

COMPUTEROME 2.0

USERS WORKSHOP

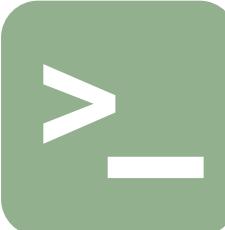
CENTER FOR HEALTH DATA SCIENCE (HEADS)
FACULTY OF HEALTH AND MEDICAL SCIENCES,
UNIVERSITY OF COPENHAGEN, FEBRUARY, 2021



PART3

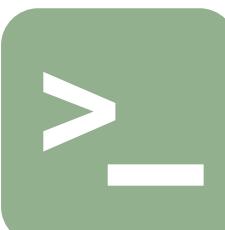
WORKING ON COMPUTEROML2.

REQUEST RESOURCES



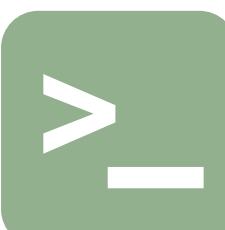
DO NOT START ANY JOB ON THE LOGIN NODE

- After you log-in, you can move around and have a look (e.g. cd, ls, cat....)
- When you know what you want to do, you need to request the resources first



INTERACTIVE MODE WITH IQSUB

- Just type **iqsub** in the command line
- This will open a window for you to put the parameters for what you need

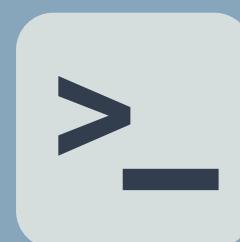


PLACE A SCRIPT IN THE QUEUE WITH QSUB

- Specify the resources needed with PBS commands (in a PBS script)
- Place the script in the queue with **qsub**
- Explored in mode details this afternoon



IQSUB PARAMETERS



PROJECT / GROUP

- As part of which project / C2 group are you working
- This affects who is paying... \$\$\$

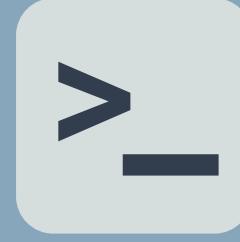
Interactive job

Select group

1	cu_10056
2	danstem
3	cu_10077
4	dan_bri
5	dan_ser
6	dan_gra

↓(+) 26%

< OK > <Cancel>



TIME NEEDED

- This is what we call wall time. After this time, the resources are closed.
- Everything you are doing that is not saved is lost.
- Better to set time a bit longer than what you think you need.
- If you have no idea how long something takes do a small test first.
- If you are done, you can exit with command exit ;-)

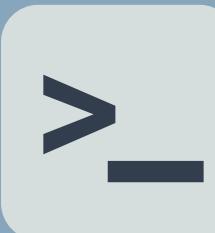
Interactive job

Select time needed (non extendable)

1	1 hour
2	2 hours
3	4 hours
4	8 Hours
5	24 hours
6	Custom

< OK > <Cancel>

IQSUB PARAMETERS

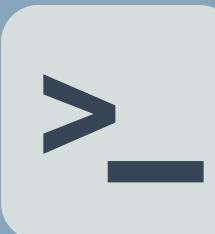


SPECIFY PROCESSORS

- Only useful for jobs that are parallelized and can benefit from several cores
- If you don't know, you can keep processor to 1
- In interactive mode you can max. get 1 thin node (2 CPUs, i.e. 40 cores).

Interactive job
Enter number of Processors needed
(1-40)

< OK > <Cancel>

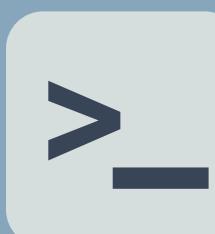


SPECIFY GPUs

- Unless you know you need some GPU, leave it to 0
- If you want to use GPU, this would be for multithreading purposes, you put 1

Interactive job
Enter number of GPUs needed (0-1)

< OK > <Cancel>



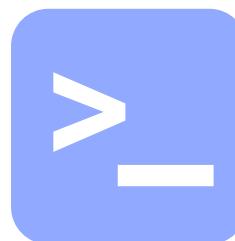
MEMORY NEEDED

- Depends on the methods / software you use
- E.g. mapping with STAR, you might want to increase to 100g
- Recall that one thin node has 192GB BUT only 180GB can be used!

Interactive job
Enter amount of memory needed

< OK > <Cancel>

FILE TRANSFER: scp & FileZilla



Copy data from/to C2 via SCP command

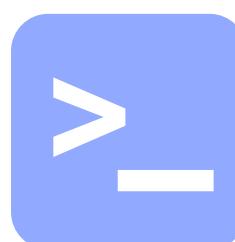
- From local to computerome 2.0:

```
scp /Users/path/to/file  
username@ssh.computerome.dk:/home/path/to/the/destination/
```

- From computerome 2.0 to local:

```
scp username@ssh.computerome.dk:/home/path/to/file  
/Users/path/to/destination/
```

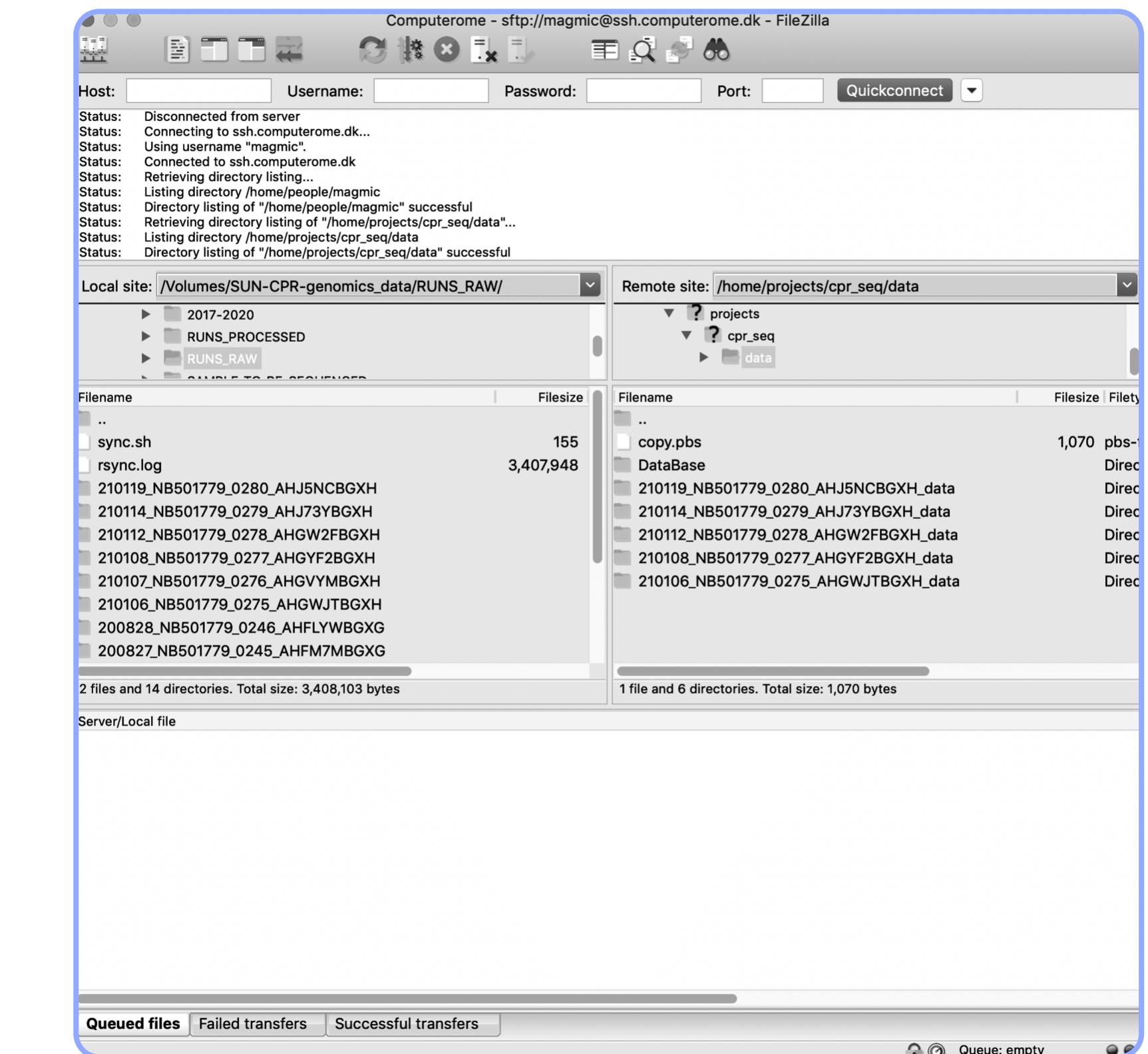
- If it's a whole folder, use -r
- For more info, study the scp command (man scp)



Use FileZilla graphical interface

- You can also use a software with a graphical interface
- Find on the wiki how to set up the connection

(<https://www.computerome.dk/display/C2W/Getting+Started++new+users>)



Filezilla configuration

SFTP Client Configurations

In order to use most FTP/SFTP clients on a 2 factor system you will need to limit the maximum simultaneous connections to avoid multiple login prompts.

Here you can see how to setup the mostly used clients

Filezilla

⚠️ Changes has been made in resent versions which means that Quickconnect no longer works with 2 factor authentication

GLOBAL

Go to Edit->Settings->Transfers

Change Maximum simultaneous transfers to 1

SITE PROFILE / BOOKMARK

Go to File->Site Manager->(your profile)->Transfer settings

Check Limit number of simultaneous connections

Change Maximum number of connections to 1

Change Login type to Interactive

MODULES



SEARCHING FOR A MODULE: MODULE AVAIL

- First load the “tools” module: module load tools
- Use the avail function with the start of your software name:
- module avail bowtie

```
[magmic@g-12-10002 ~]$ module avail bowtie
----- /cm/local/.modulefiles_cache/tools/modulefiles ---
bowtie/1.1.1    bowtie2/2.2.4  bowtie2/2.3.2
bowtie/1.2.1.1  bowtie2/2.2.5  bowtie2/2.3.4.1
[magmic@g-12-10002 ~]$
```



LOADING A MODULE: MODULE LOAD

- You need to load each software you want to use (in its specific version)
- module load bowtie/2.3.2

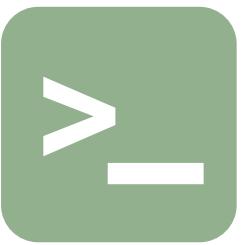
```
[[magmic@g-12-10002 ~]$ module load R/4.0.3
Loading R/4.0.3
ERROR: R/4.0.3 cannot be loaded due to missing prereq.
HINT: the following module must be loaded first: gcc
[[magmic@g-12-10002 ~]$ module load gcc R/4.0.3
Loading R/4.0.3
ERROR: R/4.0.3 cannot be loaded due to missing prereq.
HINT: the following module must be loaded first:
intel/perflibs
[[magmic@g-12-10002 ~]$ module load gcc intel/perflibs R/4.0.3
[magmic@g-12-10002 ~]$
```



ADDING THE DEPENDENCIES

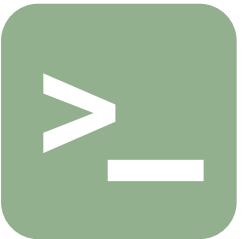
- When there is a missing dependency, follow the suggestions.

Troubleshooting and FAQ



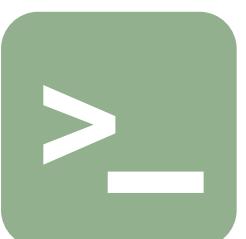
It does not work...

- Did you first load the tools? module load tools
- Did you check the spelling?



Do I have to specify the version of the software?

- YES, you do!
- In some cases, it might work without but this feature is old and is not maintained, i.e. always put the version you want



MORE TO READ ON THE C2 WIKI:

- <https://www.computerome.dk/display/C2W/Installed+Software>