HPC Workshop for Beginners

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You can find the slides in www.hannokase.com/HPC/

How do I get the HPC account?

To access the HPC cluster, you need to request an account via EUI Helpdesk.

For this workshop, we have created you **test accounts**:

User name: **cmatlab01-cmatlab16**
Password:

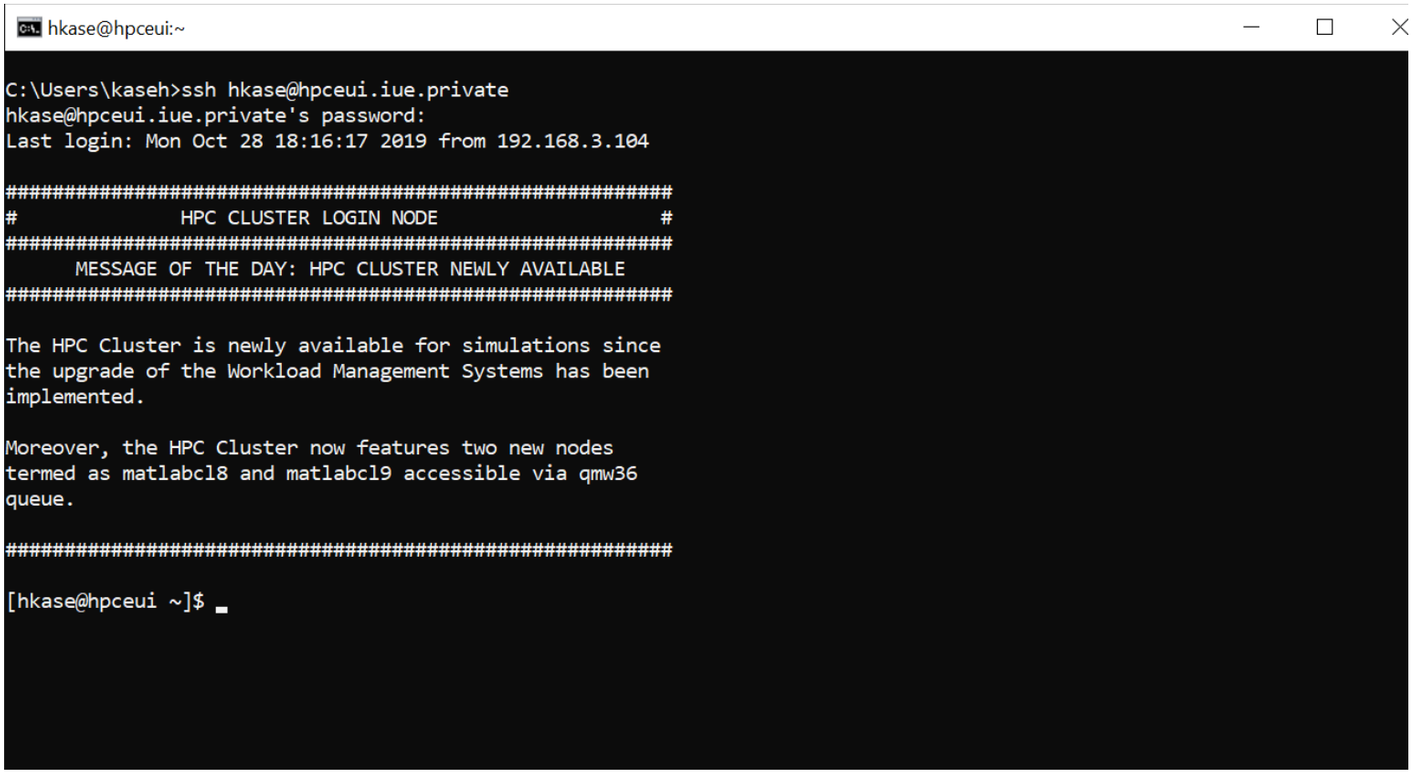
How to connect to the HPC cluster?

You can access the HPC cluster through **S**ecure **Sh**ell Protocol (SSH), using any SSH client.

On Linux, Windows 10, and Mac a SSH client is preinstalled and you can use it through command line (Terminal, Command Prompt, PowerShell).

Command for using SSH: `ssh username@host`

```
ssh hkase@hpceui.iue.private
```


hkase@hpceui:~
C:\Users\kaseh>ssh hkase@hpceui.iue.private
hkase@hpceui.iue.private's password:
Last login: Mon Oct 28 18:16:17 2019 from 192.168.3.104
##
HPC CLUSTER LOGIN NODE
##
      MESSAGE OF THE DAY: HPC CLUSTER NEWLY AVAILABLE
##
The HPC Cluster is newly available for simulations since
the upgrade of the Workload Management Systems has been
implemented.
Moreover, the HPC Cluster now features two new nodes
termed as matlabcl8 and matlabcl9 accessible via qmw36
queue.
##
[hkase@hpceui ~]$

Are you tired of typing your password?

To avoid typing your password every time you enter the HPC cluster you can add your **public SSH key** to `~/.ssh/authorized_keys` file on the HPC cluster.

On Windows 10 you can find your public SSH key in:

`C:\Users\<username>\.ssh\id_rsa.pub`

This is the default location, it might be somewhere else. If you don't find it, you can generate one by `ssh-keygen` command. Choose the location (default location is usually fine), choose a password (or leave it empty).

Some essential Linux commands

Command	What does it do?
`man [COMMAND]`	Manual page for [COMMAND]
`passwd`	Change your password
`pwd`	Current working directory
`cd [FOLDER]`	Change directory to [FOLDER]
`cd ..`	Move to parent directory
`cd ~`	Change directory to home directory
`ls`	List files in the folder
`mv [SOURCE] [DESTINATION]`	Move or rename files
`cp [SOURCE] [DESTINATION]`	Copy files
`rm [FILE]`	Delete file
`mkdir [FOLDER]`	Make a directory named [FOLDER]
`rm -r [FOLDER]`	Recursively delete the folder and all files in it
`nano [FILE]`	Open text editor (nano)

How to transfer files to the HPC cluster

- Command Line
    - SFTP
    - SCP
- Graphical User Interface
    - Using a SFTP client (FileZilla, WinSCP)
    - Map a network drive*

*Easy on Linux, but a bit tricky on Windows 10 and Mac

- Windows 10 : install WinFsp and SSHFS-Win
- Mac : this might be helpful

Transfering files - Command Line: SFTP

Interactive command, that opens a connection for submiting several commands for transfering files.

Command for opening SFTP connection: `sftp username@hpceui.iue.private`

```
sftp hkase@hpceui.iue.private
```

SFTP interactive commands

Command	What does it do?
`cd`	Change the active directory on REMOTE machine
`lcd`	Change the active directory on LOCAL machine
`ls`	List files in the active folder on REMOTE machine
`lls`	List files in the active folder on LOCAL machine
`rm`	Remove files on REMOTE machine (there is no `lrm`)
`mv`	Move files on REMOTE machine (there is no `lmv`)
`cp`	Copy files on REMOTE machine (there is no `lcp`)
`put [FILE]`	Put a file from the LOCAL machine to the REMOTE machine
`get [FILE]`	Get a file from the REMOTE machine to the LOCAL machine

Close the connection by typing `exit` or `bye` or pressing CTRL+C.

SFTP Example

```
sftp hkase@hpceui.iue.private
```

Let's try to transfer `file1.txt` file from local machine to the remote machine.

```
put file1.txt
```

The file `file1.txt` from the active directory on our local machine got transfered to the active directory on the remote machine.

Transfering files - Command Line: SCP

Non-interactive command. Takes only one command and then exits.

Command for using SCP: `SCP [SOURCE] username@hpceui.iue.private:[TARGET]`

```
scp file1.txt file2.txt hkase@hpceui.iue.private:~/demo
```

For faster file transfer, we can use compression `-C`.

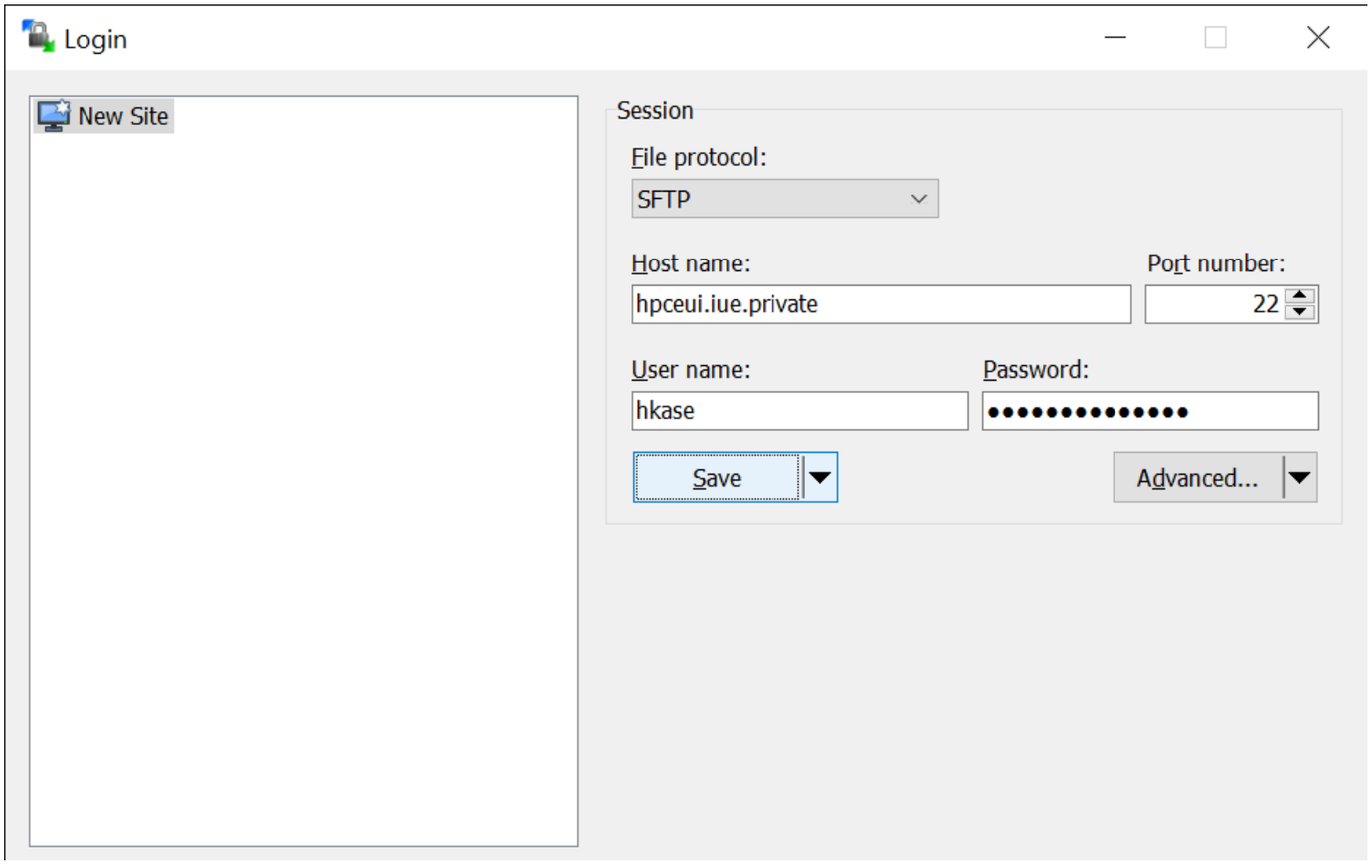
```
scp -C file1.txt hkase@hpceui.iue.private:~/demo/file_rename.txt
```

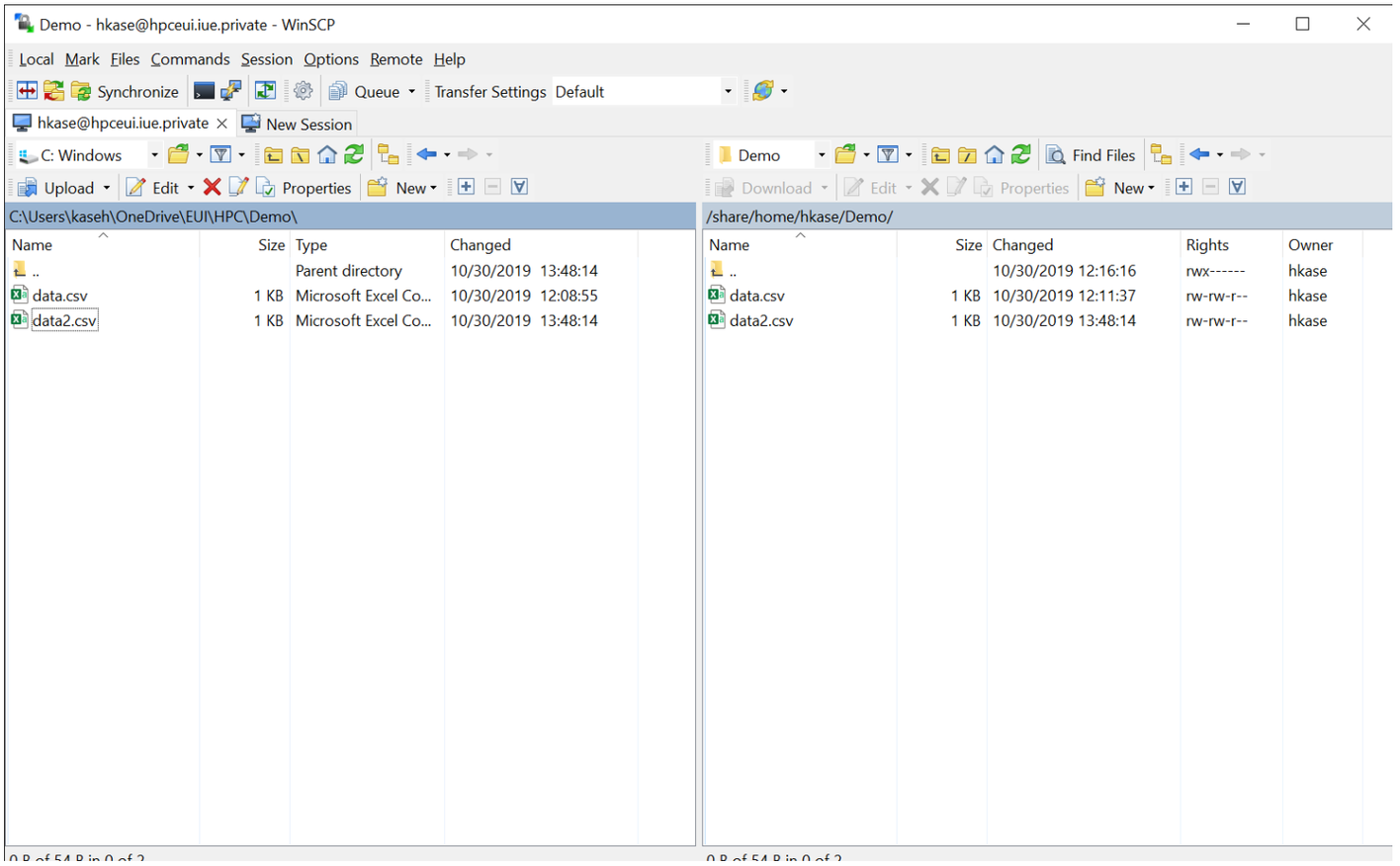
Add `-r` flag to copy the whole folder.

```
scp -r folder hkase@hpceui.iue.private:~/new_folder
```

Transfering files - GUI: WinSCP

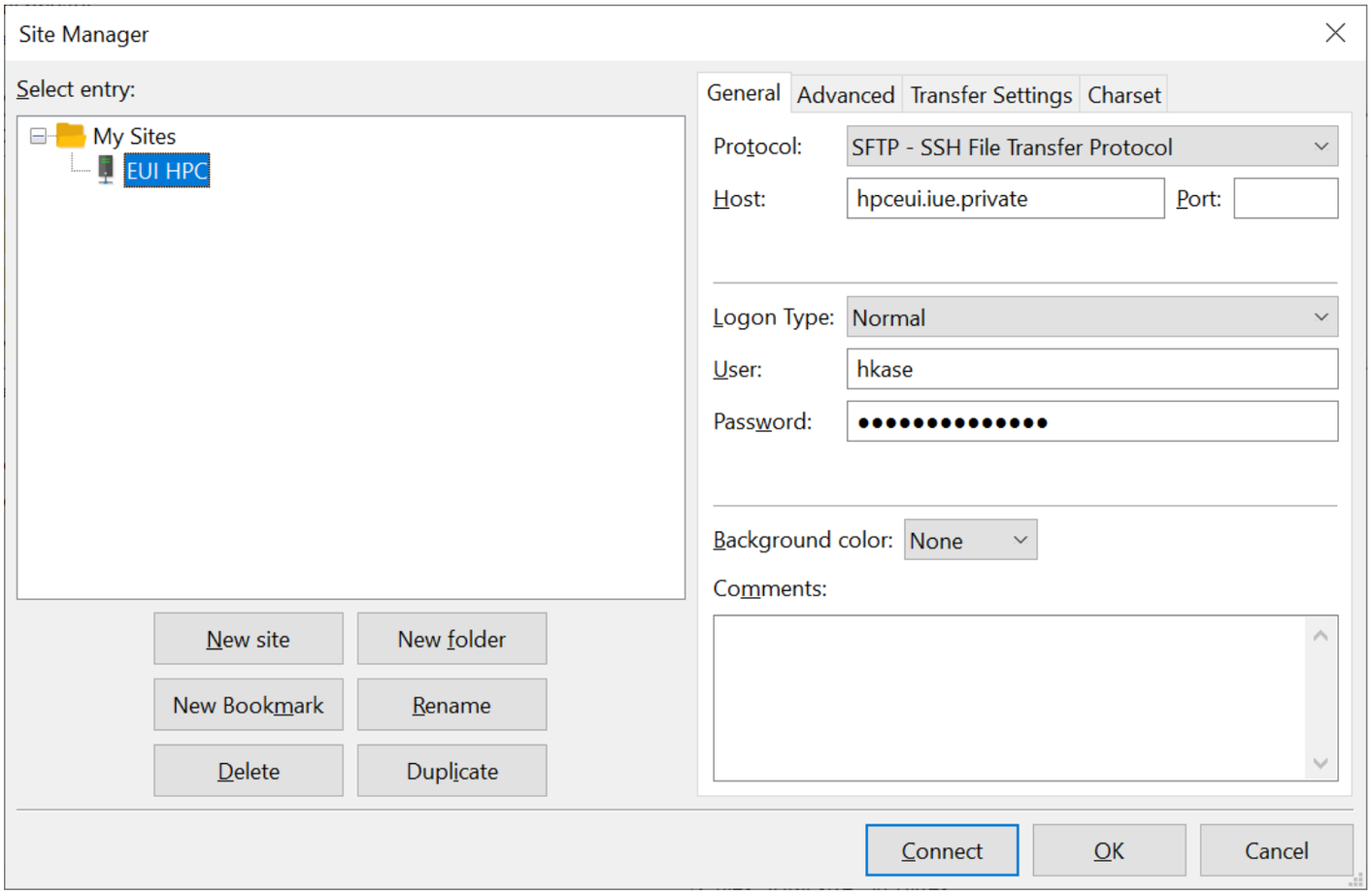
Free software for Windows 10.

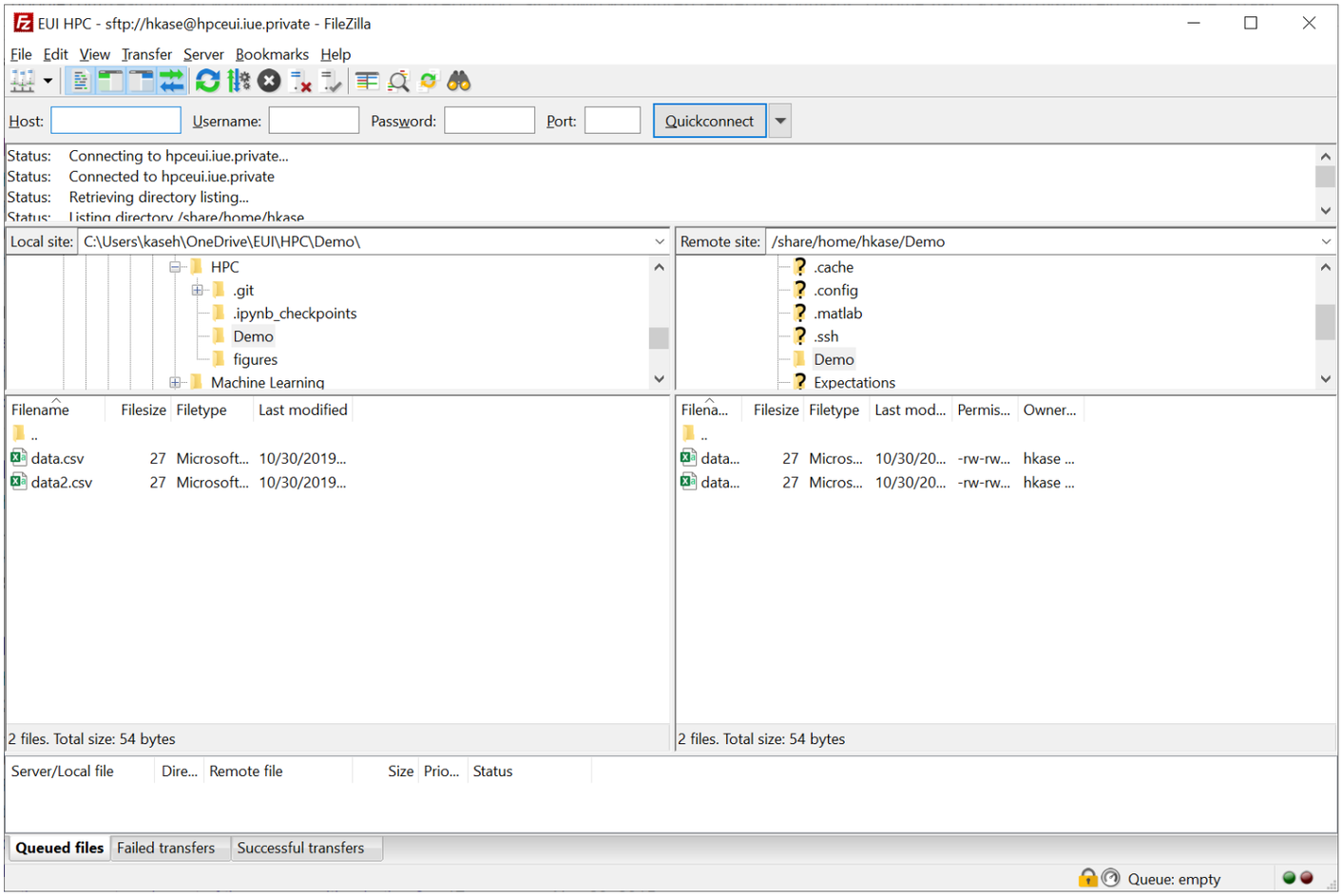



Demo - hkase@hpceui.iue.private - WinSCP
Local Mark Files Commands Session Options Remote Help
Synchronize
Queue
Transfer Settings Default
hkase@hpceui.iue.private
New Session
C: Windows
Upload
Edit
Properties
New
C:\Users\kaseh\OneDrive\EUI\HPC\Demo\
Name Size Type Changed
.. Parent directory 10/30/2019 13:48:14
data.csv 1 KB Microsoft Excel Co... 10/30/2019 12:08:55
data2.csv 1 KB Microsoft Excel Co... 10/30/2019 13:48:14
Demo
Find Files
Download
Edit
Properties
New
/share/home/hkase/Demo/
Name Size Changed Rights Owner
.. 10/30/2019 12:16:16 rwx------ hkase
data.csv 1 KB 10/30/2019 12:11:37 rw-rw-r-- hkase
data2.csv 1 KB 10/30/2019 13:48:14 rw-rw-r-- hkase

Transfering files - GUI: FileZilla

Free software available for Linux, Mac, Windows 10.
Careful when installing it. You probably don't want the included Avast Antivirus.




EUI HPC - sftp://hkase@hpceui.iue.private - FileZilla
File Edit View Transfer Server Bookmarks Help
Host: Username: Password: Port: Quickconnect
Status: Connecting to hpceui.iue.private...
Status: Connected to hpceui.iue.private
Status: Retrieving directory listing...
Status: Listing directory /share/home/hkase
Local site: C:\Users\kaseh\OneDrive\EUI\HPC\Demo\
HPC
.git
.ipynb_checkpoints
Demo
figures
Machine Learning
Remote site: /share/home/hkase/Demo
.cache
.config
.matlab
.ssh
Demo
Expectations
Filename Filesize Filetype Last modified
..
data.csv 27 Microsoft... 10/30/2019...
data2.csv 27 Microsoft... 10/30/2019...
Filena... Filesize Filetype Last mod... Permis... Owner...
..
data... 27 Micros... 10/30/20... -rw-rw... hkase ...
data... 27 Micros... 10/30/20... -rw-rw... hkase ...
2 files. Total size: 54 bytes
2 files. Total size: 54 bytes
Server/Local file Dire... Remote file Size Prio... Status
Queued files Failed transfers Successful transfers
Queue: empty

Transfering files - Map a network drive

Windows 10

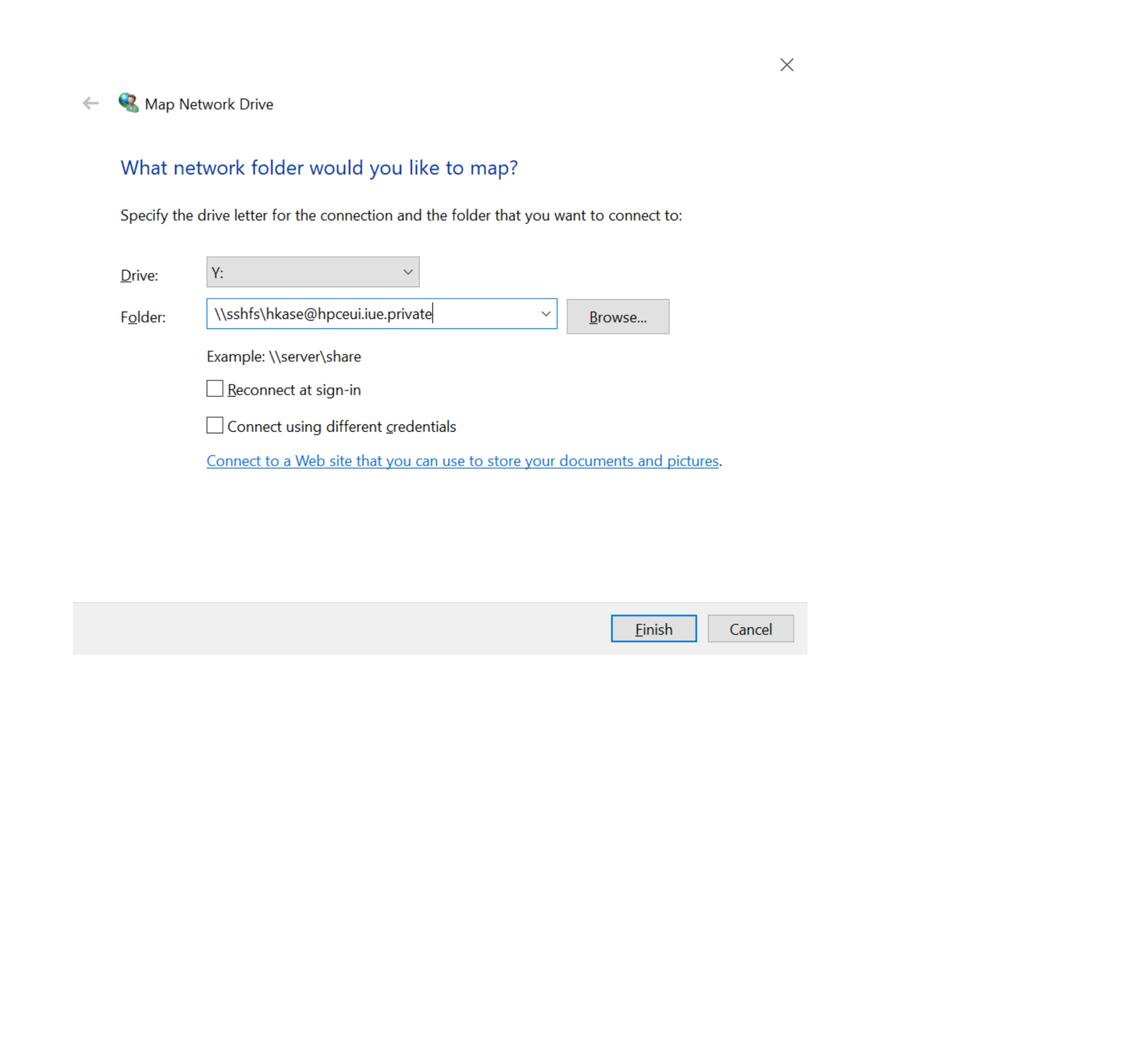
- Install WinFsp and SSHFS-Win. Look for *latest release* tag and *.msi* files.
- Map a network drive `sshfs//<username>@hpceui.iue.private`

Linux - Ubuntu 18.04

- Add remote location `sftp://<username>@hpceui.iue.private/`

Mac

- This might be helpful


Map Network Drive
What network folder would you like to map?
Specify the drive letter for the connection and the folder that you want to connect to:
Drive:
Y:
Folder:
\\sshfs\hkase@hpceui.iue.private
Browse...
Example: \\server\share
Reconnect at sign-in
Connect using different credentials
Connect to a Web site that you can use to store your documents and pictures.
Finish
Cancel

Queues in the HPC cluster

At the heart of the cluster is a workload management system (PBS Professional); a program that allocates computational resources.

You use the cluster by first asking for resources. Depending on your computational needs, you will choose from which **queue** to ask the resources from.

The EUI HPC cluster is designed such that there is a direct mapping from queues to computing nodes (servers). All the resources you request are allocated within one node.

Queue	Slots	Nodes	CPU cores	Memory	GPU	Walltime
`qwe36`	4	matlabcl6-9	36	128GB	No	12h
`qwe24`	2	matlabcl4-5	24	128GB	No	12h
`qwe12`	1	matlabcl3	12	32GB	Yes	72h
`qwe36long`	?	matlabcl6-9	36	128GB	No	168h
`qwe24long`	?	matlabcl4-5	24	128GB	No	168h

Which queue should I choose?

`qstat -Q` or `qstat -q` to find out what kind of queues are there.

`qstat` or `qstat -n1` to monitor the queues.

`pbsnodes -av` to get a detailed overview of all the nodes.

How to submit a batch job to the HPC cluster?

The most common use of the cluster is to submit a **batch job**.
For this we will need to specify for the workload manager:

1. what kind of resources we need and ...
2. what program we would like to run.

We do it all by creating a **PBS script** (like a bash script), that contains some special instructions for the workload manager.

Then we submit the job into the queue using `qsub [pbs_script]` command. When there are available resources, it will get executed.

Script for running MatLab code (CPU)

```
#!/bin/bash
# 1. Job name
#PBS -N MATLAB

# 2. Request resources
# set the number of nodes and processes per node
#PBS -q qmw12

# use submission environment
#PBS -V

# 3. Run the program
# start the job from the directory it was submitted
cd $PBS_O_WORKDIR

# set some environment variables for MatLab
source /apps/Matlab_var_R2019a.sh

# Run your the matlab code
matlab -batch "R2019a_mod_paralleldemo_parfor_bench" >& matlab.log
```

Script for running MatLab code (GPU)

```
#!/bin/bash
# 1. Job name
#PBS -N MATLAB

# 2. Request resources
# set the number of nodes and processes per node
#PBS -q qmw12

# use submission environment
#PBS -V

# 3. Run the program
# start the job from the directory it was submitted
cd $PBS_O_WORKDIR

# set some environment variables for CUDA and MatLab
source /apps/cuda-10.1.sh
source /apps/Matlab_var_R2019a.sh

# Run your the matlab code
matlab -batch "paralleldemo_gpu_backslash" >& matlab_gpu.log
```

Script for running Julia code

```
#!/bin/bash

# 1. Job name
#PBS -N Julia

# 2. Resource request
#PBS -q qmw12 -l walltime=12:00:00,select=1:ncpus=12

# use submission environment
#PBS -V

# 3. Program to run
# start the job from the directory it was submitted
cd $PBS_O_WORKDIR

# set some environment variables for Julia
source /apps/Gnu_var_4.9.4.sh
export PATH=/opt/pkgs/julia-1.1.0/bin:$PATH

# Run your Julia code
export JULIA_NUM_THREADS=4
julia -O3 -- spectralnorm.julia 5500 >& spectralnorm.julia.log
```

Script for running FORTRAN code (OpenMP)

```
#!/bin/bash

# set the number of nodes and processes per node
#PBS -q qmw12 -l select=1:ncpus=12

# set name of job
#PBS -N Fortran

# OMP Environment Variable #
export OMP_NUM_THREADS=12
export OMP_THREAD_LIMIT=12

# use submission environment
#PBS -V

# start job from the directory it was submitted
cd $PBS_O_WORKDIR

# compile the Fortran Source....
echo "Running gfortran on `hostname`: gfortran -fopenmp matrix_mult.f -o matri
x_mult.exe"
gfortran -fopenmp matrix_mult.f -o matrix_mult.exe
# run my_application over a compute node within the PBS ring (pbsnodes -av)
echo "Running line on `hostname`: ./matrix_mult.exe > 12_cores_output_file "
./matrix_mult.exe > 12_cores_output_file
```

I would like to run R/STATA/Python...

You can find many other PBS script samples on the cluster in `/share/apps`

Monitoring your job

Command	What does it do?
`qstat`	Shows the status of all the jobs
`qstat -n1`	Shows the status of all the jobs and their nodes
`qstat -u [username]`	Shows the status of the jobs belonging to [username]
`qstat -f [jobid]`	Shows the detailed information about [jobid]
`qdel [jobid]`	Delete the [jobid]
`tail -f [output_file.log]`	Prints the output file in the terminal as it is being written

How is my code doing?

If you are not quite sure that your code is running nicely in parallel, you can log into the compute node and check the task manager `htop`.

1. Find the node where your job is running using `qstat -u [username] -n1`.
2. Log into the node `ssh [node name]`, for example `ssh matlabcl3`.
3. Run `htop` to open the task manager
4. Close the task manager by pressing `F11`
5. Close the SSH connection by typing `exit`

How to use the cluster interactively?

Using cluster interactively can be useful for developing your code or debugging.

Add `-I` to the requlars `qsub` command. The following command will start an interactive job with the parameters specified in the `pbs_script`.

```
qsub -I pbs_script
```

You can start an interactive session without a PBS script.

```
qsub -I -N MyInteractiveJob -q qmw12 -l select=1:ncpus=12:host=matlabcl3
```

Thank you!

E-mail us if you have questions: hpc.support@eui.eu
Request an account via EUI Helpdesk.