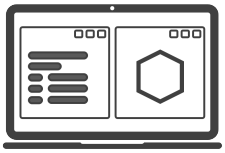

Introduction to Computational Chemistry
Handout Part 1

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1 Accessing Euler

Windows

- Open MobaXterm
- Click on Sessions - New Session
- Click on SSH and type in the remote host (euler.ethz.ch). Tick the specify username box and type your username. Then click OK.
- Type your ETH password

You can later skip this step and just select euler.ethz.ch from Recent sessions when you open MobaXterm.

Mac/Linux

Open your terminal and type `ssh username@euler.ethz.ch` and then enter your password.

2 Accessing files

Windows

- Open MobaXterm
- Click on Sessions - New Session
- Click on SFTP and type in the remote host (euler.ethz.ch). Type your username. Then click OK.
- Type your ETH password

You can again later skip this step and just select euler.ethz.ch from Recent sessions when you open MobaXterm (it will have a different icon to distinguish it from the SSH connection).

Mac/Linux

- Open FileZilla
- Type in the Host (euler.ethz.ch).
- Type your username and password, and the port (22).
- Click on Quickconnect

3 Bash commands and tricks

- The tab button will either auto-complete the command/path or show all possibilities (double-tap).
- Use > to write the output of a command into a file:
  `command input > output` *or* `command > output`
- You can use the up and down keys to navigate your bash history in case you want to reuse a command you recently typed.

A selection of useful bash commands:

Command	**Description**
Directories	
`pwd`	prints current working directory
`cd ..`	changes the directory to one level up
`cd dummy`	changes the directory to "dummy"
`cd -`	change to previous directory
`cd`	changes the directory to home
`mkdir dummy`	makes a directory "dummy"
Content management	
`ls (or ll)`	prints list of folders and files in current directory (with details)
`ls -a`	show hidden files
`cp source dest`	copy file "source" to directory "dest" (if exists) or to a new file called "dest"
`cp -r source dest`	same as above, but also works on folders
`mv source dest`	move file/directory "source" to directory "dest" (if dest exists) or to a new file/directory called "dest"
`rm dummy`	removes the file called "dummy" (cannot remove directories)
`rm -ri dummy`	removes the file or directory called "dummy" (must confirm with y/n)
	N.B. Be careful with `rm` commands—you cannot undo the remove command (nor any other commands, for that matter).
Modules and jobs	
`module avail`	prints the list of available modules
`module avail dummy`	prints all the available options for the module dummy
`module load dummy`	loads the module "dummy"
`module unload dummy`	unloads the module "dummy"
`module list`	prints the list of loaded modules
`sbatch --wrap="dummy"`	submits job of a command called "dummy"
`squeue`	prints the list of submitted jobs
`scancel <id>`	stop the job with the job id number "id"
File viewing and editing	
`vi dummy`	opens the file "dummy" in vim
`cat dummy`	prints the content of a file "dummy" on the screen
`git`	
`git clone URL`	downloads the `git` repository from URL
`git pull origin main`	downloads the latest version of the `git` repository at URL
Miscellaneous	
`man command`	shows the manual for the command; exit by pressing `q`
`lquota`	prints the storage quota information (for Euler)

3.1 File permissions

The `chmod` command allows you to change the permissions for a file for the three user classes, owner (yourself), group, and public. For instance,

```
chmod 744 dummy
```

will give yourself reading, writing, and executing permissions, and only reading permissions for the two other user classes (group and public). You can change the permission level with the help of the table below.

Octal Digit	rwx	Permission
4	100	Read only
5	101	Read and execute
6	110	Read and write
7	111	Read, write, and execute

4 Submitting a job

If no options are specified, `sbatch` submits for 4 hours with 1 core, 1024 MB of memory and 0 MB of scratch space. See the submission line advisor link in Section 6 for the options. As an example, the following line would submit the command acting on an input file and writing to an output file for 24 hours (the `--time` flag) with 4 cores (the `-n` flag specifies tasks, the default is one task per node, thus resulting in 4 cores) and 2048 MB of memory per core.

```
sbatch --time=24:00:00 -n 4 --mem-per-cpu=2048 --wrap="command input > output"
```

5 Common errors

- Necessary modules for the command are not loaded.
- Windows files are not converted to Linux format.
- Executables are not given the necessary permissions.

6 Useful links

- `https://scicomp.ethz.ch/`
  ETH scientific computing homepage. Contains tutorials and information about Euler.
- `https://scicomp.ethz.ch/public/lsla/index2.html`
  Generates the submission command with the necessary flags for Euler.
- Prof. Hünenberger's `lecture notes` and `exercise` about `UNIX`.