

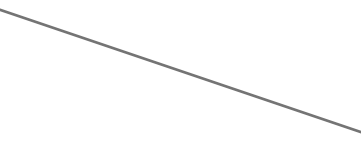
First Steps with UNIX and Science Cluster

Fanny Wegner
2023-03-21

Learning outcomes

- Connecting to Science Cluster
- Get familiar with the UNIX environment
- Use the most common UNIX commands
- How to write simple bash scripts
- Run singularity containers
- How to submit a job to Science Cluster

Connecting to Science Cluster

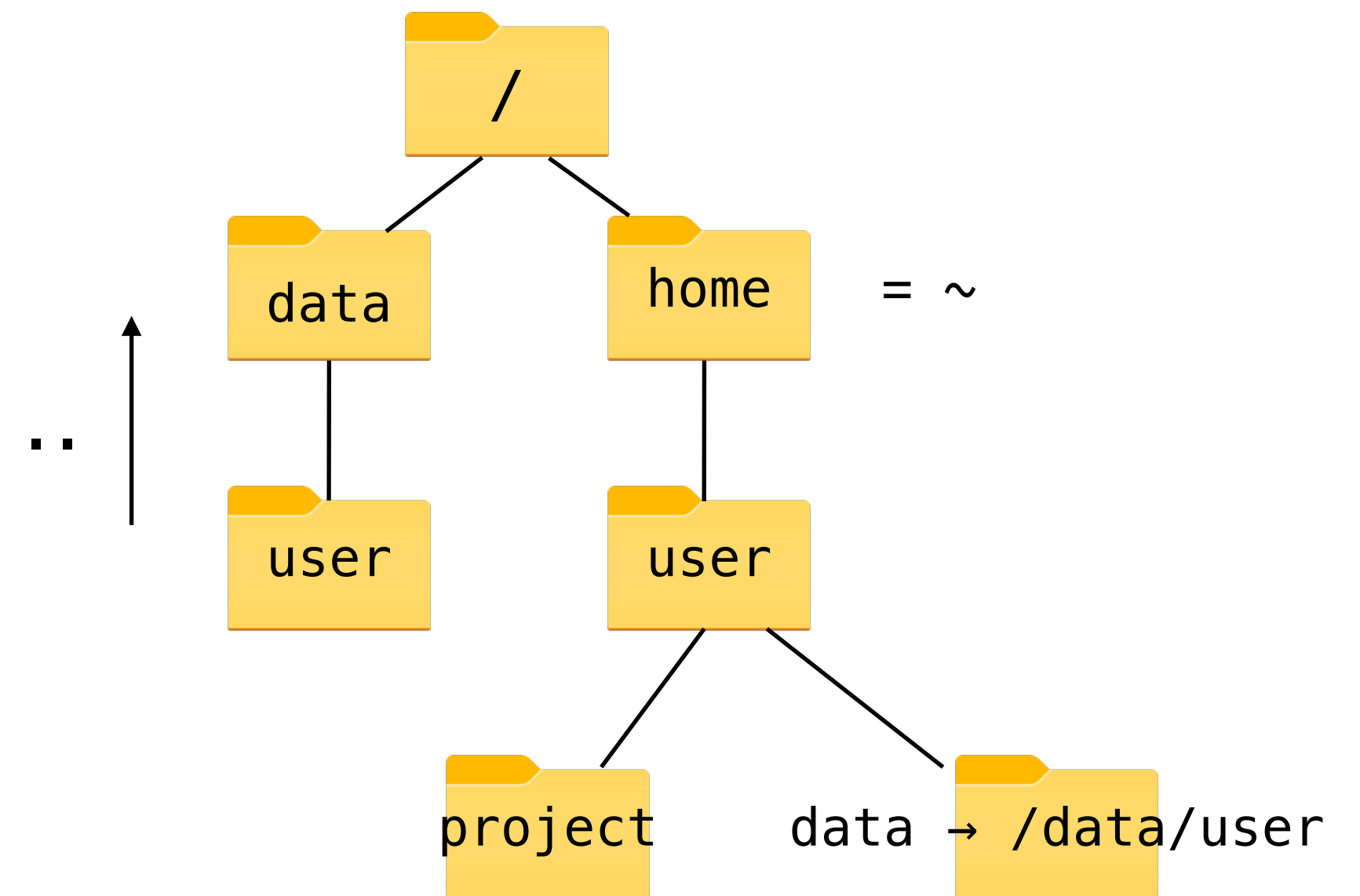
- High performance computing environment of UZH
- Many tools with different advantages available for remote connection
- To connect on command line: `ssh <shortname>@s3it.cluster.uzh.ch` Hostname
- However, graphical tools with SFTP make things a lot easier:
For Mac e.g., **Termius**
For Windows e.g., **MobaXterm**
- Transfer of files on command line:
`scp my_local_file.txt <shortname>@cluster.s3it.uzh.ch:<target directory>`
- To disconnect just type `exit`

Science Cluster

- Science Cluster uses **bash** as shell (= command line interface)
others: zsh (Mac), csh, sh, tcsh ...
- Four filesystems for data storage
 - your **home** filesystem: `/home/cluster/$USER` or `~` 15 GB/100k files
 - your personal **data** filesystem: `/data/$USER` or `~/$USER` 200 GB
 - scratch** filesystem: `/scratch/$USER` 20 TB
 - group**-specific shared filesystem Do you all see `amr.imm.uzh`?
- SSH connection is to login nodes, computations are done on computational nodes

Navigating

- `pwd` - print working directory
- `cd` - change directory
`cd /`
`cd ~`
`cd ..`
- `ls` - list files
- Directories behave similar to files in UNIX
- Symlinks can be used for files and directories
- `[tab]` will autocomplete any commands or available files



EXERCISE 1

Files and directories

- `cp` - copy files and directories
- `mv myfile target_directory/` - move file (or directory)
`mv myfile newname` - rename file (or directory)
- `mkdir` - create a new directory
- `rm` - delete files and directories
- `ln -s file link_to_file` - create a symbolic link for a file (or directory)

EXERCISE 2

Read and manipulate files

- **cat** - print all content of a file
- **less** or **more** - print some content
for **less**: **g** - go to top of file, **SHIFT+g**, go to bottom of file, **/word** to search for 'word'
- **head** - look at the first 10 lines
tail - look at the last 10 lines
- **touch** - create an empty file or change the “modified by” date of existing file
- **nano** - simple editor
vi or **vim** - advanced editor
- **wc** - count lines, words and bytes
-l lines
-w words
-c characters
- **cut -d [delimiter] -f [field]** - cut out a specified field by separated by delimiter
- **grep** - print lines in a file that match pattern

Input and output

- `echo "some statement"` - print statement to standard output
- `echo "Hello world!" > hello.txt` - print statement and direct to (new) file
- `cat myfile.txt > mynewfile.txt` - print content of file and direct it to new file
`cat anotherfile.txt >> mynewfile.txt` - print content and concatenate it to existing file
- `command1 | command2` - Directs output from command1 as standard input into command2 ("piping")
example: count number of files in current directory
`ls | wc -l`

EXERCISE 3

Variables

- You can store text or numbers in variables to use in scripts or on the CLI
- Definition `myvar="Hello world"`
No space around the “=”!
- Calling `$myvar` or `${myvar}`
example: `echo $myvar`
 `"Hello world"`
- Pre-defined variables in UNIX: `$USER`, `$HOME`, `$PATH` etc.
- Can be concatenated with other variables or strings, for example
 `sample_id="ESC000142"`
 `./make_alignment.sh ${sample_id}.fastq.gz ${sample_id}_reference.fasta`
- Output from commands can also be stored into a variables
 `output=$(command)`

 `numfiles=$(ls | wc -l)`

Control structures

- **for loop** - do something for a specified number of times

```
for i in {1..n}
do
    command $i
done
```

Defined sequence of numbers

Is a number

```
for i in *
do
    command $i
done
```

For all files in your working directory

Is a filename

example1: print the names of all files starting with A

```
for i in A*; do echo $i; done
```

One-liner syntax

- **while loop** - do something while some condition is TRUE

```
while [ condition ]
do
    command1
    command2
done
```

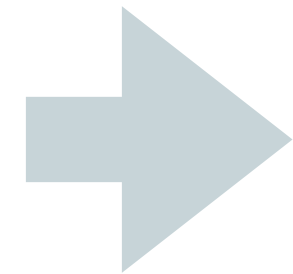
Space around the [] !

Ideally one of these commands changes the condition as some point, otherwise you'll end up with an infinite loop

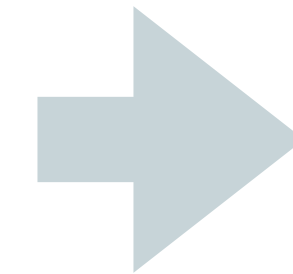
Control structures

- **if else** - do something if a condition is true

```
if [ condition ]  
then  
    command1  
    command2  
fi
```



```
if [ condition ]  
then  
    command1  
else  
    command2  
fi
```



```
if [ condition ]  
then  
    command1  
elif [ condition2 ]  
    command2  
else  
    command3  
fi
```

- Also possible to nest if statement

Arrays

- Data structure that stores multiple elements

- Definition `myarray=(1 2 3 4 5 6)` Curly brackets required

- Calling `echo ${myarray[@]}` All elements are accessed with "@"
 `1 2 3 4 5 6`
 `echo ${myarray[0]}` Indexing starts at 0, so this accesses the first element
 `1`

This expression gives you the indices of each element

- Looping through array elements

```
for i in ${myarray[@]}
do
    command $i
done
```

Looping through array indices

```
for i in ${!myarray[@]}
do
    command ${myarray[$i]}
done
```

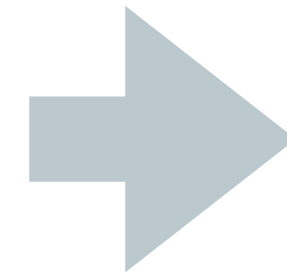
Writing simple scripts

- A script is just the concatenation of a series of commands that are executed one after the other
- A shell script always starts with the shebang `#!/`, defining the shell it will operate in

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

```
command1  
command2  
command3
```

```
# this will do X
```



myscript.sh

- To run a script
`./myscript.sh`

You can explain your code (to yourself and others) using comments (good practice!)

A quick note: Scope of variables

- **Local variables:** If you define variables on your command line, it will only be available in this instance of your shell, not anywhere else or when you re-login in
- Similarly, variables defined within scripts only exist in there
- **Global variables:** Valid everywhere. For example, \$USER

EXERCISE 4

Singularity containers

- Singularity = container platform, that packages up pieces of software
- A container = an image (.sif or sometimes .img)
- Portable and reproducible, safe
- To execute the software from an image: `singularity_image.sif command [parameters]`
- On Science Cluster, we “install” most our software as singularity images.
To run them, you need to load a required module
`module load singularityce`
- Note: singularity does not work for Mac command line, only on UNIX/linux systems!

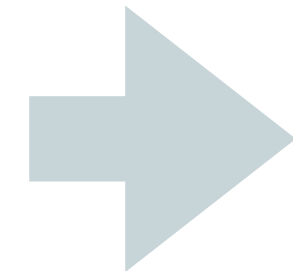
Submission of jobs on Science Cluster

- Jobs can either be single commands or scripts
- Submissions scripts are bash scripts with a special header defining parameters for the job we request to run

```
#!/usr/bin/env bash
#SBATCH --cpus-per-task=[number]
#SBATCH --mem=[memory]
#SBATCH --time=[hr:min:sec]
#SBATCH --job-name=[name]
#SBATCH --output=[name]_%j.out
#SBATCH --error=[name]_%j.err
```

```
# load any required modules
module load [module name]
```

```
command1
command2
command3
```



More specific example for our use case

```
#!/usr/bin/env bash
#SBATCH --cpus-per-task=8
#SBATCH --mem=5G
#SBATCH --time=02:00:00
#SBATCH --job-name=myJob
#SBATCH --output=myJob_%j.out
#SBATCH --error=myJob_%j.err
```

```
# load any required modules
module load singularityce
```

```
path/to/singularity/module.sif command [parameters]
```

Submission of jobs on Science Cluster

- Submission: `sbatch myJob.sh`
- What's happening: `queue -u $USER`
- Output from the script (which is normally printed to standard output) can be directed to `.out` and `.err` files

EXERCISE 5