

Using HPC of HHU

Create an account

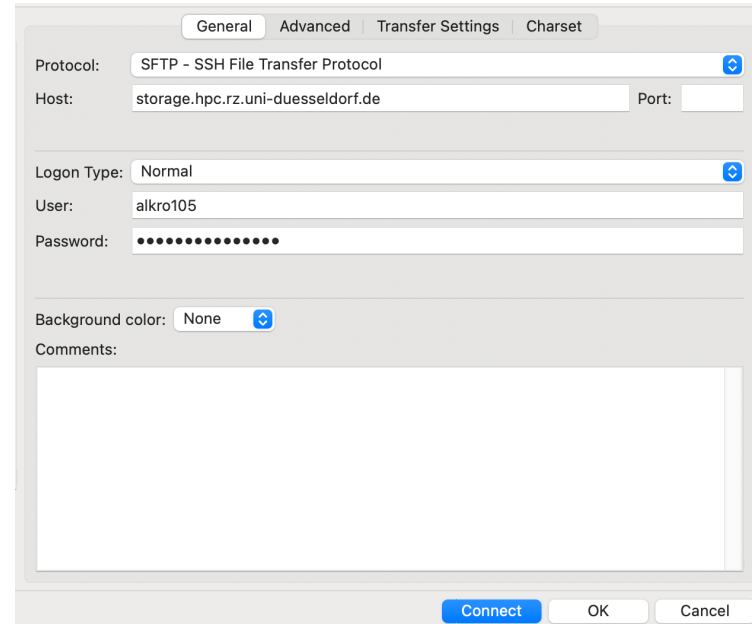
- You need to create an account on <https://www.zim.hhu.de/forschung/high-performance-computing/antrag>. Fill in the following information:
 - Institut: Institut für Informatik – Computational Cell Biology
 - Institutsleiter: Prof. Dr. Martin Lercher
 - Verantwortlicher des Projekts: Alexander Kroll
 - Zustand des Projekts: "Neues Projekt"
 - Projektkürzel: DL4MoleculesCourse
 - Kurze Projektbeschreibung: "This account will be used for small programming tasks that are part of the lecture 'Applications of Transformer Networks in Bio- and Cheminformatics' by Alexander Kroll."

Requirements to log in to HPC

- You need to be in the campus network to log in to HPC. Options:
 - Connect to university wifi
 - Connected to campus network via VPN:
 - Follow instructions on <https://www.zim.hhu.de/en/servicekatalog/networks/vpn>

Managing files with FileZilla

- You need to move files between your PC and the HPC
- You can do this using FileZilla: <https://filezilla-project.org/> (available for all platforms)
 - Download the FileZilla Client
- Log in to HPC using FileZilla:
 - Connect to new server (ctrl + s / cmd + s) by entering the information on the right
 - User is your university username



The image shows the 'General' tab of the FileZilla settings dialog box. The 'Protocol' is set to 'SFTP - SSH File Transfer Protocol'. The 'Host' is 'storage.hpc.rz.uni-duesseldorf.de'. The 'Port' is empty. The 'Logon Type' is 'Normal'. The 'User' is 'alkro105'. The 'Password' is masked with dots. The 'Background color' is 'None'. There is a 'Comments' text area at the bottom. At the bottom right are 'Connect', 'OK', and 'Cancel' buttons.

General Advanced Transfer Settings Charset

Protocol: SFTP - SSH File Transfer Protocol

Host: storage.hpc.rz.uni-duesseldorf.de Port:

Logon Type: Normal

User: alkro105

Password:

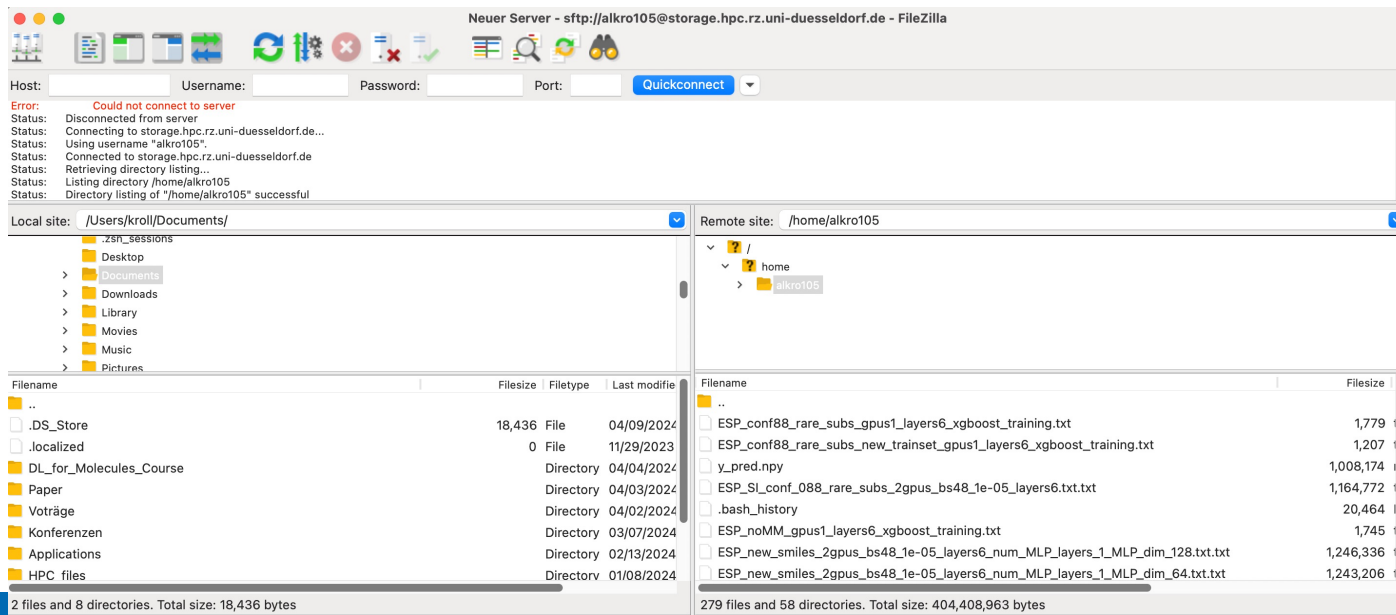
Background color: None

Comments:

Connect OK Cancel

Managing files with FileZilla (2)

- After you are connected you can see
 - Left side: The files on your PC
 - Right side: Files in your HPC folder “/home/user”
- You can move files by right clicking on them



Jobs are submitted via Bash scripts

■ Example for bash script that installs the python package torch

```
1  #!/bin/bash
2  #PBS -l select=1:ncpus=1:mem=6GB  ← Required resources: 1 CPU and 6GB RAM
3  #PBS -l walltime=05:00:00  ← Required runtime: After 5 hours the job will quit if not already finished
4  #PBS -A kcat-prediction  ← Project name that you entered when registering for the HPC
5  #PBS -N package_install  ← Job name; choose a suitable name
6  #PBS -j oe
7  #PBS -o "package_install.log"  ← After job is finished you will find the logs in a file with this name
8
9  cd /home/alkro105/  ← Move to your home folder
10
11 module load Python/3.8.3  ← Load Python version for which you want to install the Python package
12 module load CUDA/11.7.1  ← Load CUDA to install torch with CUDA enabled
13
14 pip install --user -i http://pypi.repo.test.hhu.de/simple/ --trusted-host pypi.repo.test.hhu.de torch==2.0.0+cu117 --upgrade
```

← Command to install Python package "torch" version 2.0.0 with CUDA enabled

■ You need to upload this file to HPC via FileZilla if you want to execute it

Submitting jobs via terminal

- You need to connect to HPC via your terminal:

```
kroll — alkro105@hpc-login7:~ — ssh alkro105@hpc.rz.uni-duesseldorf.de — 88x41
[(base) kroll@MacBook-Air-von-Administrator ~ % ssh alkro105@hpc.rz.uni-duesseldorf.de ]
[alkro105@hpc.rz.uni-duesseldorf.de's password: ]
Last login: Tue Apr  2 06:10:57 2024 from 134.99.174.99
[alkro105@hpc-login7 ~]$
```

- Once logged-in, you will be in your home folder “/home/user”
 - Operating system is Linux:
 - You can see all the files in your current folder using the command `ls`
 - You can submit a job using the command `qsub name_of_bash_script.sh`
 - You can see the status of your jobs
 - `qstat -u username`
 - Status “Q” stands for queued; “R” stands for running; After job is executed it will vanish from this list
 - You can monitor your jobs on myjam3.hhu.de

Running a Python Script

- Implement Bash script to execute Python script:

```
1  #!/bin/bash
2  #PBS -l walltime=01:30:00
3  #PBS -l select=1:ncpus=1:mem=8GB
4  #PBS -A kcat-prediction ← Chang to project name that you entered when registering for the HPC
5  #PBS -N run_python_script
6  #PBS -j oe
7  #PBS -o "run_python_script.log"
8
9  cd /home/alkro105
10 module load Python/3.8.3
11 python3 /home/alkro105/python_script.py
```

- Upload your Python script and your bash script to your HPC folder via FileZilla
- Submit Bash script via terminal