_CLUSTER`' in your terminal). The name 'victini' refers to a Pokémon. Actually all Ghent University clusters named after Pokémon. At the moment there are 5 Tier-2 clusters available: phanpy, golett, swalot, skitty and victini. QuantumEspresso is installed on all of these clusters. You can check the different specifications of these clusters here: https://www.ugent.be/hpc/en/infrastructure.

You can change the cluster you are submitting to by the command:

```
module swap cluster/<NameOfCluster>.
```

To check which version of QuantumEspresso is installed, enter the following:

```
module avail QuantumEspresso
```

Normally you will see that two or more versions of QuantumEspresso are installed. The one that is followed by a (D) is the default one. Unless you voluntarily want to use an older version of QuantumEspresso, you can load the newest (default) version by simply typing:

```
module load QuantumEspresso
```

However if you want to use a specific version, you have to specify it, e.g.:

```
module load QuantumESPRESSO/6.5-intel-2019b
```

However as we will perform our calculations on the compute nodes and not on the login nodes, it is not necessary to load the QuantumEspresso on the login nodes. Rather, the QuantumEspresso module should be loaded on the compute nodes from within the job script.

Creating a job script

The job scripts we will create are bash shell scripts which we give the .sh extension. In order to make such a script with e.g. the name 'NaCl', one should enter the following in the terminal:

```
nano NaCl.sh
```

This means you use the (rather intuitive) 'nano' editor. A popular alternative in the Linux world is:

```
vi NaCl.sh
```

With the *vi* command, you are using the *Vim editor* to create your job script. Before you can type in the editor one should press *i* on your keyboard. Now the insert mode is activated and you can simply type the text you want to add to the file. After adapting the file, press *esc* to exit the insert mode.

Then type *:x* to save the changes to your file. If you did not change the file you can exit the Vim editor by entering *:q*. If you did adapt the file but you do not wish to save the changes, then exit the Vim editor using *:q!* .

More information on the Vim editor can be found here: http://www.vim.org/

The job script contains three sections:

1. The first line is called the hashbang(#!) line and specifies in what programming language the script is written. This way it is more probably that the job script will also work on other computers using a different OS. As mentioned we will use the bash shell language here. Therefore the first line should look like:

   ```
   #!/usr/bin/env bash
   ```

2. In the following lines one should specify the requested resources for the calculations (name of the calculation, output file, error file, walltime, number of nodes, number of cores per node, the requested memory, whether or not you want to be notified when the job ends, ..). The user has to specify this so that the resource manager can check whether or not the requested resources are available or not. If not, the user will have to wait until the requested resources become available before the calculation can start. The software used in order to achieve this is called PBS/Torque (Portable Batch System). Requesting certain resources can be done using PBS directives. An example is given below:

   ```
   #PBS -N jobNaCl
   #PBS -o outputNaCl.file
   #PBS -e errorNaCl.file
   #PBS -l walltime=11:59:00
   #PBS -l nodes=1:ppn=16
   #PBS -l mem=4gb
   #PBS -m be -M user@hotmail.com
   ```

   Line 1: The name ‘jobNaCl’ is appointed to the job.
   Line 2: A filename is chosen to which the standard output (stdout) is redirected.
   Line 3: A filename is chosen to which the standard error messages (stderr) are redirected.
   Line 4: A walltime (maximum calculation time for job) of 11u59min is requested (max = 72u).
   Line 5: 1 node is requested and 16 cores per node will be used (delcatty: max ppn = 16).
   Line 6: 4GB of memory is requested for the job
   Line 7: Ask to send a message to a given email address when job begins (b) and ends (e).

   More information can be found here:
   https://docs.vscentrum.be/gent/tier2_hardware.html#ugentt2-hardware

3. The third part contains the tasks you actually want to perform. This is what you would normally enter in your terminal if you were working on a login node or on your personal computer (using LINUX). The execution of your job always begins in your home directory, regardless of what directory your script resides in or where you submitted the job from. It is however often desired to work in the directory you submitted the job from. One can easily navigate to this directory using the environment variable $PBS_O_WORKDIR. This can be done by writing the following in your jobscript:

   ```
   cd $PBS_O_WORKDIR
   ```

The next thing we should do is to load the QuantumEspresso module in the compute node:

```
module load QuantumESPRESSO/6.2-intel-2017b
```

Finally we have to run the QuantumEspresso command. Here we make use of the ‘mpirun’ software to parallelize our calculations. This can be done as follows:

```
mpirun –np $PBS_NP pw.x –input NaCl.in > NaCl.out
```

pw.x is the QuantumEspresso executable we will use most often. The –np flag specifies the number of processes to which the calculation should be parallelized. This information is contained in the environment variable $PBS_NP which is simply the multiplication of the number of nodes and the cores per node. The –input flag is used to specify the input file and the output is redirected to a file with the specified name ‘NaCl.out’ using the ‘>’ symbol.

It is always very useful to put comments in your job script stating what you are aiming to do using each command. These comments can be added in a job script using a ‘#’ at the start of the line.
An example of a complete job script is given below:

```
#!/bin/sh
#
#
#PBS -N jobFe
#PBS -o outputFe.file
#PBS -e errorFe.file
#PBS -l walltime=0:30:00
#PBS -l nodes=1:ppn=8
#

# change to directory you were working when submitting job
cd $PBS_O_WORKDIR

#load QE
module load QuantumESPRESSO/5.2.1-intel-2015b

#run QE command
mpirun -np $PBS_NP pw.x -input Fe.in > Fe.out
```

How to make a QuantumEspresso input file such as ‘Fe.in’ and what its contents should be will be explained in a different document that you can also find on the www.compmatphys.org website.