

# COMPUTEROME 2.0

## USERS WORKSHOP

FACULTY OF HEALTH AND MEDICAL SCIENCES,  
UNIVERSITY OF COPENHAGEN, FEBRUARY, 2021



# WELCOME TO THE C2 USERS WORKSHOP - ANDERS

# WHO ARE WE

## CENTER FOR HEALTH DATA SCIENCE:

- Anders Krogh, Professor, Head of Center
- Thilde Terkelsen, Data Scientist



ANDERS KROGH



THILDE TERKELSEN



MAGALI MICHAUT

## DANSTEM:

- Magali Michaut, Research Consultant

## GLOBE INSTITUTE:

- Bent Petersen, Associate Professor
- Shyam Gopalakrishnan, Associate Professor



BENT PETERSEN



SHYAM GOPALAKRISHNAN



ALLAN HAVE

## KU IT:

- Allan Have Sørensen, Head of Section

PART1

INTRODUCTION

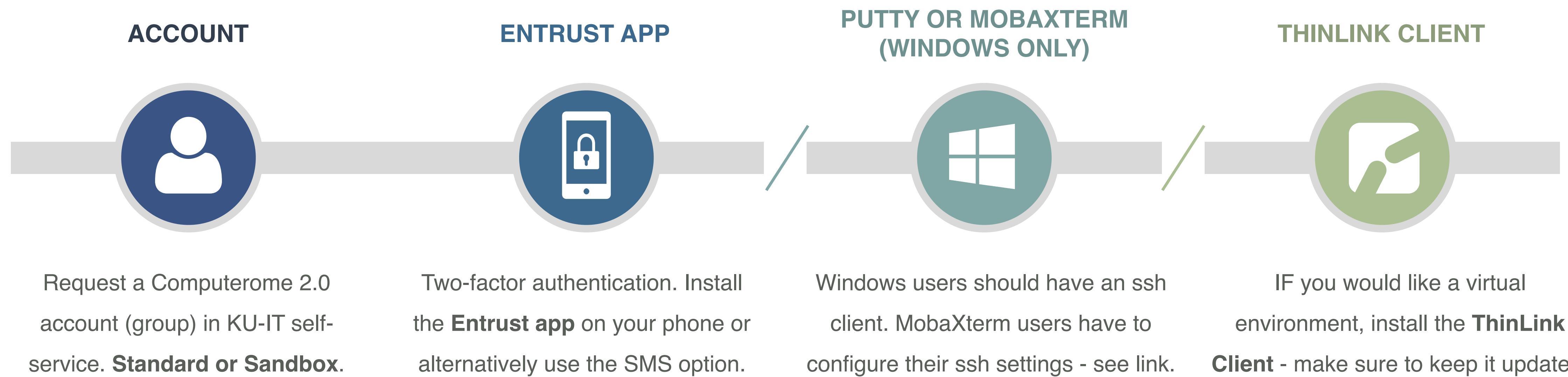
# INTRODUCTION TO C2 - BENT

PART 2

THE BASICS

# BEFORE LOG IN TO COMPUTEROME 2.0

**GETTING STARTED:** <https://www.computerome.dk/display/C2W/Getting+Started+-+new+users#GettingStarted-newusers-SSHlogintoComputerome2.0>



# LOG IN TO COMPUTEROME 2.0

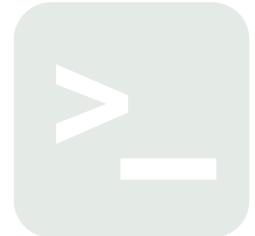
## 2.0

### LOG IN WITH THINLINC

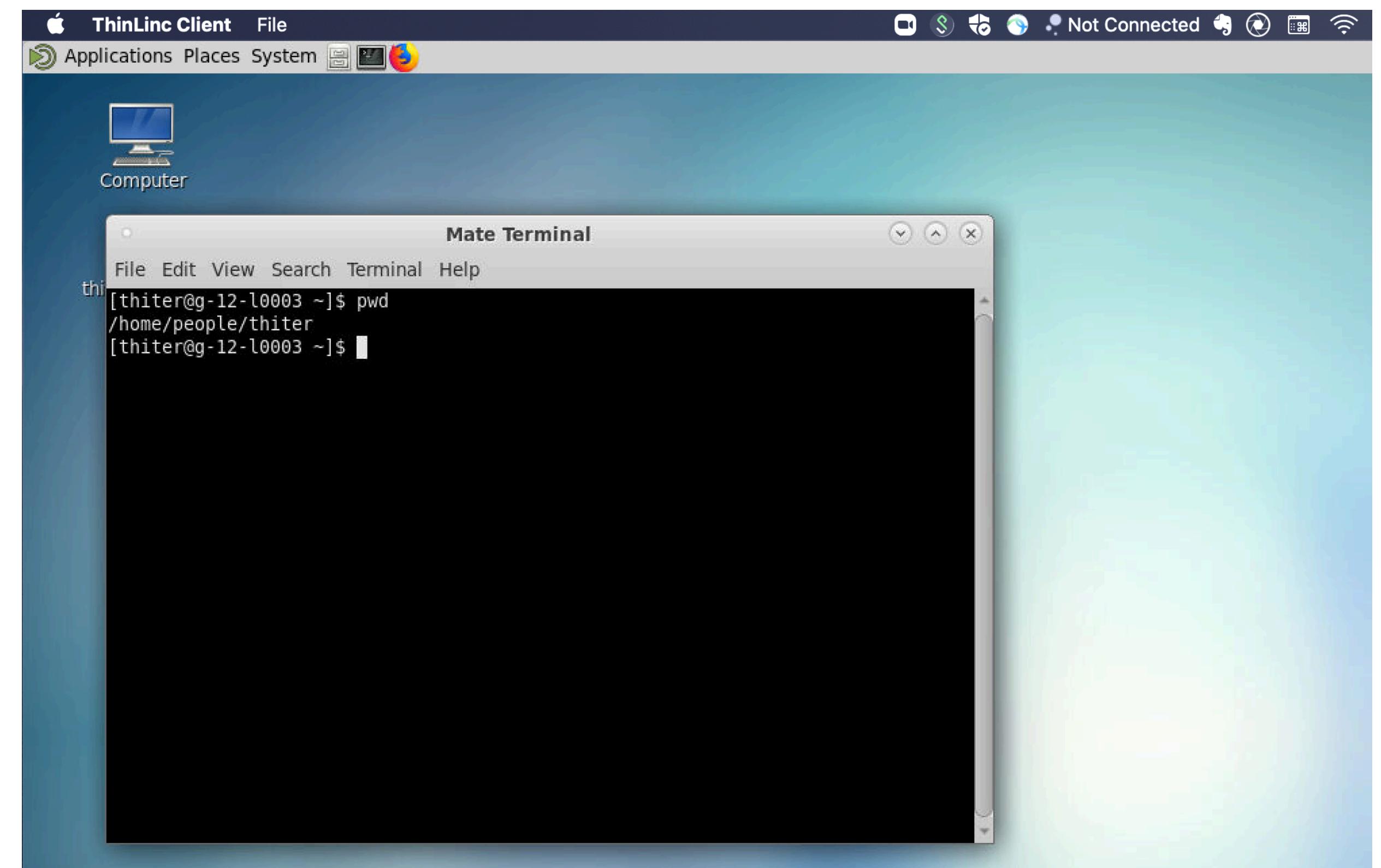


- Download and install the **ThinLinc Client**
- Open and enter your **Username + Password**
- It make take a couple of minutes to connect
- Enter the token from the Entrust App (or Confirm)
- Open a terminal or click your way around
- Exit a full screen - press the F8 key

### LOG IN WITH SSH



- Open a terminal
- ssh [username@ssh.computerome.dk](ssh://username@ssh.computerome.dk)
- Enter your password
- Enter the token from the Entrust App (or Confirm)



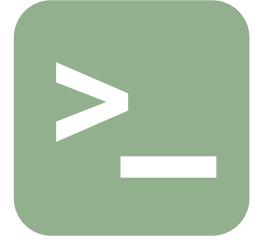
# LOG IN TO COMPUTEROME 2.0

## 2.0



### LOG IN WITH THINLINC

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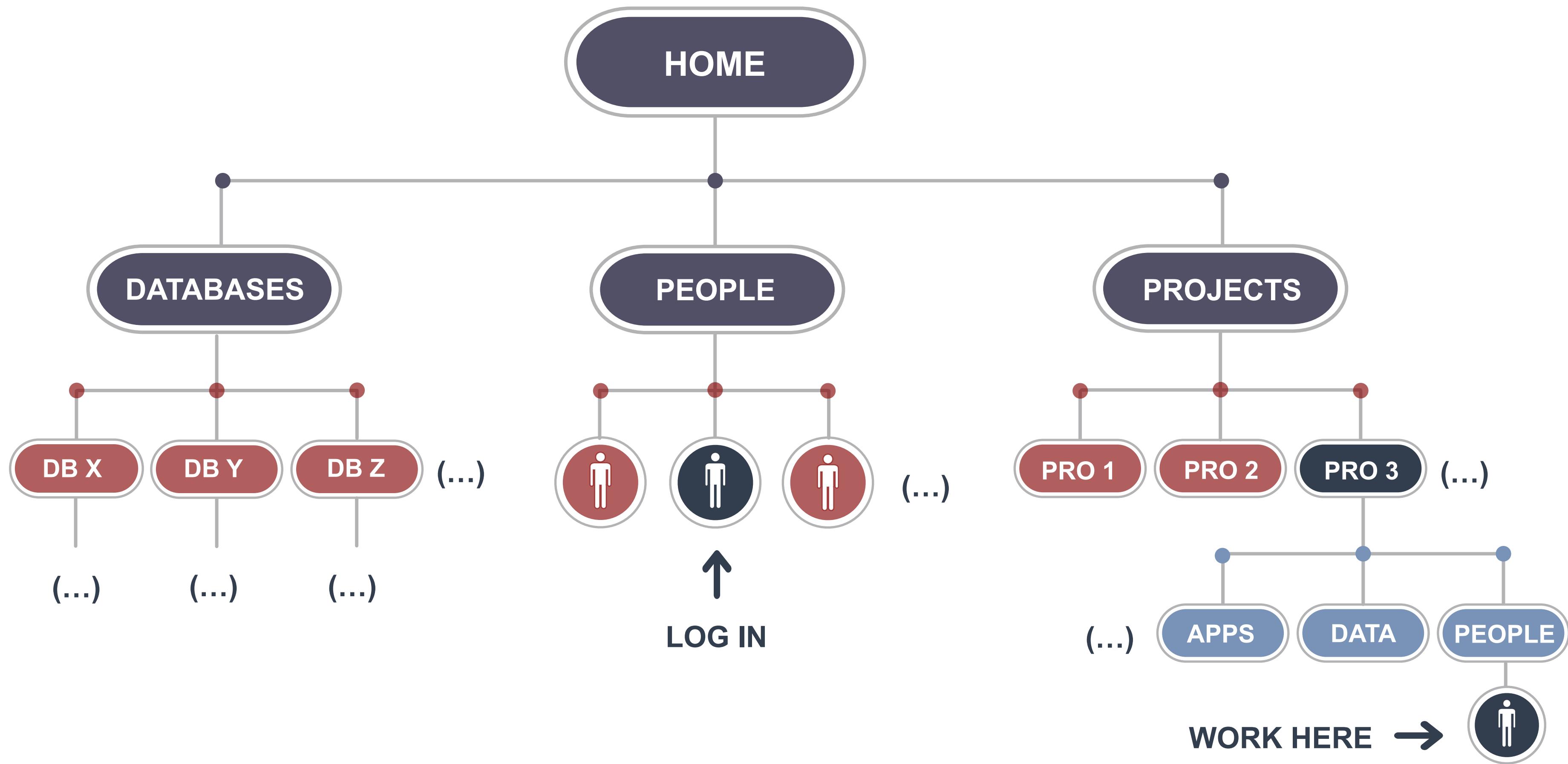


### LOG IN WITH SSH

- Open a terminal
- ssh [username@ssh.computerome.dk](ssh://username@ssh.computerome.dk)
- Enter your password
- Enter the token from the Entrust App (or Confirm)

```
Last login: Mon Jan  4 15:31:24 on ttys000
[kgx936@SUN1007442 ~ % ssh thiter@ssh.computerome.dk
#####
#                                     #
#             Welcome to Computerome 2.0          #
#                                     #
#               NOTICE !!!                      #
#               This system requires 2-factor authentication   #
#                                     #
#               To login, type your password and press Enter.    #
#               This sends either an SMS passcode to your mobile   #
#               or a push-notification to Entrust IdentityGuard app.   #
#               If the push-notification times out, a new prompt line   #
#               asks for the 8 digit security code shown in the app.   #
#                                     #
#               BY LOGGING INTO THIS SYSTEM YOU ACCEPT          #
#               COMPUTEROME'S TERMS AND CONDITIONS OF USE.      #
#                                     #
#               Send support requests to computerome@dtu.dk       #
#                                     #
#####
[Password:
Last login: Mon Jan  4 13:47:55 2021 from 2.111.76.128
[[thiter@g-12-10002 ~]$ pwd
/home/people/thiter
[thiter@g-12-10002 ~]$ ]
```

# C2 SANDBOX STRUCTURE

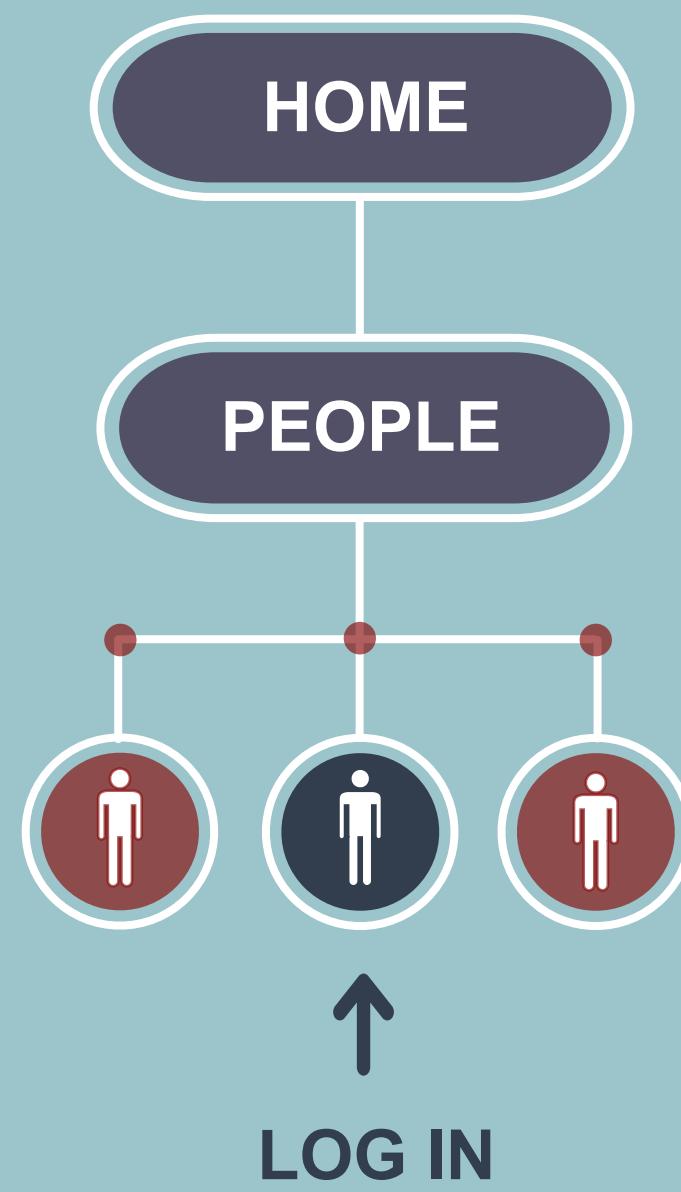


# C2 SANDBOX STRUCTURE

1

/home/people/username

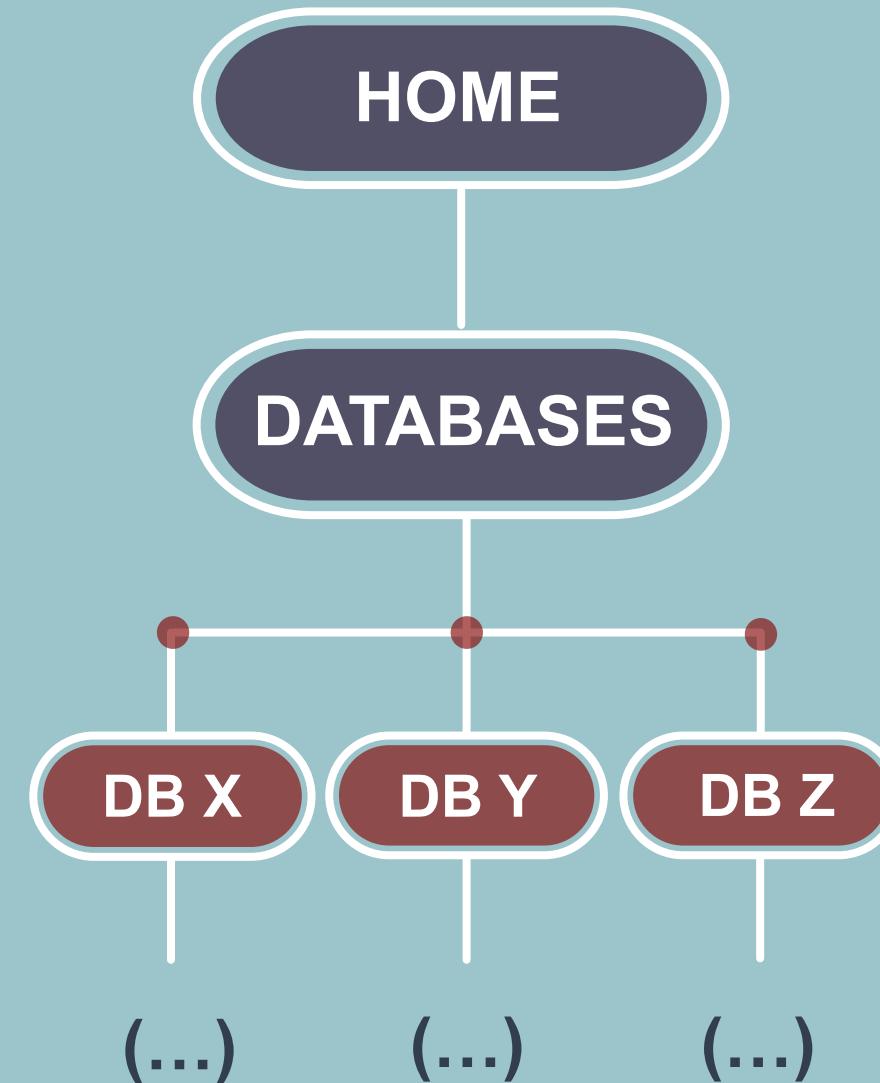
- Your private directory.
- This space is meant for configuration files.
- Do NOT store data here (max 10G)
- Do NOT run jobs from here.



2

/home/databases

- Shared database resource
- Databases include:
  - Human genomes
  - Blast
  - TCGA / GTEx
  - dbSNP
  - ClinVar / COSMIC
  - ...

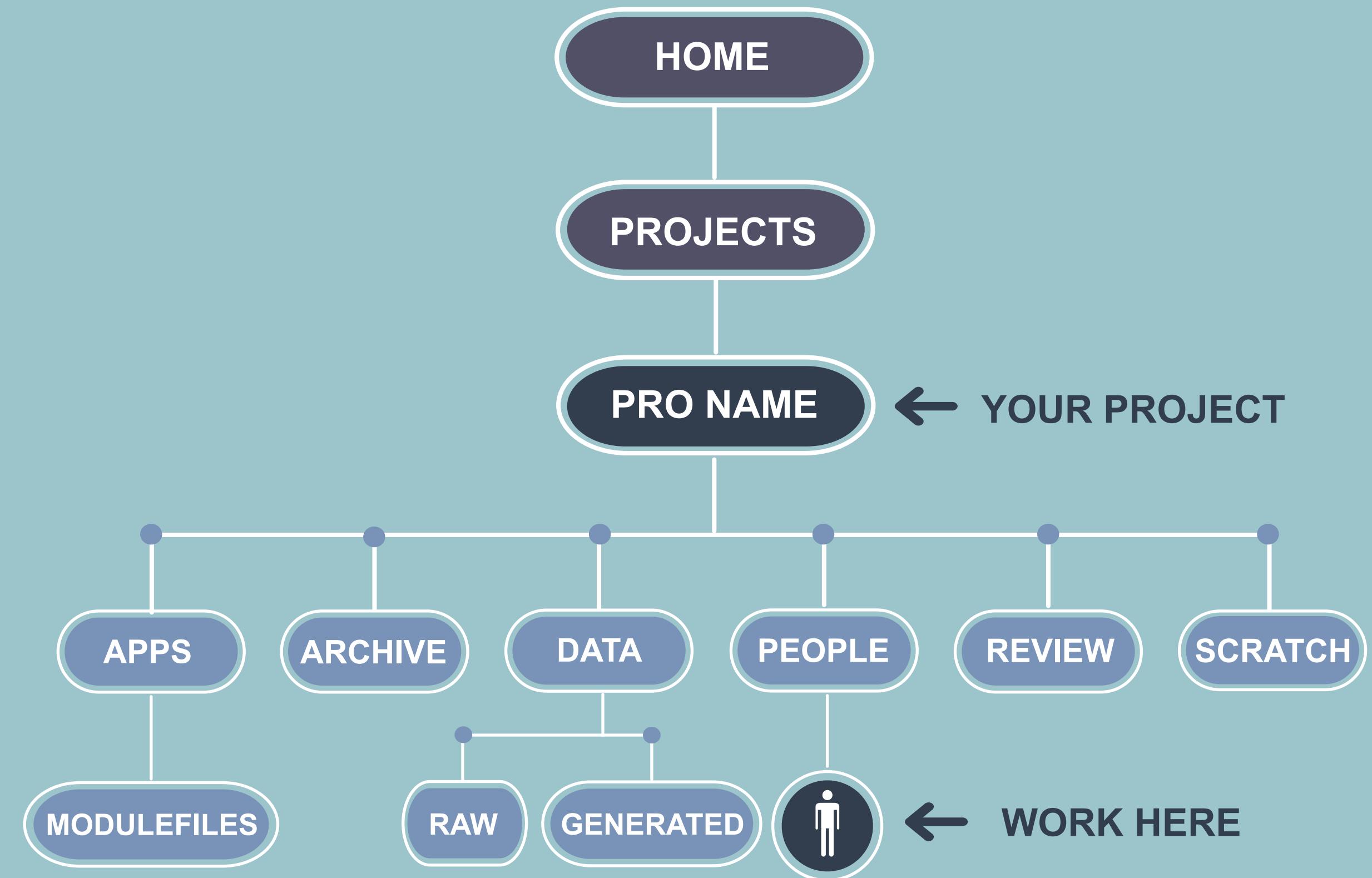


# C2 SANDBOX STRUCTURE

3

/home/projects/project

- Your project directory.
- ./apps : project specific applications & modulefiles
- ./archive: dataproject specific data
- ./scratch: temporary & re-creatable data N.B will not be backed up!
- ./review used for peer-review.



# YOUR PROJECT AND GROUP

## PROJECT

<project> usually refers to the projects funding.



## USERNAME

<username>  
Your unique user ID. Can be connected to multiple projects and groups.

## PROJECT NAME

<project\_name> is the name given by the C2 team. Almost exclusively the same as <project>.

## GROUP NAME

<group\_name>  
ID assigned by DTU.  
Refers to the UNIX group, e.g. the projects/users access to resources.  
Often the same as <project\_name>.

Type in <id> to get this information

```
#####
#           Welcome to Computerome 2.0
#
#           NOTICE !!!
#           This system requires 2-factor authentication
#
#           To login, type your password and press Enter.
#           This sends either an SMS passcode to your mobile
#           or a push-notification to Entrust IdentityGuard app.
#           If the push-notification times out, a new prompt line
#           asks for the 8 digit security code shown in the app.
#
#           BY LOGGING INTO THIS SYSTEM YOU ACCEPT
#           COMPUTEROME'S TERMS AND CONDITIONS OF USE.
#
#           Send support requests to computerome@dtu.dk
#
#####
Password:
Last login: Wed Jan  6 13:04:54 2021 from 2.111.76.128
[[thiter@g-12-10002 ~]$]
[[thiter@g-12-10002 ~]$ id
uid=113800351(thiter) gid=113800351(thiter) groups=113800351(thiter),113800352(ku_00033)
[thiter@g-12-10002 ~]$ ]
```

# GOOD TO KNOW

COMPUTEROME 2.0 WIKI - FIND EVERYTHING HERE

<https://www.computerome.dk/>

VIDEO TUTORIALS - HELPFUL TO WINDOWS USERS

<https://www.computerome.dk/display/C2W/Video+Tutorials>

BRUSH UP ON YOUR UNIX SKILLS

[https://www.computerome.dk/display/C2W/Getting+Started++new+users?  
preview=42205237/42205239/Hackinars\\_in\\_Computerome-wiki.pdf](https://www.computerome.dk/display/C2W/Getting+Started++new+users?preview=42205237/42205239/Hackinars_in_Computerome-wiki.pdf)

CHECK YOUR USAGE ON C2

module load tools usage\_script/2.0  
usage -u username

GETTING HELP

Write to [computerome@dtu.dk](mailto:computerome@dtu.dk)

- Subject description
- System, e.g. Computerome main, sandbox, or <named> cloud system
- Login issues, ThinLinc vs SSH login, username & error message(s)
- Command line(s) used
- Describe the problem including error messages

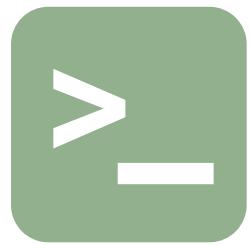
PART3

WORKING ON COMPUTEROME 2.0



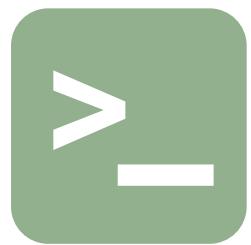
# WORKING ON COMPUTEROME 2.0 - MAGALI

# REQUEST RESOURCES



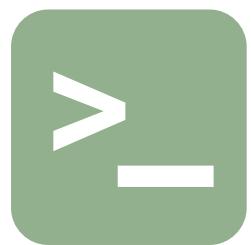
## DO NOT START ANY JOB ON THE LOGIN NODE

- 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

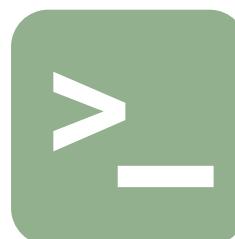
- Just type iqsub in the command line
- This will open a window for you to put the parameters for what you need



## PLACE A SCRIPT IN THE QUEUE WITH QSUB

- Specify the resources needed with PBS commands (e.g. 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

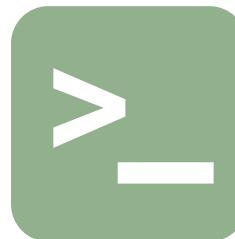
Select group

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

↓(+)

26%

< OK > <Cancel>



## TIME NEEDED

- This is the wall time. After this time, the resources are close.
- Everything you are doing that is not saved is lost.
- Better to put a bit longer than what you think you need (you can close before the end)
- If you are done, you can exit with command exit ;-)

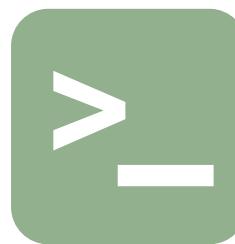
Interactive job

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

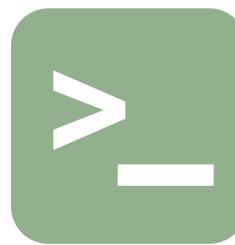


## NUMBER OF CPUs

- Only useful for jobs that are parallelized and can benefit from several CPUs
- If you don't know, you can leave 1

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

< OK > <Cancel>

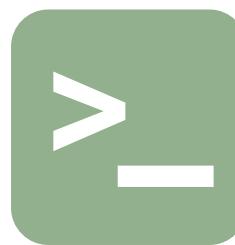


## NUMBER OF GPUs

- Unless you know you need some GPU, leave it to 0
- If you want to use GPU, you put 1

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

< OK > <Cancel>



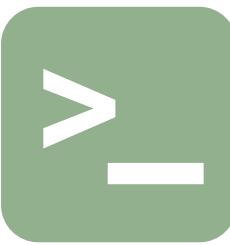
## MEMORY NEEDED

- Depends on the methods / software you use
- E.g. mapping with STAR, you might want to increase to 60-80g

Interactive job  
Enter amount of memory needed

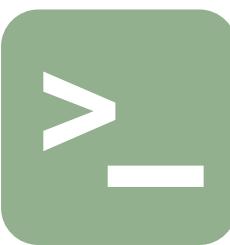
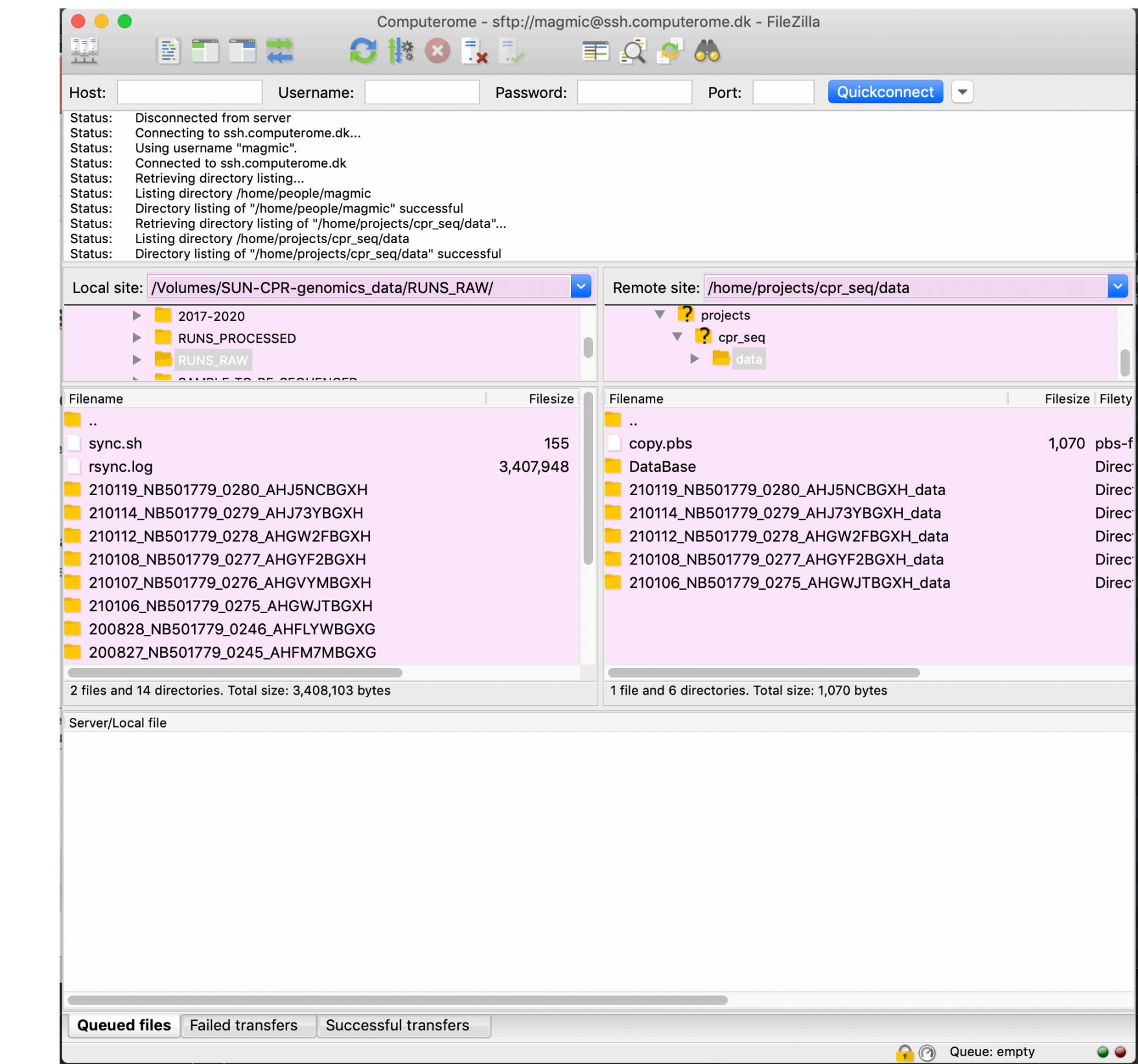
< OK > <Cancel>

# FILE TRANSFER: scp & FileZilla



## COPY DATA FROM/TO C2 via SCP command

- From local to computerome:  
•scp /Users/path/to/file username@ssh.computerome.dk:/home/path/to/the/destination/
- From computerome 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

# 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

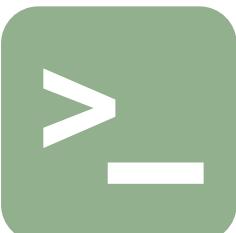
Go to Edit->Settings->Transfers  
Change Maximum simultaneous transfers to 1

#### 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

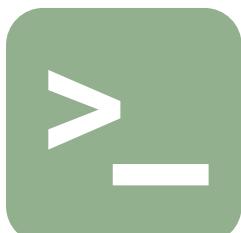
From C2 wiki: <https://www.computerome.dk/display/C2W/SSH+login+to+Computerome+2.0>

# MODULES



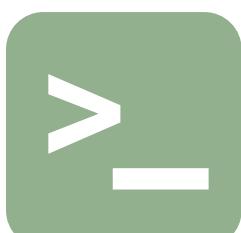
## LOADING A MODULE: MODULE LOAD

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



## SEARCHING FOR A MODULE: MODULE AVAIL

- Use the avail function with the start of your software name
- module avail bowtie



## ADDING THE DEPENDENCIES

- When there is a missing dependency, follow the suggestions

```
[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 ~]$ ]
```

```
[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 ~]$ ]
```

More on C2 wiki: <https://www.computerome.dk/display/C2W/Installed+Software>

PART4

A BRIEF TECHNICAL INTERMEZZO



# A BREIF TECHINCAL INTERMEZZO - ALLAN

**PART5**

**C2 MODULES & QUEING SYSTEM**

# MODULES, QUEING SYSTEM & SCRIPTS - SHYAM

# PART6

## OPTIMIZATION OF TIME & COST

# OPTIMIZATION OF TIME AND COST ON C2 - SHYAM