Introduction to the I2BC cluster

I2BC file system

For the new comers

« Partages » storage system, aka. /store/

- ➔ A space designed for **storage**
- ➔ Accessible everywhere
- ➔ Regularly backed up (snapshot system)

3 subspaces:

- ➔ **EQUIPES** (team space, 1Tb)

  read/write for all team members except MEMBERS subdirectory

  MEMBERS: 1 folder per team member, read-only for others
- ➔ **USERS** (personal space, 20Gb)
- ➔ **plateformes** (project space, 5Tb)

  Useful for projects across teams or with external collaborators (ask SICS)

https://intranet.i2bc.paris-saclay.fr/outils/informatique/#stock => about storage @I2BC

https://intranet.i2bc.paris-saclay.fr/procedures/info/#file => how to access outside I2BC

S.O.S.

For the new comers

Need help with your **computer, internet, some software, the cluster**…?

=> Contact the **SICS** – IT support team

support.informatique@i2bc.paris-saclay.fr

(be clear and concise in the email and email subject)

Questions on **specific bioinformatics tools & practices**? Help on setting up an analysis pipeline? Etc.

=> Contact **BIOI2**: contact-bioi2@i2bc.paris-saclay.fr

=> Ask around you e.g. using our **FramaTeam** group: more information

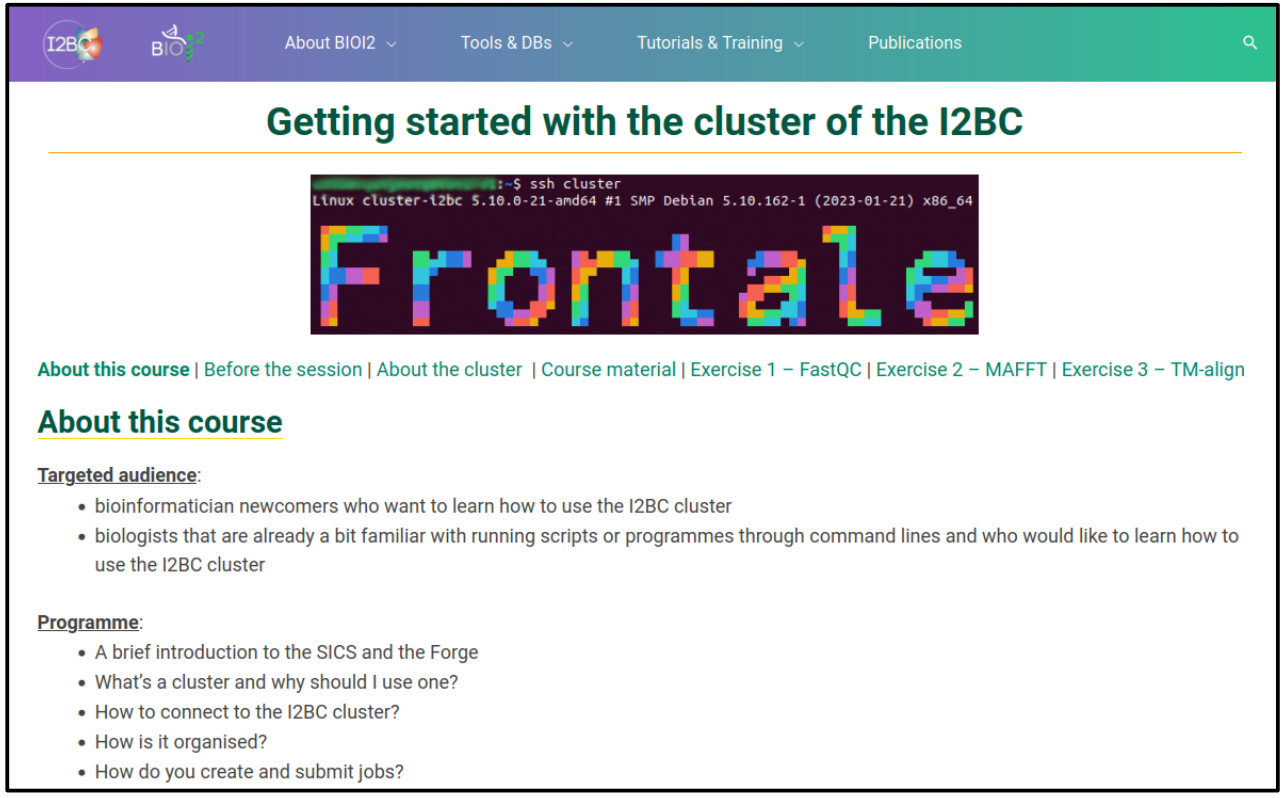
=> Search through the **intranet** (tools & procedures)

=> Search & contribute to the **Wiki** on the Forge: here

BIOI2 website

Anything linked to this training session can be found on the BIOI2 website:

https://bioi2.i2bc.paris-saclay.fr/training/i2bc-cluster/



Goals

You, processing your data with your own computer

You, processing your data with the help of the cluster

Goals

You, processing your data
with your own computer

You, processing your data
with the help of the cluster

I2BC cluster

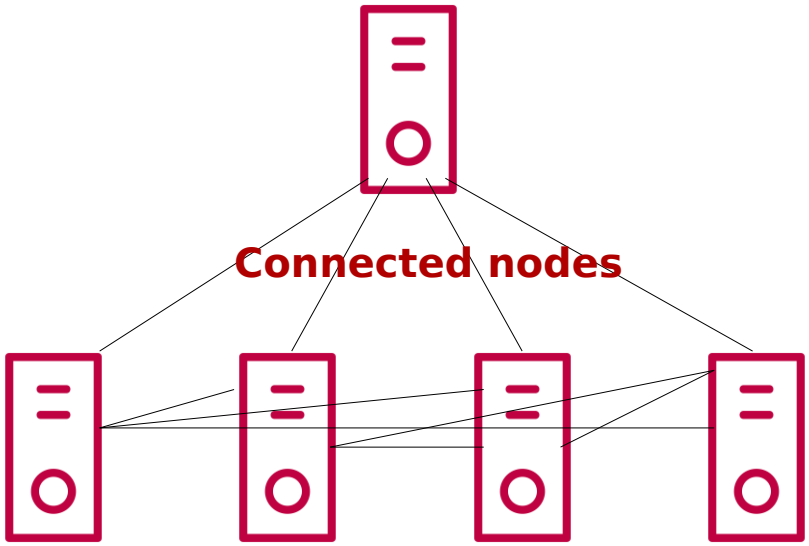
Goals

- what’s a cluster?
- how to connect?
- how it is structured?
- how to use it?
- practice makes perfect!

What is a cluster?

A computer cluster:

* is a set of computer servers (=**nodes**) connected together

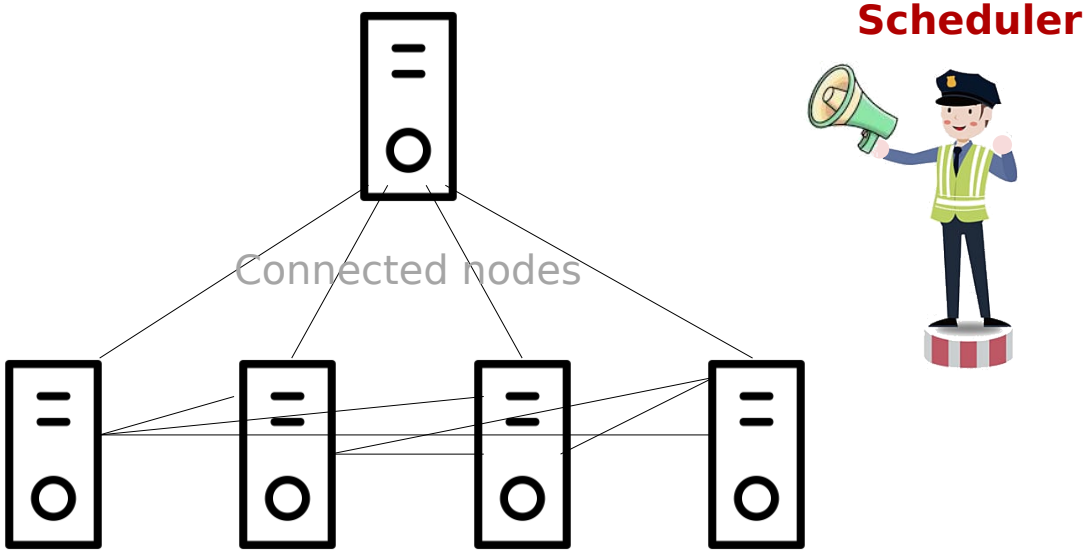


What is a cluster?

A computer cluster:

* is a set of computer servers (=**nodes**) connected together

* communication between nodes goes through a centralised **scheduler**

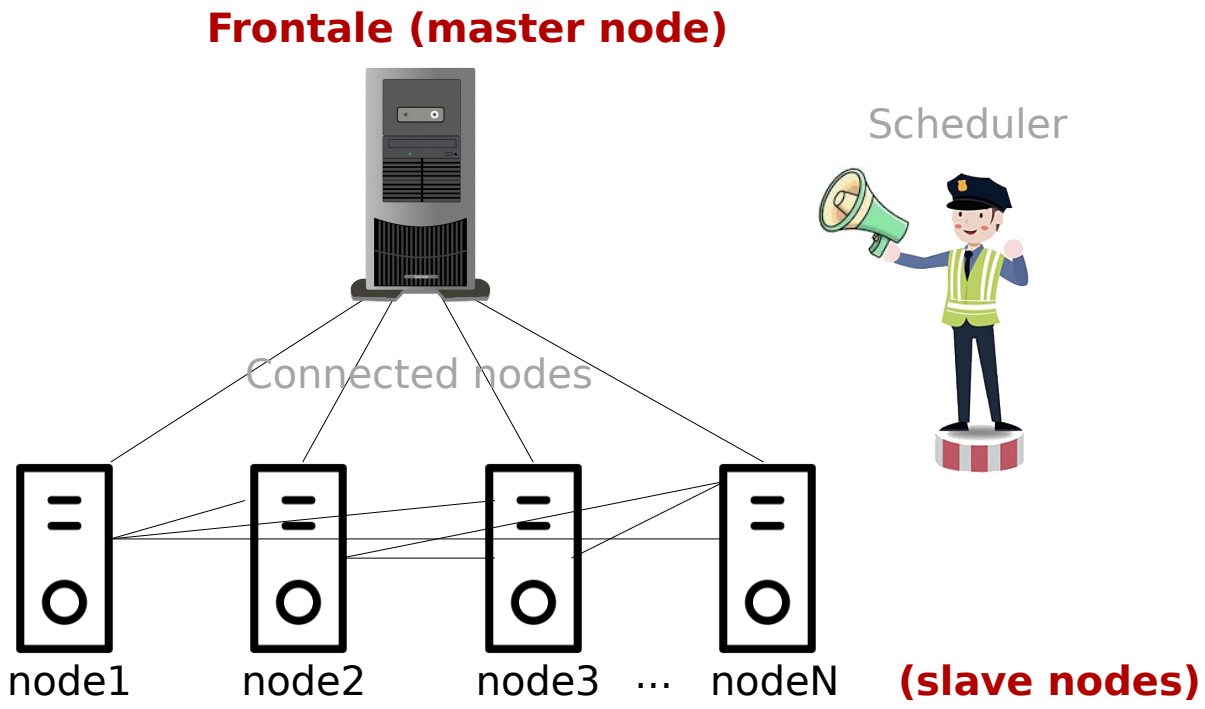


Scheduler

What is a cluster?

A computer cluster:

* is a set of computer servers (=**nodes**) connected together
* communication between nodes goes through a centralised **scheduler**
* there are **master node(s)** (=main nodes) and **slave nodes** (=workers)



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A computer cluster:

* is a set of computer servers (=**nodes**) connected together
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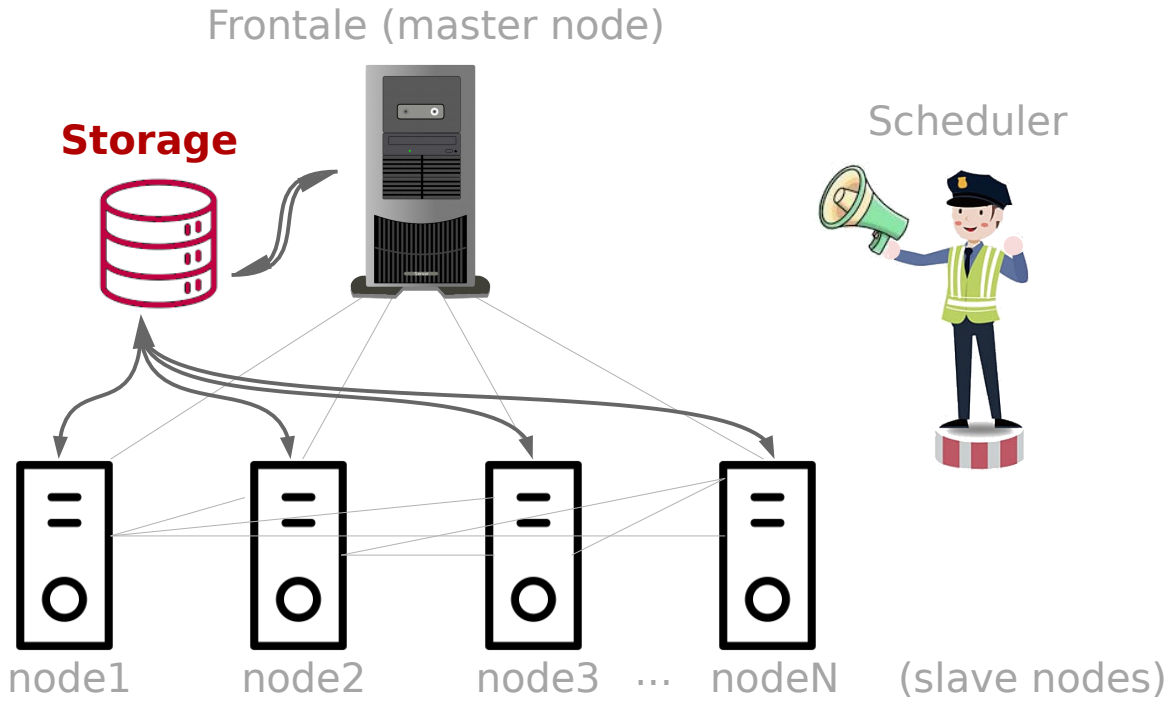
* there are **master node(s)** (=main nodes) and **slave nodes** (=workers)
* all nodes have **access** to the **storage** system

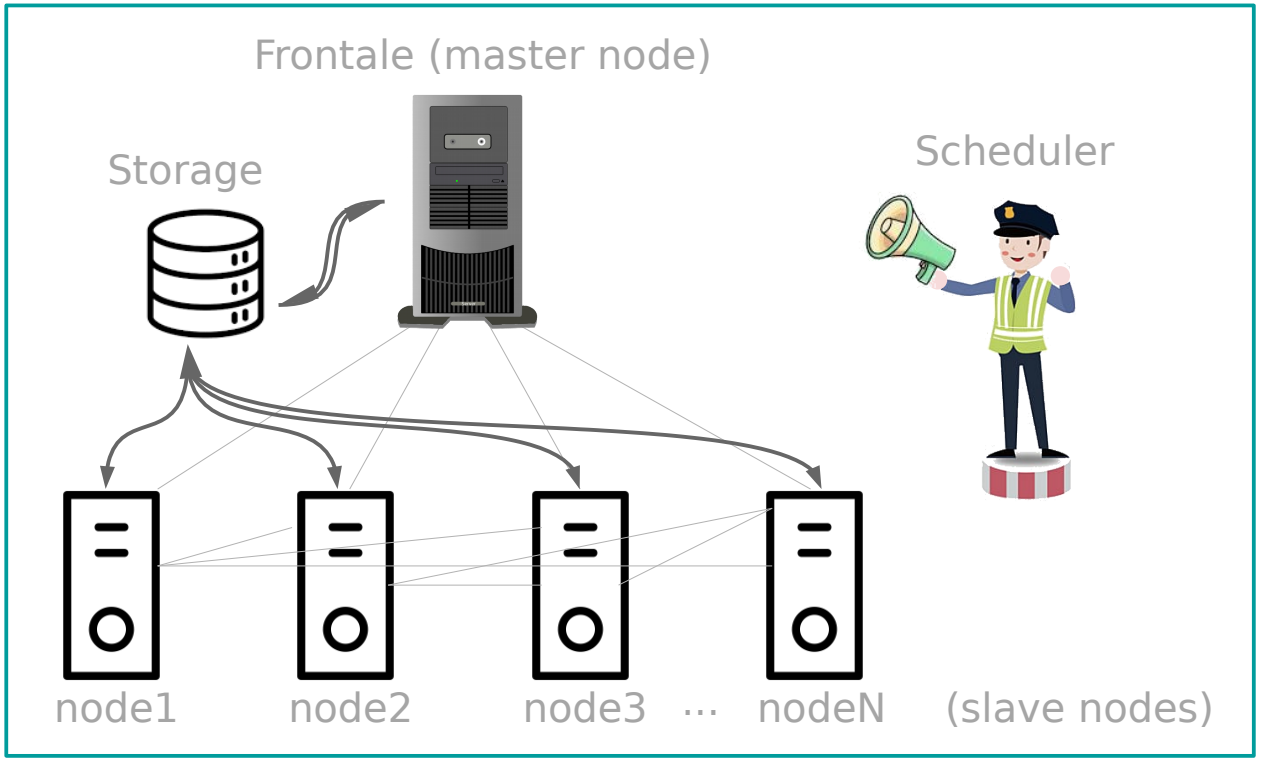


What is a cluster?

A computer cluster:

=> *The master node gives orders to the slave nodes through the scheduler*

=> *The slave nodes do all the work.*



Why use a cluster?

You, processing your data with your own computer

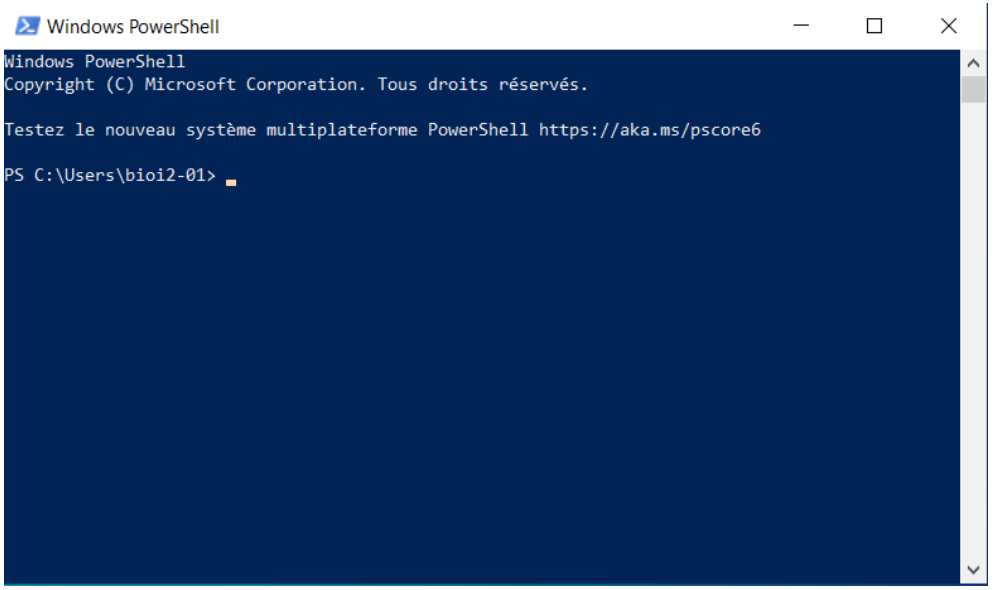
You, processing the same data with the cluster

* A computer cluster is often **more powerful** than a personal computer.
* You can **dispatch & parallelise the workload** onto several nodes = faster.
* Clusters **handle heavy data better** than your own computer would.
* When using a cluster, you save the resources of your PC for other stuff (i.e. you don't slow it down) and you also don't have to leave it on while you're waiting for computations to finish

NB: You *can* use a computer cluster but you don't *have to*. Your own PC might be good enough, it will depend on the tools and on your data.

Connect to the cluster

Several ways of doing it, we'll be using the "Terminal" / "Windows Power Shell"



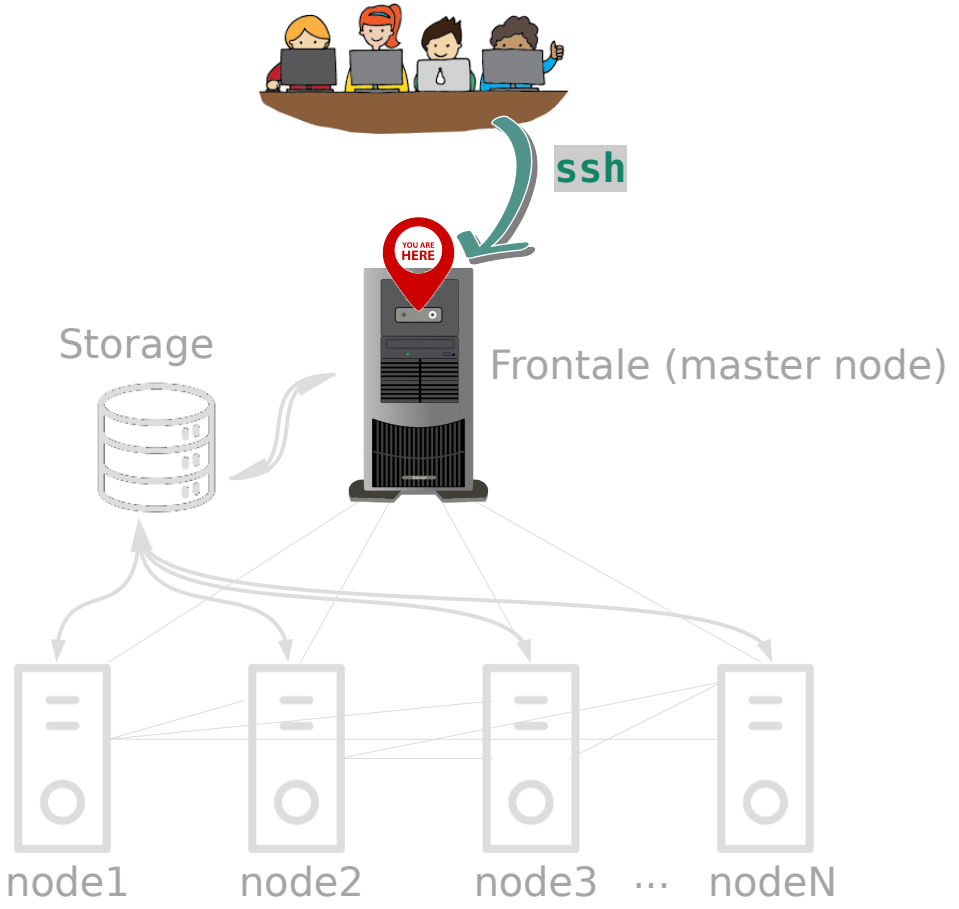
...and the SSH command line:

```
ssh john.doe@passerelle.i2bc.paris-saclay.fr
ssh john.doe@i2bc-cluster.calcul.i2bc.paris-saclay.fr
```

Connect to the cluster

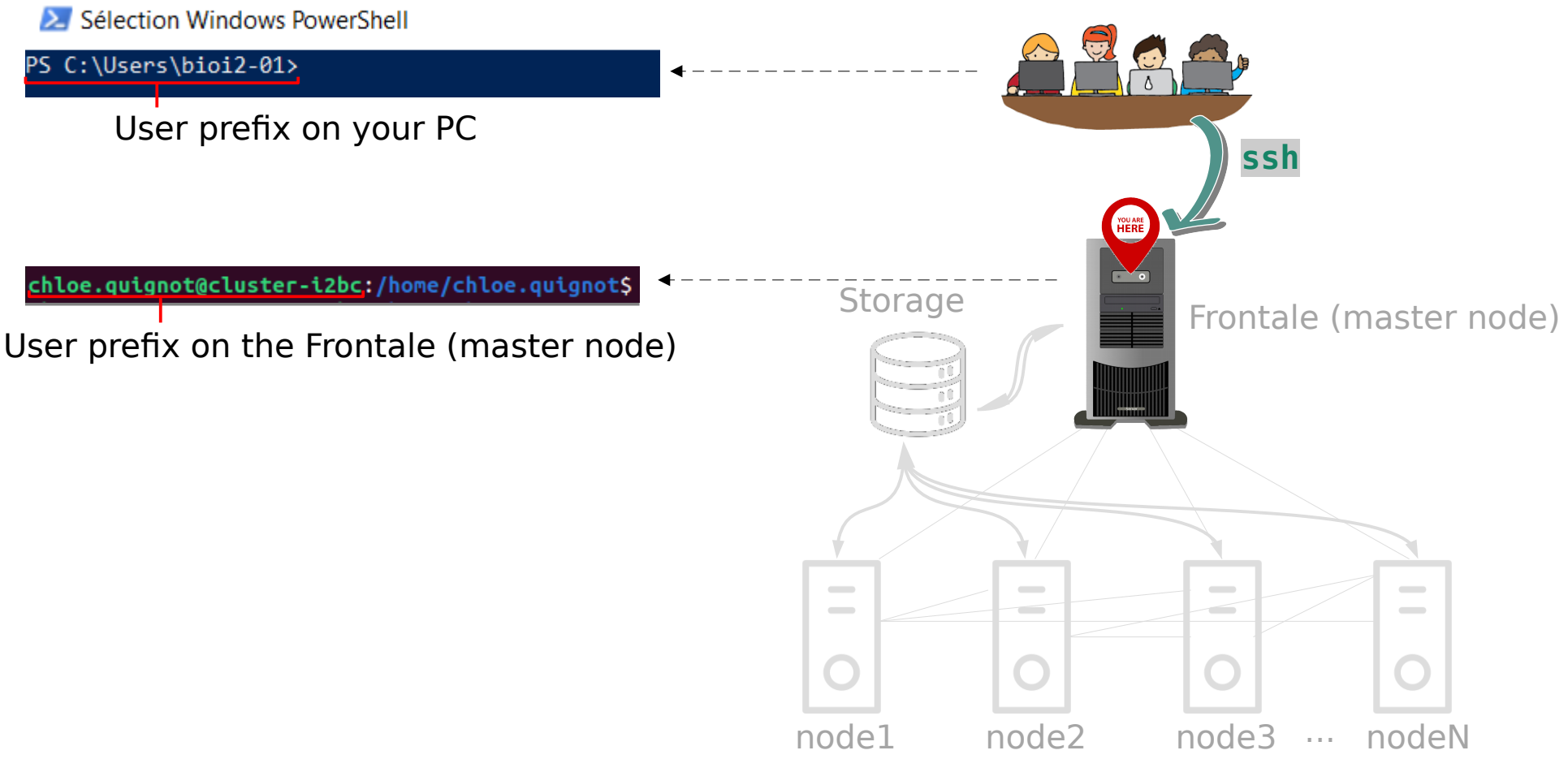
Then you land on the Frontale => the master node of the I2BC cluster

```
Linux cluster-i2bc 5.10.0-21-amd64 #1 SMP Debian 5.10.162-1 (2023-01-21) x86_64

The programs included with the Debian GNU/Linux system are free software;
the exact distribution terms for each program are described in the
individual files in /usr/share/doc/*/copyright.

Debian GNU/Linux comes with ABSOLUTELY NO WARRANTY, to the extent
permitted by applicable law.

Frontale

================================================================================
=                                                                              =
= Documentation: https://intranet.i2bc.paris-saclay.fr/intranet/sics/Main/Calcul =
= Pour voir l'état du Cluster  veuillez utiliser la commande   qshow ( ou qs ).  =
=                                                                              =
================================================================================
```



Connect to the cluster

Note the changes in your **shell prefix**! It will tell you where you are.



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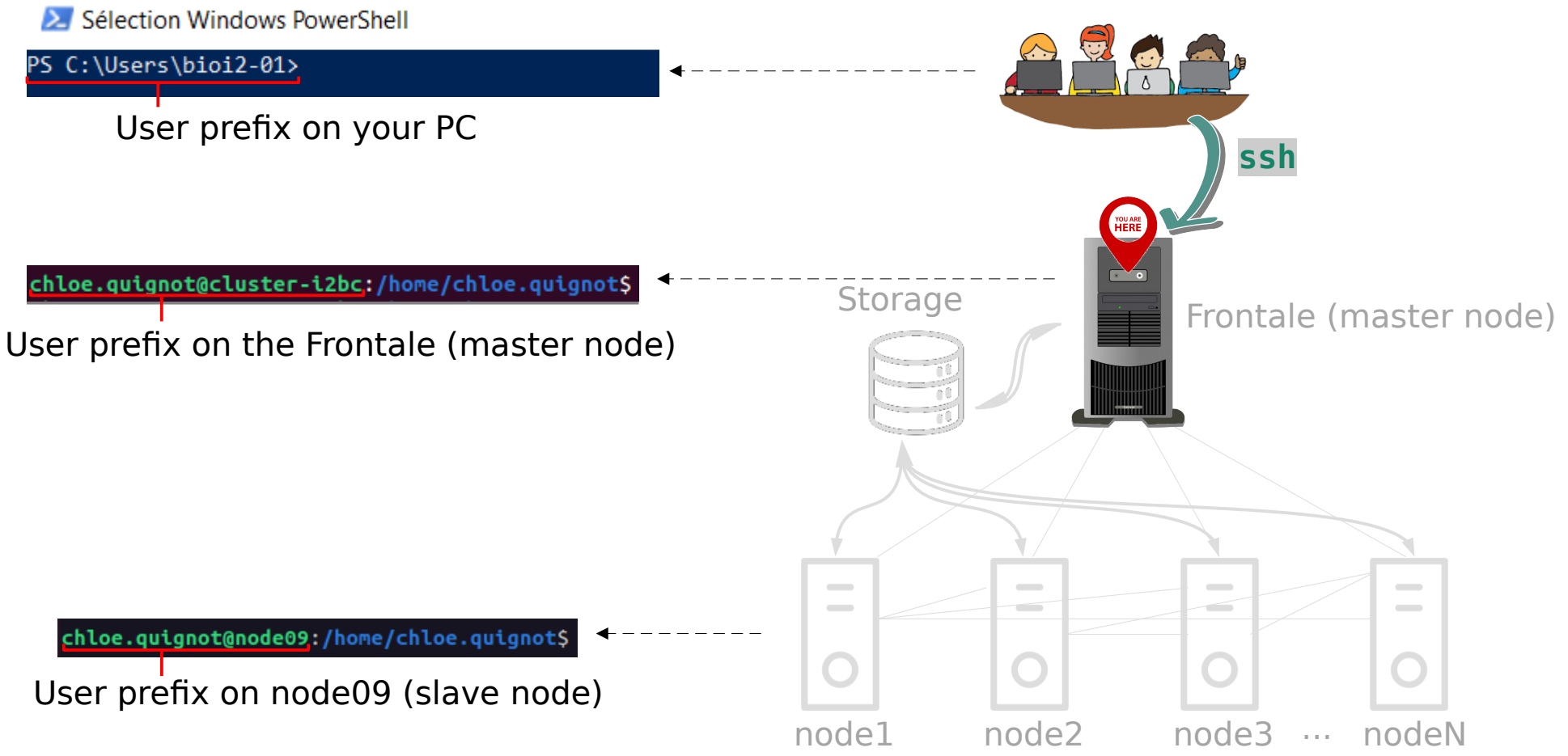
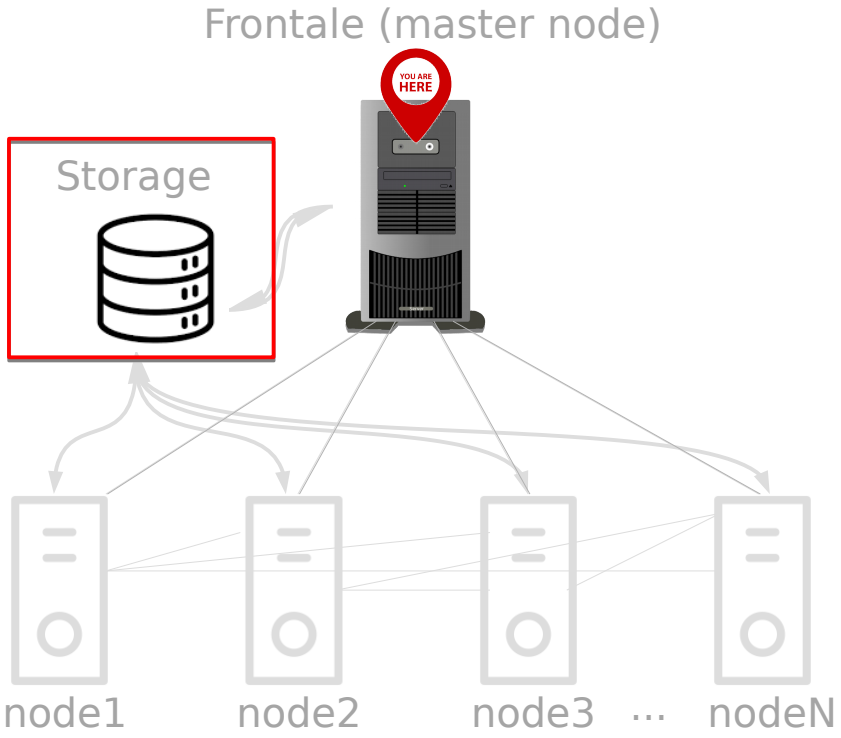


Storage system

From here, you have access to all of the I2BC's "storage" systems:

- `/store/EQUIPES/<team accronym>/`
- `/store/USERS/<your login>/`
- `/store/plateformes/<project name>/`

} "partages" => for storage



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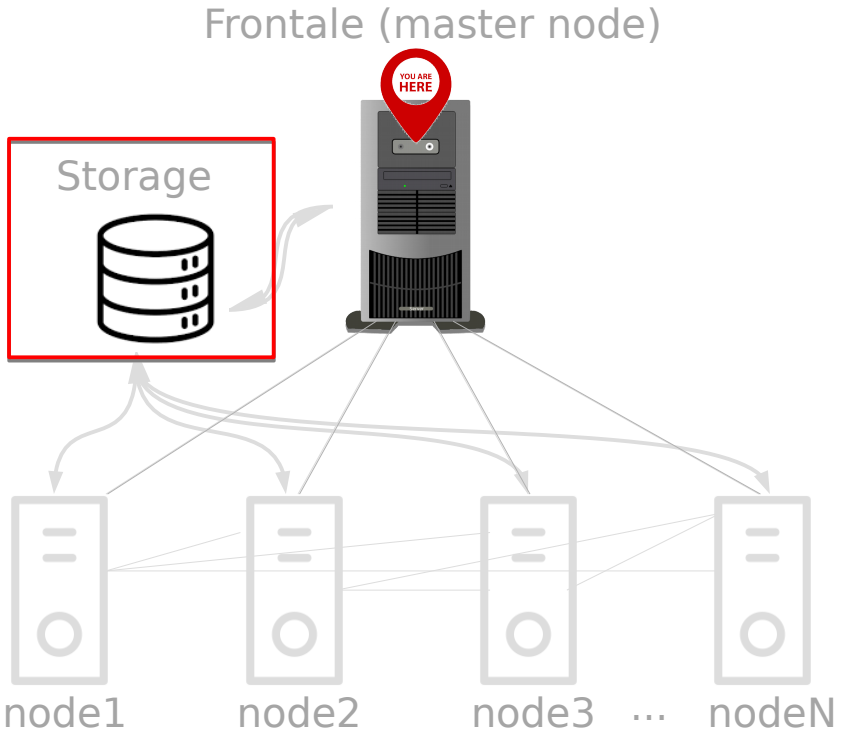

+ 3 computing spaces:

`/home/<your login>/` => your "home"

`/data/work/I2BC/` => "temporary"

`/scratchlocal/` => "temporary"

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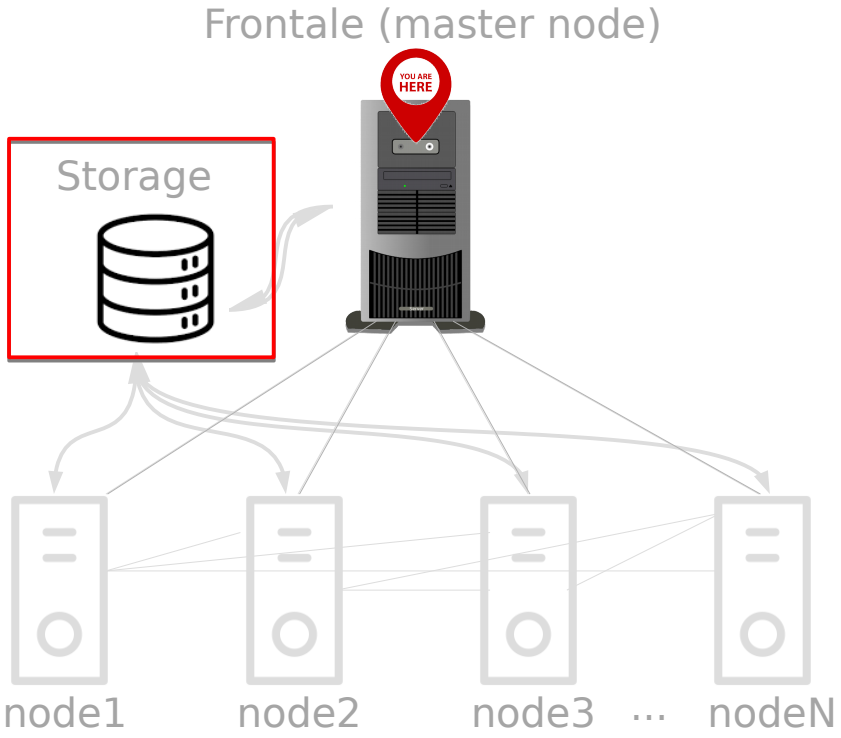

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Storage system

« Partages » storage system, aka. /store/

A space designed for **storage**

Folder	Quota	Usage	Accessibility
`/store/USERS/<your login>`	20 GB	For personal (but professional) use	Only you (read & write)
`/store/EQUIPES/<team acronym>` with a `MEMBERS` subdirectory	~~>5 TB~~ <1 TB	Shared team space	Team members only (read & write for everyone except MEMBERS)
`/store/EQUIPES/<team acronym>/MEMBERS/<your login>`		Your dedicated space within the team space	Read for everyone in the team, write only for you
`/store/plateformes/<project name>`	5 TB	For collaborations or specific projects, created on demand	People you've selected (read & write)

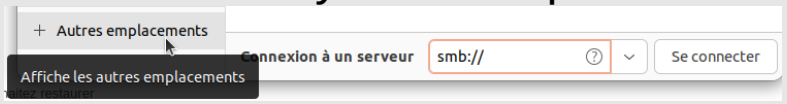
https://intranet.i2bc.paris-saclay.fr/outils/informatique/#stock => about storage @I2BC

Storage system

« Partages » storage system, aka. /store/

A space designed for **storage**

	Within I2BC (or with VPN)	Outside I2BC
	\\store\ in the navigation bar of your file explorer id: i2bc email address & password 	WinSCP: download the zip file from the intranet or use \\intra.i2bc.paris-saclay.fr\partages 

 	smb://store/ in your file explorer  id: login, domain: intra.i2bc.paris-saclay.fr
	Or mount from passerelle:
	`mkdir $HOME/store`
	`sshfs chloe.quignot@passerelle:/store $HOME/store`
	`sudo ln -s $HOME/store /store # optional`
	Or scp from passerelle
	`scp chloe.quignot@passerelle:/path/to/file .`
		Mount from passerelle (sshfs)
		Or scp from passerelle

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Storage system

From here, you have access to all of the I2BC's "storage" systems:

`/store/EQUIPES/<team accronym>/`
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`/store/plateformes/<project name>/`

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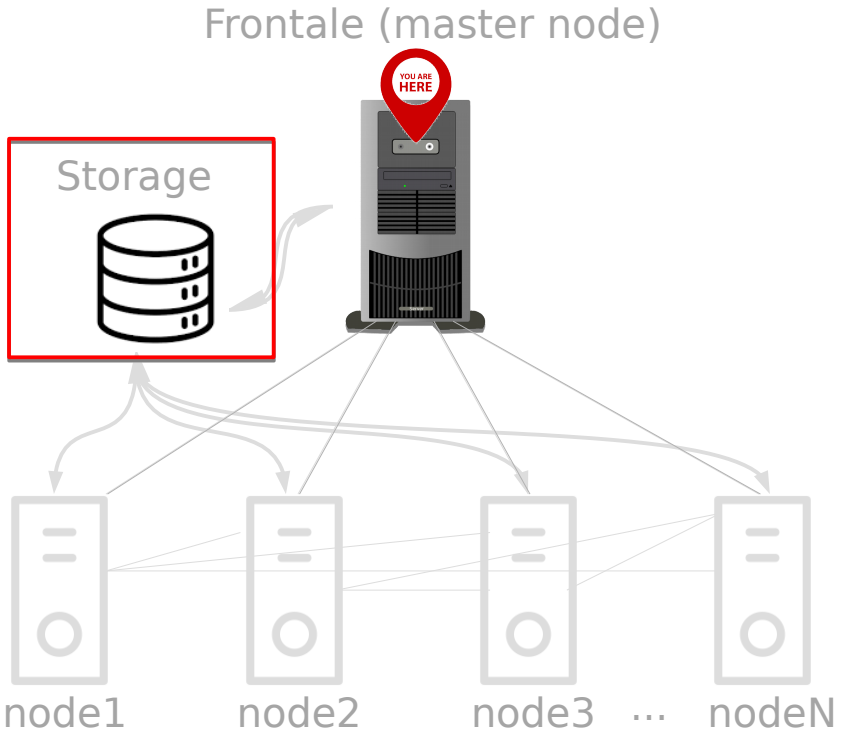

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`/scratchlocal/` => "temporary"

Storage system

«Home» directory, aka. /home/$USER

NOT for storage but for hosting configuration and login files, locally installed packages (`.local` folder), etc.

Folder	Quota	Usage	Accessibility
`/home/<your login>`	200 GB	Your home directory on the cluster, where you save e.g. config & local files	Only you (read & write)

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NOT for storage but for hosting configuration and login files, locally installed packages (`.local` folder), etc.

Folder	Quota	Usage	Accessibility
`/home/<your login>`	200 GB	Your home directory on the cluster, where you save e.g. config & local files	Only you (read & write)

	Within I2BC (or with VPN)	Outside I2BC
	Cluster home: \\data\cluster-homes in the navigation bar of your file explorer 	N/A
	smb://data/cluster-homes in your file explorer	N/A

Storage system

From here, you have access to all of the I2BC's "storage" systems:

`/store/EQUIPES/<team accronym>/`
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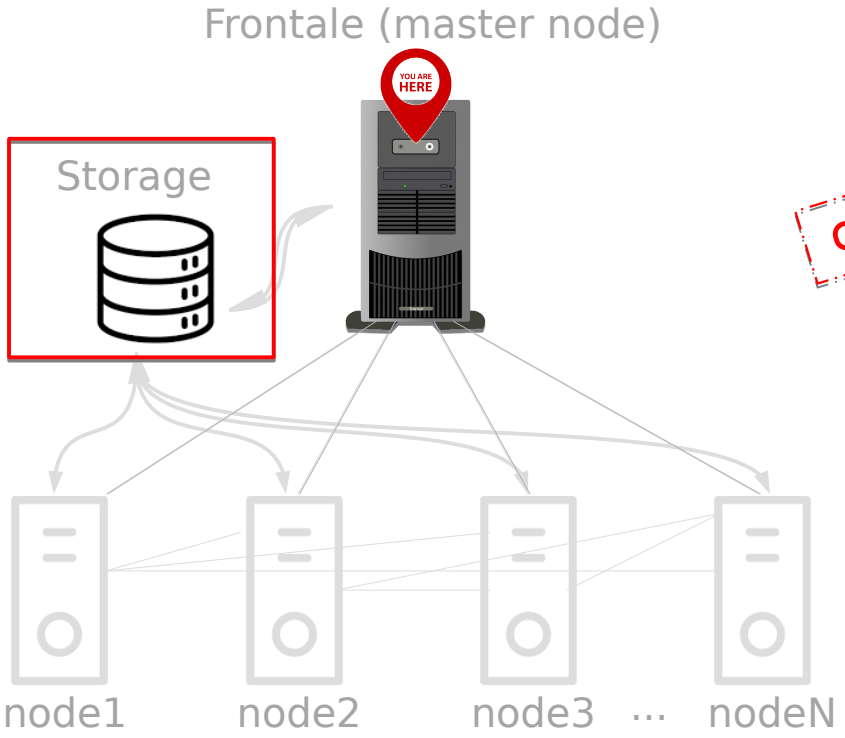

+ 3 computing spaces:

CONFIG

`/home/<your login>/` => your "home"

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Storage system - backup

Both `/store` & `/home/your_login` are **regularly backed-up**

In the terminal, put yourself in your folder and checkout the *hidden* `.snapshots/` directory
(you can run a `cp` of files and directories to retrieve them “to the present”)

```
chloe.quignot@cluster-i2bc: /home/chloe.quignot
chloe.quignot@cluster-i2bc:/home/chloe.quignot$ ls .snapshots
Jour_2023_02_27__08_00  Mois_2023_02_16__01_00     Semaine_2023_02_24__06_00
Jour_2023_02_27__12_00  rep_1677513600842          Semaine_2023_02_25__06_00
Jour_2023_02_27__16_00  Semaine_2023_02_21__06_00  Semaine_2023_02_26__06_00
Jour_2023_02_27__20_00  Semaine_2023_02_22__06_00  Semaine_2023_02_27__06_00
Mois_2023_01_19__01_00  Semaine_2023_02_23__06_00
chloe.quignot@cluster-i2bc:/home/chloe.quignot$
```

`Jour_YYYY_MM_DD__HH_MM`
`Semaine_YYYY_MM_DD__HH_MM`
`Mois_YYYY_MM_DD__HH_MM`

For more information:
https://forge.i2bc.paris-saclay.fr/redmine/projects/partage-bioinfo/wiki/B_Cluster_ressources#Backups

Storage system

From here, you have access to all of the I2BC's "storage" systems:

`/store/EQUIPES/<team accronym>/`

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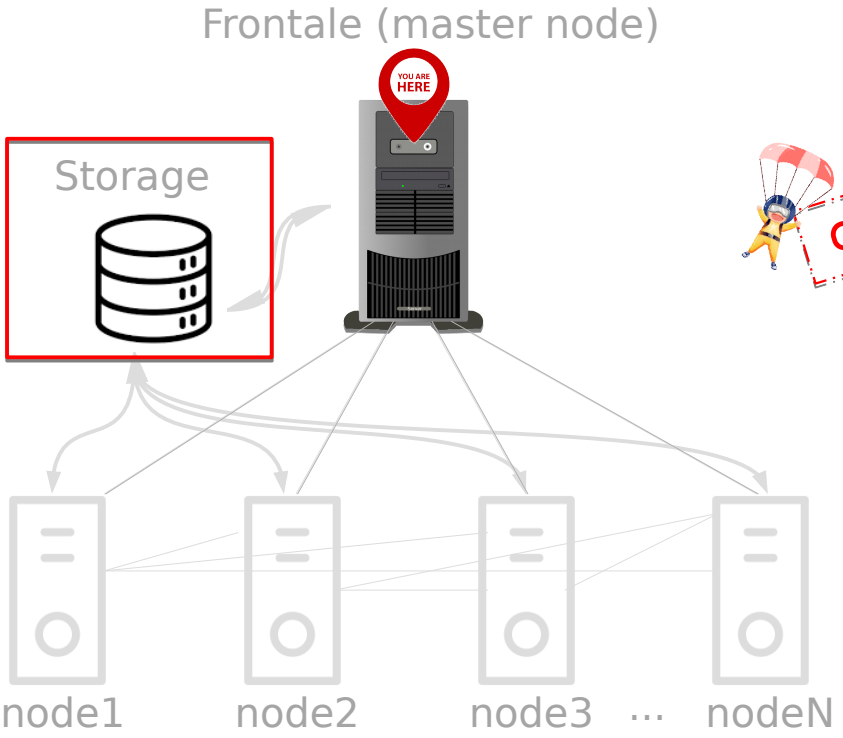

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Storage system

"Computing space":

NOT for storage but for hosting temporary/intermediate files

Not backed-up, limited space, **clean up after yourselves!**

Folder	Quota	Usage	Accessibility
`/data/work/I2BC/`	20 TB	Shared between all users (for temporary files only)	Everyone (read & write)
`/scratchlocal/`	variable from node to node	For temporary files, only on the node in question, more rapid as local to the node	Read & write only for your files & directories

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`/scratchlocal/`	variable from node to node	For temporary files, only on the node in question, more rapid as local to the node	Read & write only for your files & directories

NB1: Nothing in these spaces is deleted on its own, it's up to you to clean up after yourselves when you're done!

NB2: If you're using these spaces, it's a good habit to work within a folder with your name and/or jobid

Storage system

"Computing space":

NOT for storage but for hosting temporary/intermediate files

Not backed-up, limited space, **clean up after yourselves!**

	Within I2BC (or with VPN)	Outside I2BC
	Work: \\data\work in the navigation bar of your file explorer 	N/A
	smb://data/work in your file explorer	N/A

Storage system

From here, you have access to all of the I2BC's "storage" systems:

`/store/EQUIPES/<team accronym>/`
`/store/USERS/<your login>/`
`/store/plateformes/<project name>/`

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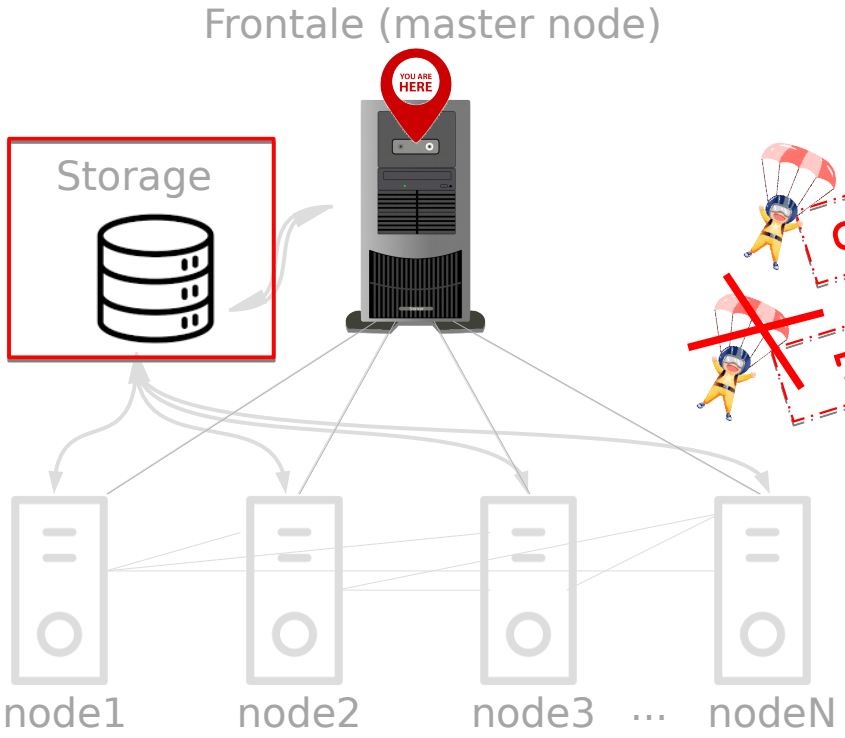


+ 3 computing spaces:

CONFIG

`/home/<your login>/` => your "home"

TEMP

`/data/work/I2BC/` => "temporary"

`/scratchlocal/` => "temporary"

Storage system

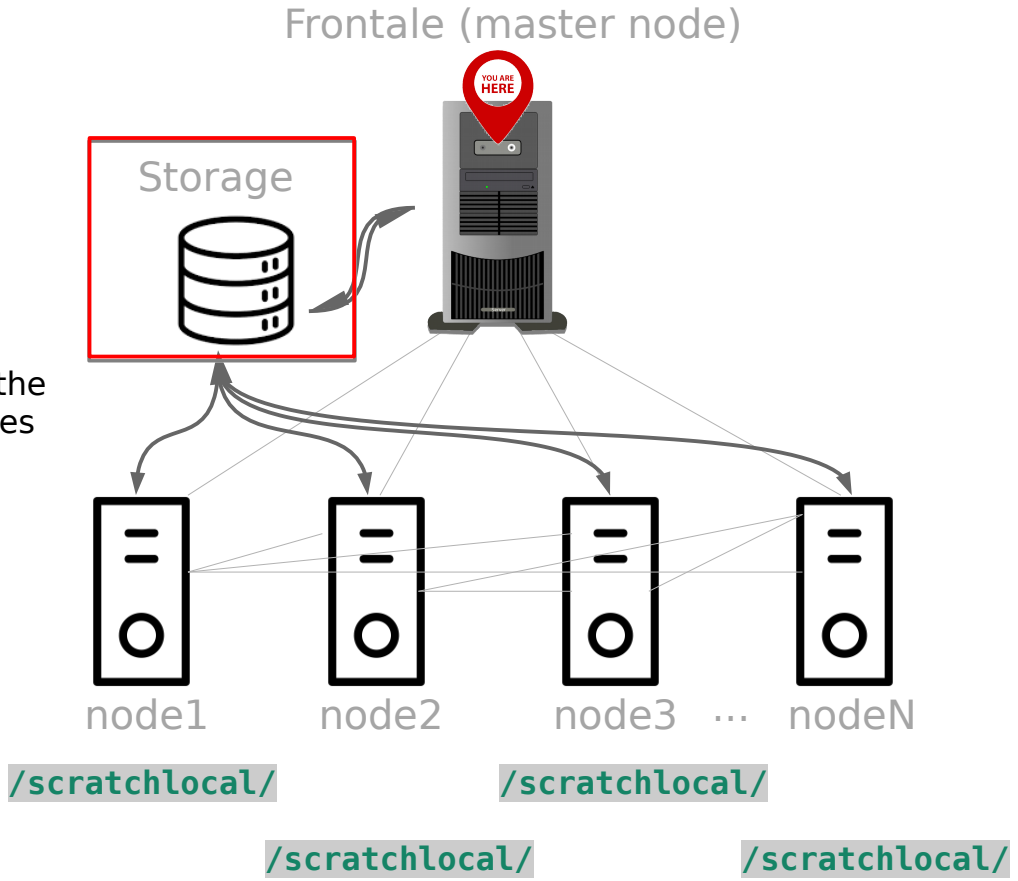
In summary: 3 spaces accessible from both the slave and the master nodes + 1 space accessible only on the nodes and specific to each node

`/home/<your login>/`,

`/store/` and

`/data/work/I2BC/`

are accessible from both the master and the slave nodes



Quotas

In the terminal, you can rapidly check the quota of the disk using the in-house `i2bc_quota` command with `-a` (all) or `-u` (only your usage).

Example: total quota on `/data/work`

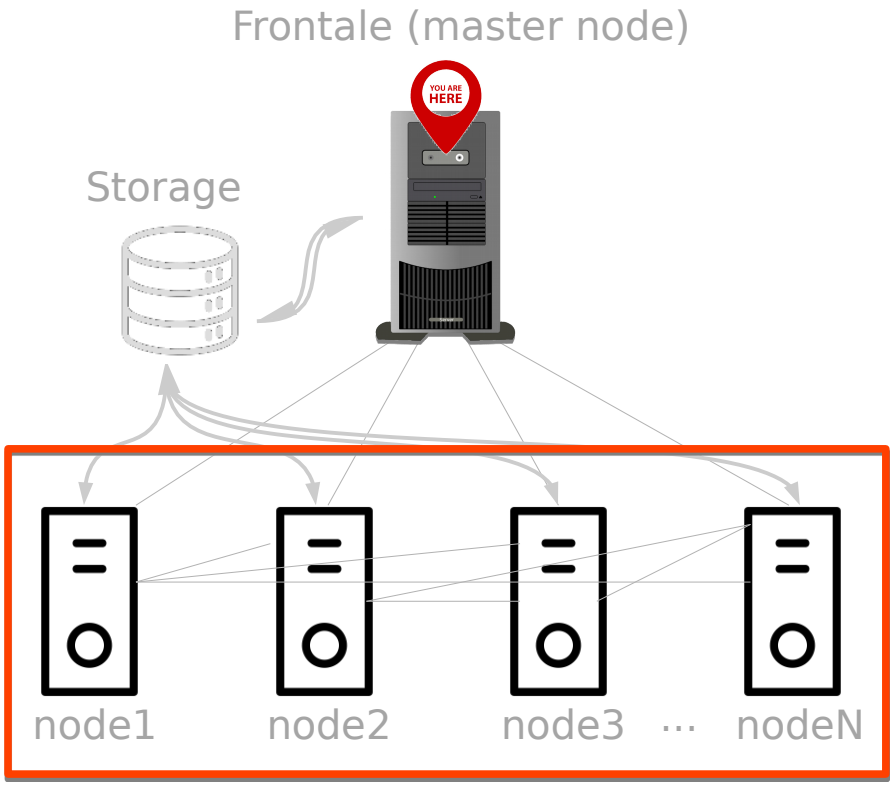
```
chloe.quignot@cluster-i2bc: /home/chloe.quignot
chloe.quignot@cluster-i2bc:/home/chloe.quignot$ i2bc_quota -s data -v WORK -a
Volume          Directory                 Free      Used     Quota    FreeGB    UsedGB   QuotaGB
work            /I2BC                 3072 GB   17.0 TB   20.0 TB      3072     17408     20480
work            /NGS                  3380 GB    6.7 TB   10.0 TB      3380      6860     10240
```

```
chloe.quignot@cluster-i2bc: /home/chloe.quignot
chloe.quignot@cluster-i2bc:/home/chloe.quignot$ i2bc_quota
usage: i2bc_quota [-h] [-u] [-a] [-s {data,store}] [-v VOLUME]

Examples:

1) i2bc_quota -v EQUIPES /SICS
Display quota information about EQUIPES/SICS on store NAS server

2) i2bc_quota -s data -v WORK -a
Display quota information for all directories in volume DATA on data NAS
server

3) i2bc_quota -v USERS -u
Display quota information about your own use on volume USERS (on store NA
S server)
chloe.quignot@cluster-i2bc:/home/chloe.quignot$
```

If you only type the "i2bc_quota" command, you'll get a help message to show you how to use it

Meet the workers

Jobs are never run on the Frontale, they should always be run on the slave nodes!!!



The slave nodes are the ones that do the job

Meet the workers

Use `pbsnodes -avS` to list all the nodes on the cluster

chloe.quignot@cluster-i2bc: /home/chloe.quignot

```
chloe.quignot@cluster-i2bc:/home/chloe.quignot$ pbsnodes -avS
vnode           state           OS       hardware host            queue       mem     ncpus   nmics   ngpus  comment
--------------- --------------- -------- -------- --------------- ---------- -------- ------- ------- ------- ---------
node01          state-unknown   --       --       node01          --             0kb       0       0       0 node_target: COMMON
node02          state-unknown   --       --       node02          --             0kb       0       0       0 node_target: COMMON
node03          state-unknown   --       --       node03          --             0kb       0       0       0 node_target: COMMON
node04          state-unknown   --       --       node04          --             0kb       0       0       0 node_target: COMMON
node05          free            --       --       node05          --          125gb      40       0       0 node_target: MICMAC
node06          free            --       --       node06          --          125gb      40       0       0 node_target: COMMON
node07          free            --       --       node07          --          125gb      40       0       0 node_target: COMMON
node08          free            --       --       node08          --          125gb      40       0       0 node_target: EMC2
node09          free            --       --       node09          --          125gb      40       0       0 node_target: AMIG
node10          job-busy        --       --       node10          --          125gb      40       0       0 --
node11          free            --       --       node11          --          125gb      40       0       0 node_target: AMIG
node12          free            --       --       node12          --          125gb      40       0       0 node_target: AMIG
node13          free            --       --       node13          --          125gb      40       0       0 node_target: COMMON
node14          job-busy        --       --       node14          --          125gb      40       0       0 node_target: COMMON
node15          job-busy        --       --       node15          --          125gb      40       0       0 node_target: COMMON
node16          job-busy        --       --       node16          --          125gb      40       0       0 node_target: COMMON
node17          job-busy        --       --       node17          --          377gb      40       0       0 --
node18          job-busy        --       --       node18          --          251gb      40       0       0 node_target: CHRODY
```

Each node has a name...

...we know if it's completely booked or if it has some free processors...

...we also have information on its properties: available memory, number of CPUs & GPUs and to what group it belongs

Meet the workers

Use `pbsnodes -aSj` to list all the nodes on the cluster and the jobs that are running on them

chloe.quignot@cluster-i2bc: /home/chloe.quignot

```
chloe.quignot@cluster-i2bc:/home/chloe.quignot$ pbsnodes -aSj
                                                    mem       ncpus   nmics   ngpus
vnode           state           njobs   run   susp      f/t        f/t     f/t     f/t   jobs
--------------- --------------- ------ ----- ------ ------------ ------- ------- ------- -------
node01          state-unknown        0     0      0       0kb/0kb     0/0     0/0     0/0 --
node02          state-unknown        0     0      0       0kb/0kb     0/0     0/0     0/0 --
node03          state-unknown        0     0      0       0kb/0kb     0/0     0/0     0/0 --
node04          state-unknown        0     0      0       0kb/0kb     0/0     0/0     0/0 --
node05          job-busy             5     5      0   115gb/125gb    0/40     0/0     0/0 224148,224149,224150,224151,224622
node06          job-busy             5     5      0   115gb/125gb    0/40     0/0     0/0 224152,224153,224154,224155,224156
node07          job-busy             5     5      0   115gb/125gb    0/40     0/0     0/0 224157,224158,224159,224160,224161
node08          free                 1     1      0   125gb/125gb   20/40     0/0     0/0 226811
node09          job-busy             5     5      0   115gb/125gb    0/40     0/0     0/0 224162,224163,224164,224165,224166
node10          job-busy             5     5      0   115gb/125gb    0/40     0/0     0/0 224167,224168,224169,224170,224171
node11          job-busy             5     5      0   115gb/125gb    0/40     0/0     0/0 224172,224173,224174,224175,224176
node12          job-busy             5     5      0   115gb/125gb    0/40     0/0     0/0 224177,224603,224604,224605,224606
```

Number of jobs that are running

Amount of free memory left

Number of CPUs that are free

Job ids of jobs that are running on that node

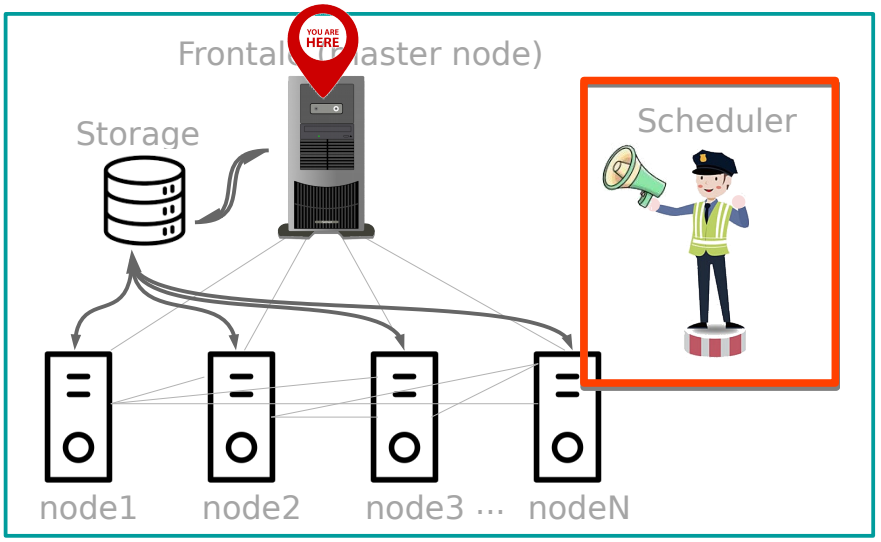
Running jobs

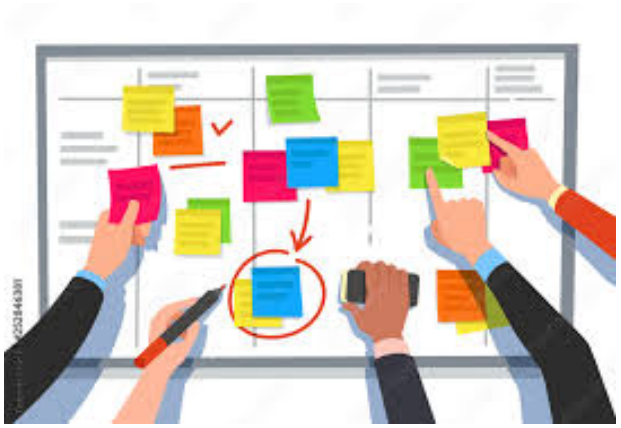
Communication between the nodes is done through the OpenPBS system (version 20.0)

Portable **B**atch **S**ystem (PBS) is a software scheduler that:

→ **manages** jobs, ressources & quotas

→ creates a job queue to organise **job priorities**

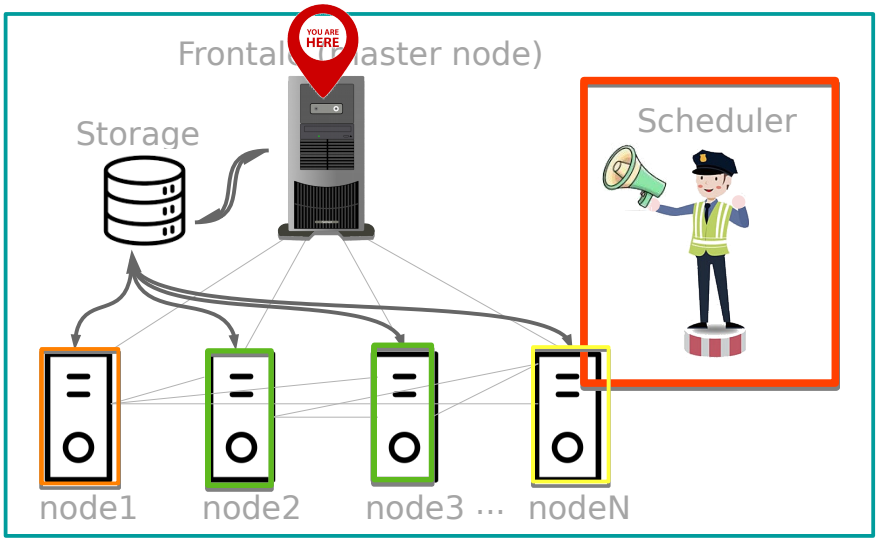




Running jobs

When you submit a job on the cluster, you submit it to a **queue**.

different queues = different properties



- **common** ← gives access to all shared nodes (“COMMON” nodes)
- **RunXX** (2,4,8,16,32) ← when several jobs, auto management to limit to XX jobs running at a time
- **<group-specific>** ← priority (or exclusive usage) for group members who financed these nodes
- **lowprio** ← access to more nodes but job could be suspended for a while (not high-priority)

Cluster status

`qshow` is an “in-house” script based on `qstat`, it’s only accessible on the Frontale

`qshow` can be used in many ways, it’s to help you get a general view of the cluster resources and their availability

For ex: `qshow -a -q` to list all node types and their associated queues

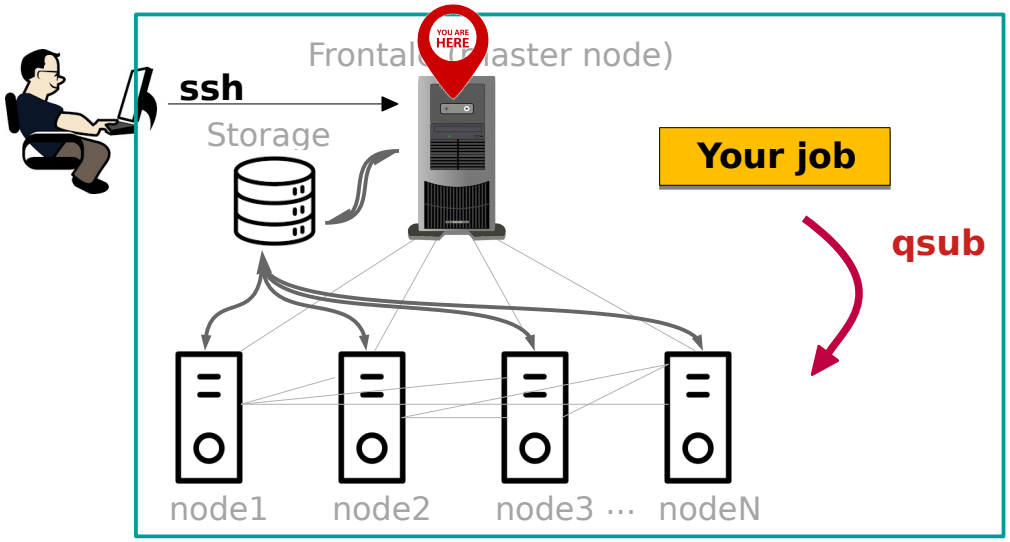
```
chloe.quignot@cluster-i2bc:/home/chloe.quignot$ qshow -a -q

-------------------------------------------------------------
Nodes AMIG :  You can use these nodes by submitting yours jobs in one of the following queues: amig
    6 node(s) can run new job
    12 of 320 Processors used
    No job blocked => Next submitted job will run immediately
    No job in restricted queues (run4, run8,...)

-------------------------------------------------------------
Nodes BIM :  You can't use these nodes!!
    2 node(s) can run new job
    2 of 176 Processors used
    No job blocked => Next submitted job will run immediately
    No job in restricted queues (run4, run8,...)
-------------------------------------------------------------
Nodes COMMON :  You can use these nodes by submitting yours jobs in one of the following queues: common,run16,run2,run32,run4,run8
    20 node(s) can run new job
    20 of 740 Processors used
    No job blocked => Next submitted job will run immediately
    No job in restricted queues (run4, run8,...)
```

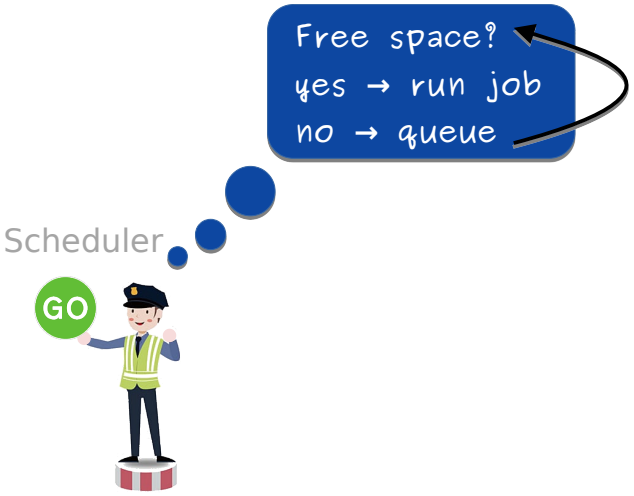
qshow --help

Running jobs

3 important commands in PBSpro:

- `qsub`: to submit the job
-
-

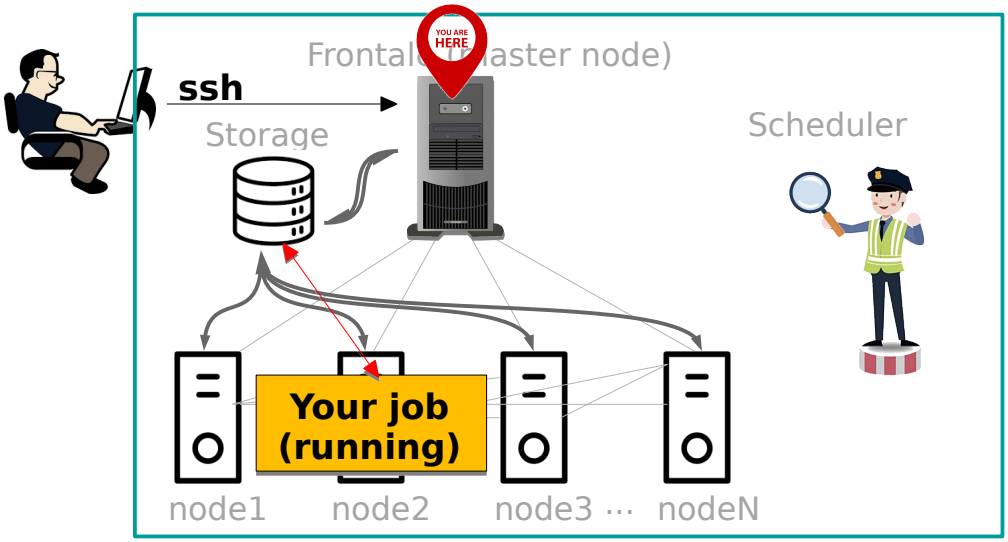




Running jobs

3 important commands in PBSpro:

- `qsub`: to submit the job
- `qstat`: to follow the job (`qshow`: more information on ressource consumption)
-

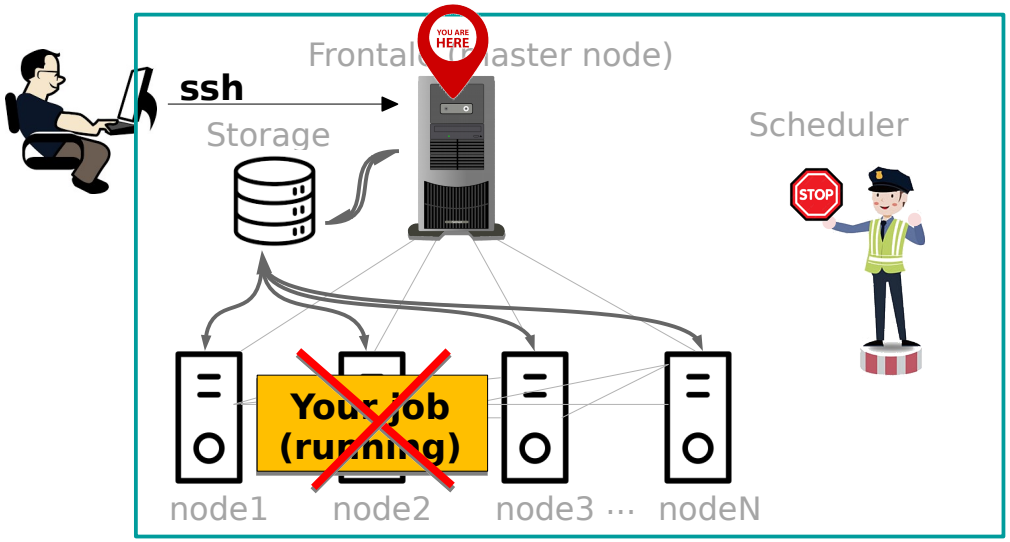


qstat *List status of submitted jobs*

Running jobs

3 important commands in PBSpro:

- `qsub`: to submit the job
- `qstat`: to follow the job (`qshow`: more information on ressource consumption)
- `qdel`: to kill the job



qdel *Kill the job that is running*

Installed programmes

There is a certain number of programmes that are arleady installed on the nodes of the I2BC cluster (/!\ not on the Frontale – only on the nodes!)

Use the module system:

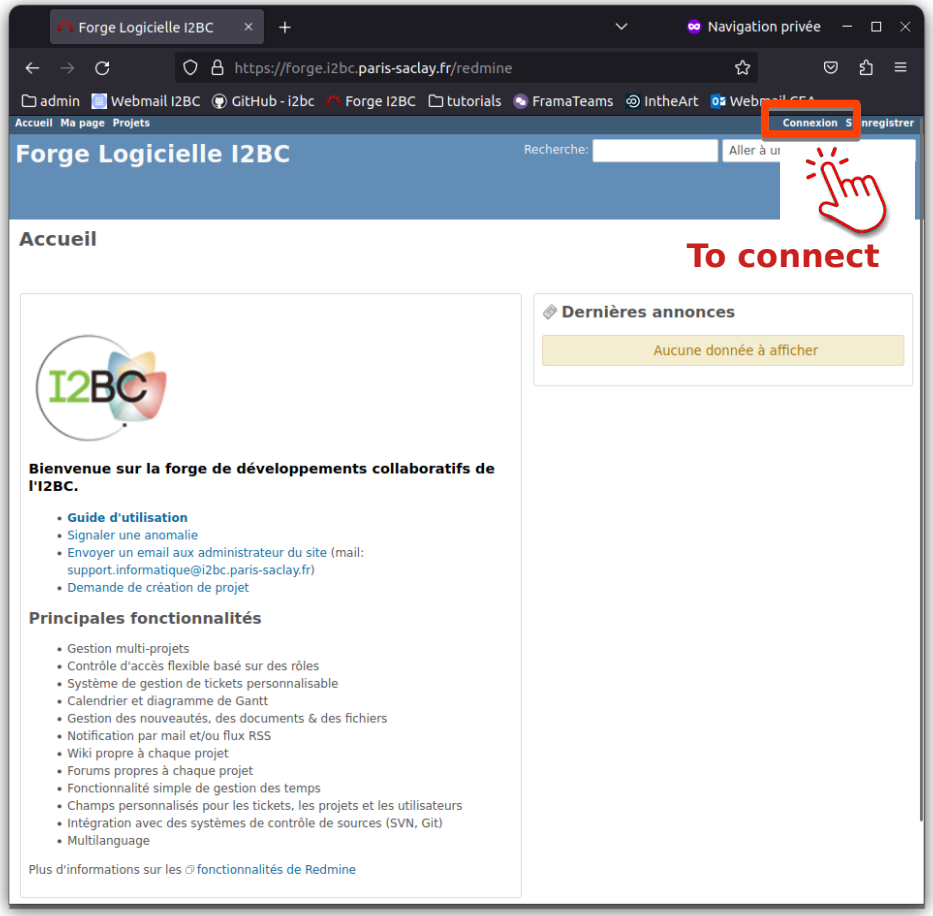
`module avail` to list all available software

`module load` to load a specific programme

Before starting the practical sessions...

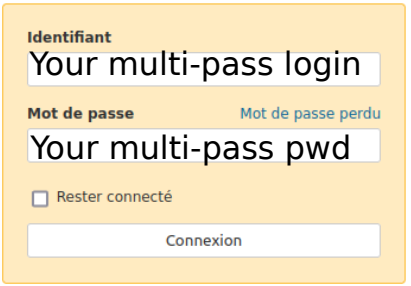
Connect to the Forge

We'll be using the Forge at the end of this session to download the example files. Let's just check you all have access to it.



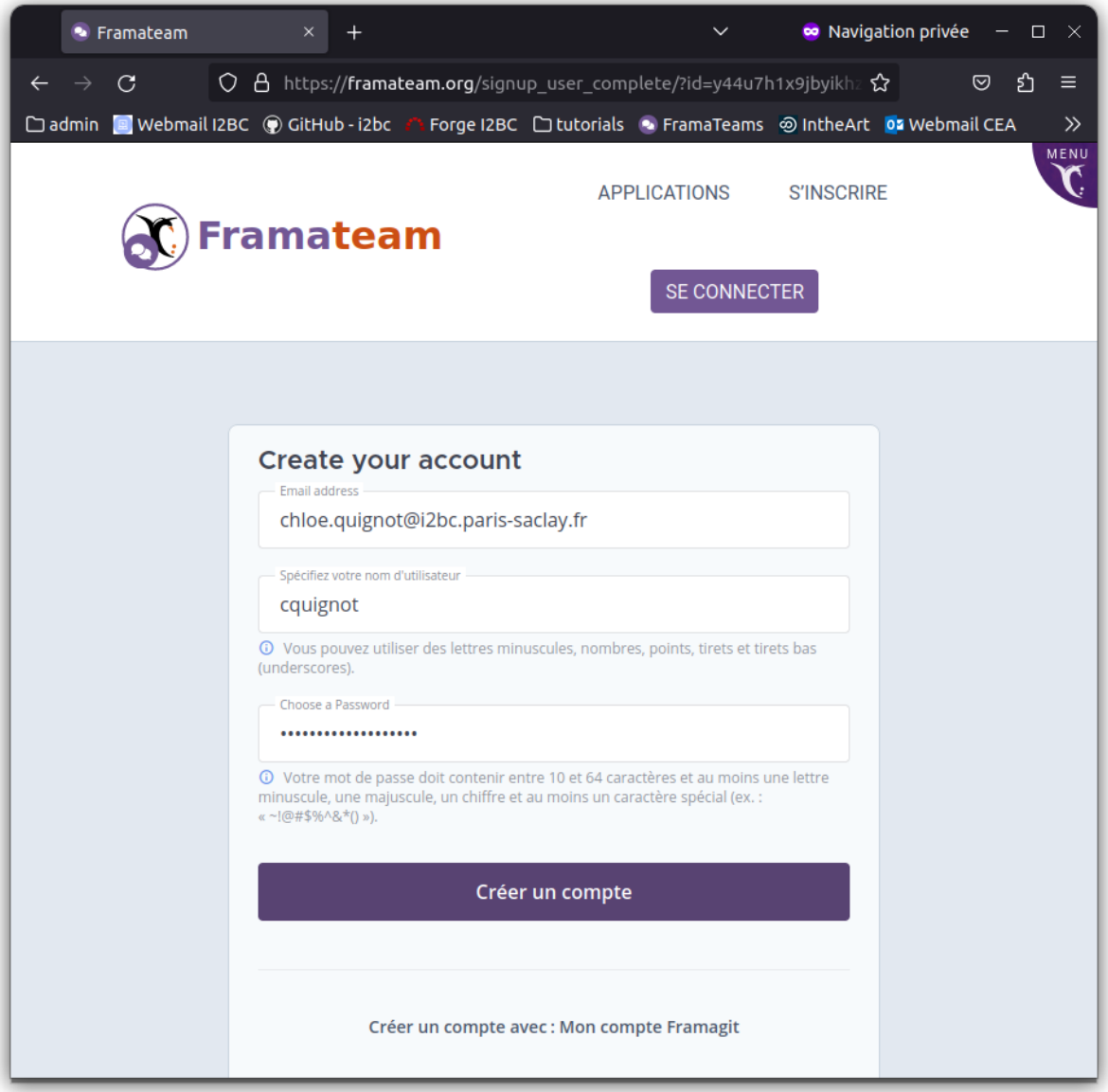
https://forge.i2bc.paris-saclay.fr/

The Forge is similar to Github but files are hosted locally on the I2BC servers



Your multi-pass login is the one that you use to connect to your I2BC account (PC, email, etc.). It's often firstname.lastname, but not always!

Let’s stay in touch



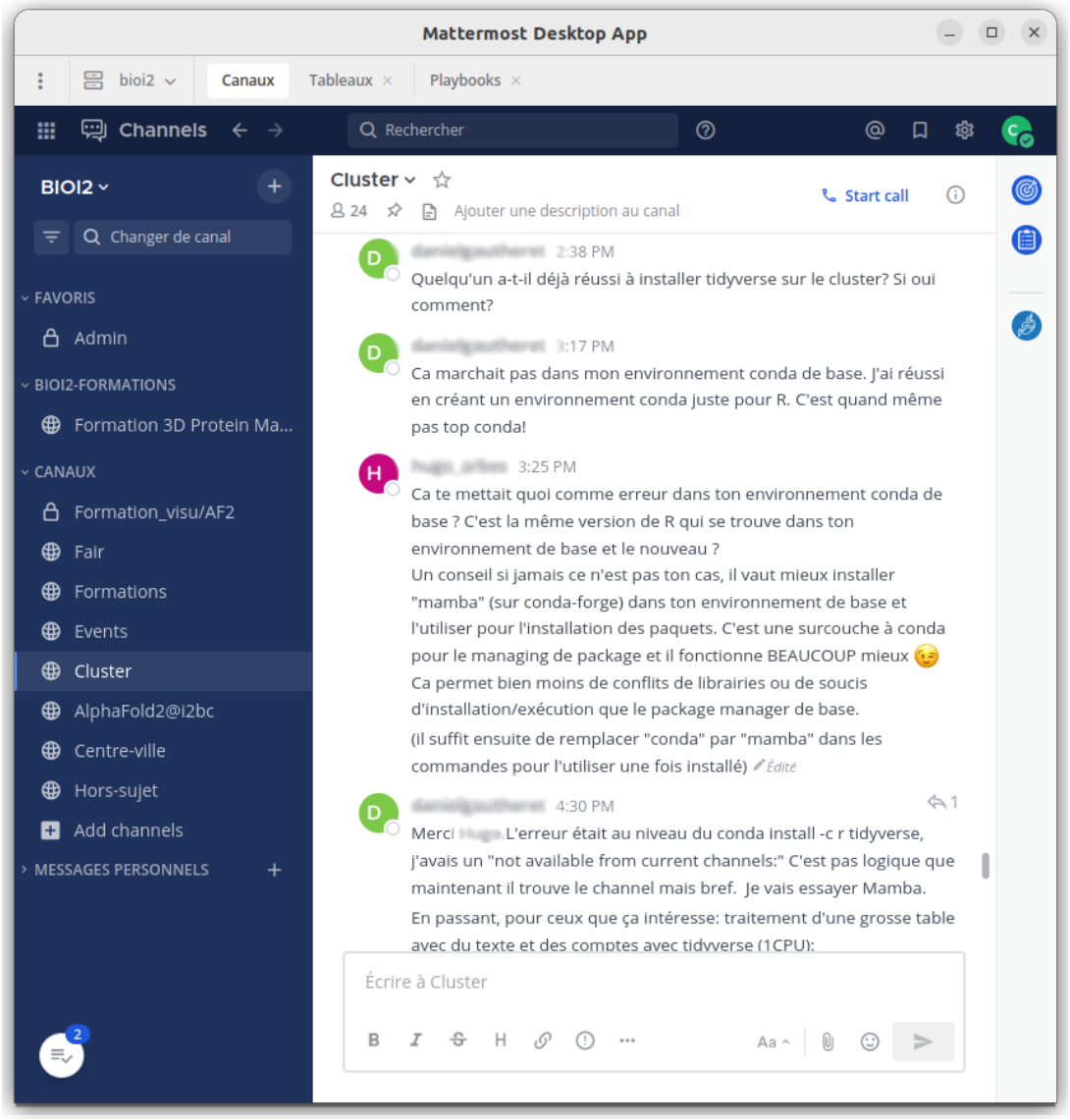
https://framateam.org/signup_user_complete/?id=y44u7h1x9jbyikhzmtbb6bw3hc

Join the Bioinformatician community of the I2BC on our FramaTeam discussion group

Just create an account with your i2bc email address and click on the link above.

You can also download the app on your computer or mobile phone (Mattermost app - specify framateam.org as the server URL)

Let’s stay in touch



There’s a channel dedicated to news and discussions about the I2BC cluster.

Don’t hesitate to join us and ask your questions here.

SICS – IT support

Need help with your computer, internet, some software, the cluster…?

=> the “Support informatique” team (SICS) is there for that
Email: support.informatique@i2bc.paris-saclay.fr

Some tips for a more efficient response:
* Be clear and concise in the email and email subject
* Start your subject with a keyword describing the problem category
(e.g. [Cluster], [Internet], [Software], etc.)

SICS – IT support

About IT resources on the intranet:

/!\ 2 pages:
- outils/informatique
- procedures/info

Information on your IT account, cluster usage, quotas, MyCore (the CNRS OneDrive), etc.

support.informatique@i2bc.paris-saclay.fr

about & procedures

about & procedures

about

https://intranet.i2bc.paris-saclay.fr/wp-content/uploads/2023/10/PBSUserGuide18.2.pdf

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about & procedures

about & procedures

about

https://intranet.i2bc.paris-saclay.fr/wp-content/uploads/2023/10/PBSUserGuide18.2.pdf

FAIR practices

Keep the FAIR practices in mind!

PID
Repository

Protocols
(free, open, auth.)

Standards
(format, vocabulary)

Metadata
License
Origin

https://doi.org/10.1038/sdata.2016.18

* Write notes, keep track of what you're doing (choose the format that suits you best e.g. text files, OneNote, Forge wiki, Joplin, eLabFTW etc.)
* Use understandable and logical filenames
* Organise your workspace (e.g. don't mix scripts and data)
* Keep track of versions used/downloaded
* ...