

HPC cluster Initiation

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<https://southgreenplatform.github.io/trainings>





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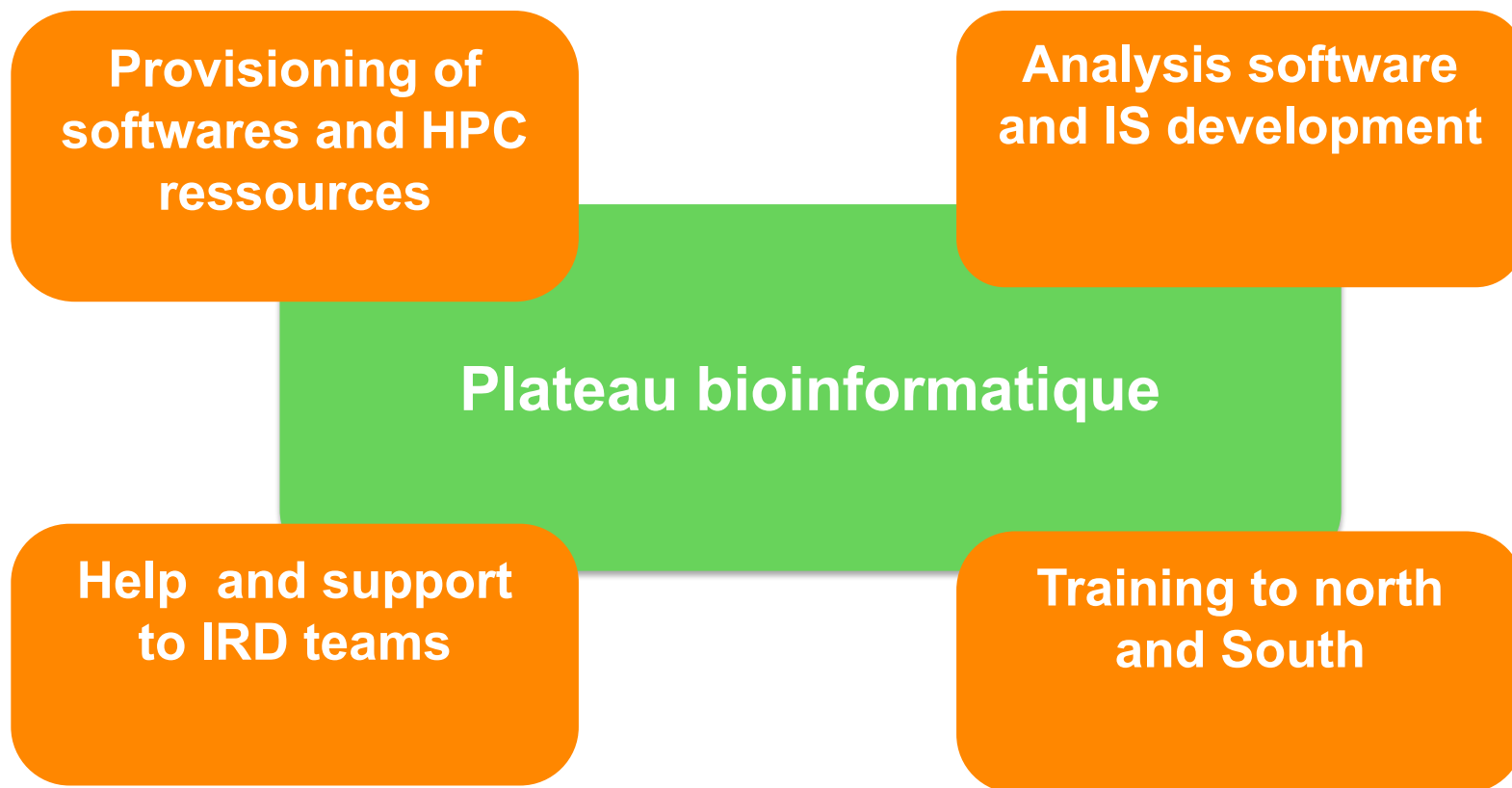
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- Request forms:

<https://itrop-glpi.ird.fr/plugins/formcreator/front/formlist.php>

- Accounts
- Softwares
- Projects

- Incidents: contact bioinfo@ird.fr

- Howtos:

<https://southgreenplatform.github.io/trainings/hpc/hpcHowto/>

- Slurm Tutorials:

<https://southgreenplatform.github.io/tutorials//cluster-itrop/Slurm/>



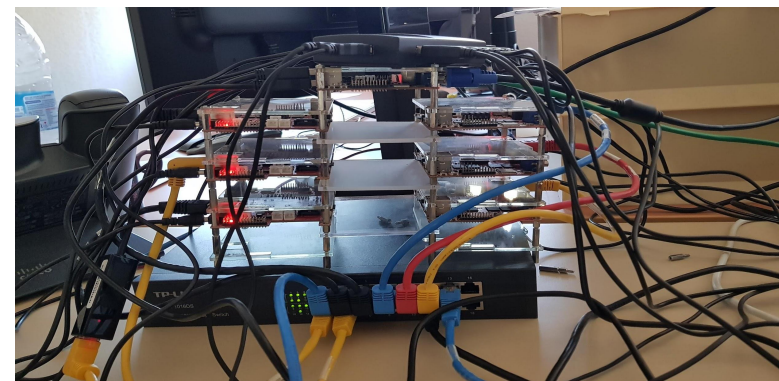
ARCHITECTURE

- A logical unit composed of several servers
- A powerful unique machine
- Allow to obtain high computing performance
- A bigger capacity storage
- More reliable
- A better resources availability

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- **Master Node**
Handle resources and jobs priorities
- **Computing nodes**
Resources (CPU or RAM memory)

COMPUTING



- **Master Node**
Handle resources and jobs priorities
- **Computing nodes**
Resources (CPU or RAM memory)

STORAGE



- **NAS Server(s)**
Storage

- **1 Master Node**



bioinfo-master.ird.fr

Role :

- Launch and prioritize jobs on computing nodes
- Accessible from the Internet
- Connection :

```
ssh login@bioinfo-master.ird.fr
```

- **1 Master Node**



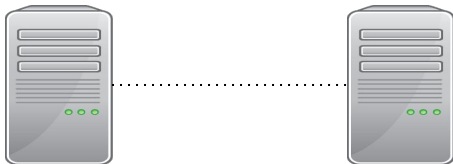
bioinfo-master.ird.fr

Role :

- Launch and prioritize jobs on computing nodes
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```
ssh login@bioinfo-master.ird.fr
```

- **27 computing nodes**



nodeX
X : 0..26

Role :

- Used by the master to execute jobs
- Not accessible from the Internet
- node0 to node26

- **1 Master Node**



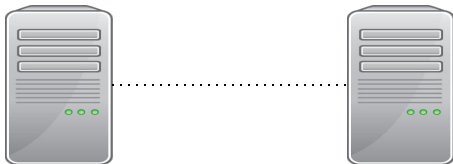
bioinfo-master.ird.fr

Role :

- Launch and prioritize jobs on computing nodes
- Accessible from the Internet
- Connection :

```
ssh login@bioinfo-master.ird.fr
```

- **27 computing nodes**



nodeX
X : 0..26

Role :

- Used by the master to execute jobs
- Not accessible from the Internet
- node0 to node26



Interactif node (node6)

- Accessible from the Internet: bioinfo-inter.ird.fr
- Connection :

```
ssh login@bioinfo-inter.ird.fr
```



Practice

Step 1: Connection, qhost

1

Go to the [Practice 1](#) of github

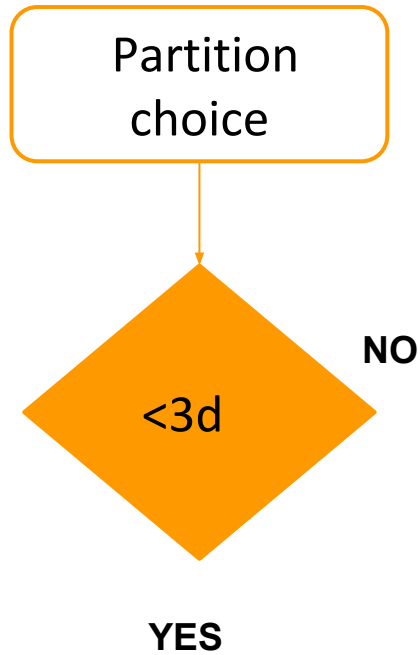
Connection
to
bioinfo-mas
ter.ird.fr
and
resources
reservation



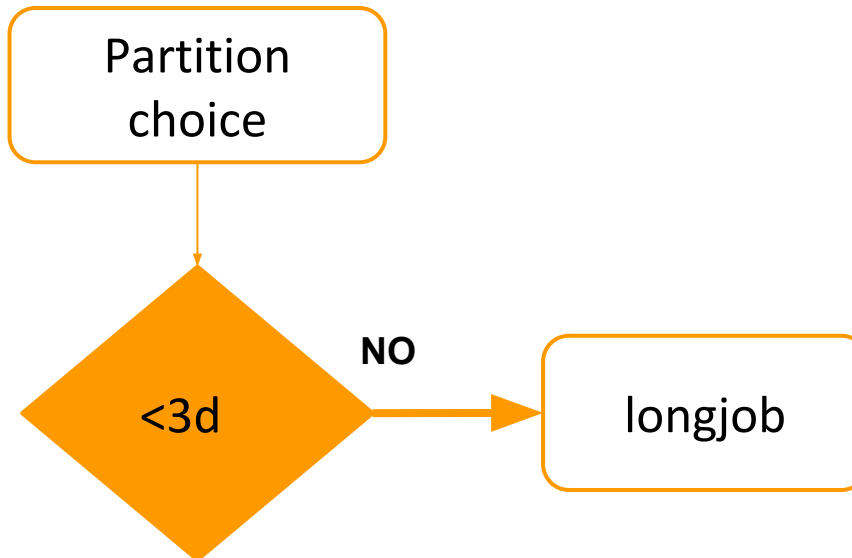
Step 1
salloc/srun
ou sbatch

Partitions	Use	RAM on nodes	Core on nodes
short	Short Jobs < 1 day (higher priority, interactive jobs)	48 to 64 GB	12 cores
normal	Short Jobs max 3 days	64 Go to 96 GB	12 to 24 cores
long	45 days >long jobs > 3 days	48 GB	12 to 24 cores
highmem	Jobs with more memory needs	144 GB	12 to 24 cores
supermem	Jobs with much more memory needs	1TB	40 cores
gpu	Need for analyses on GPU cores	192GB	24 cpus and 8 GPUs cores

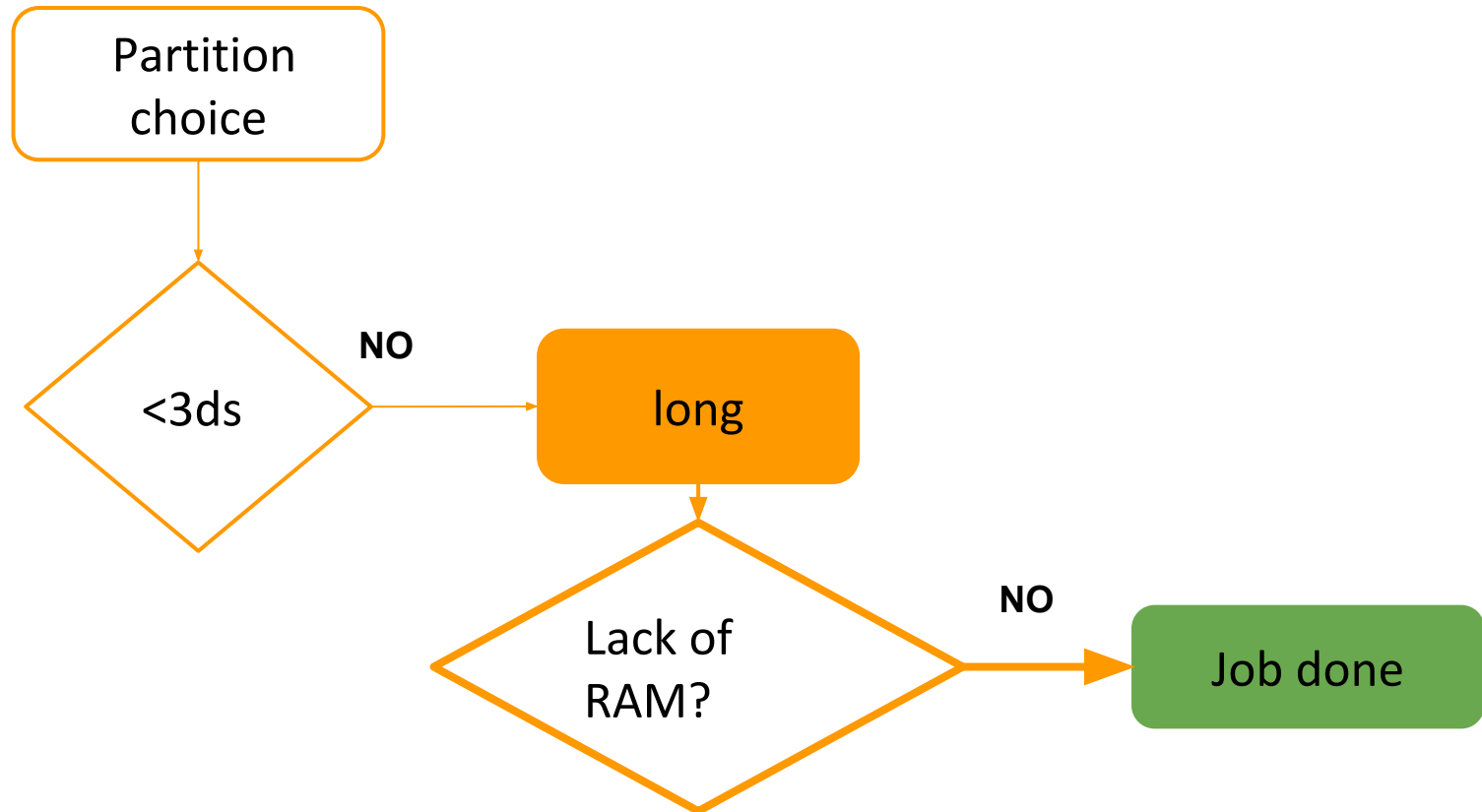
How do I choose the partition?



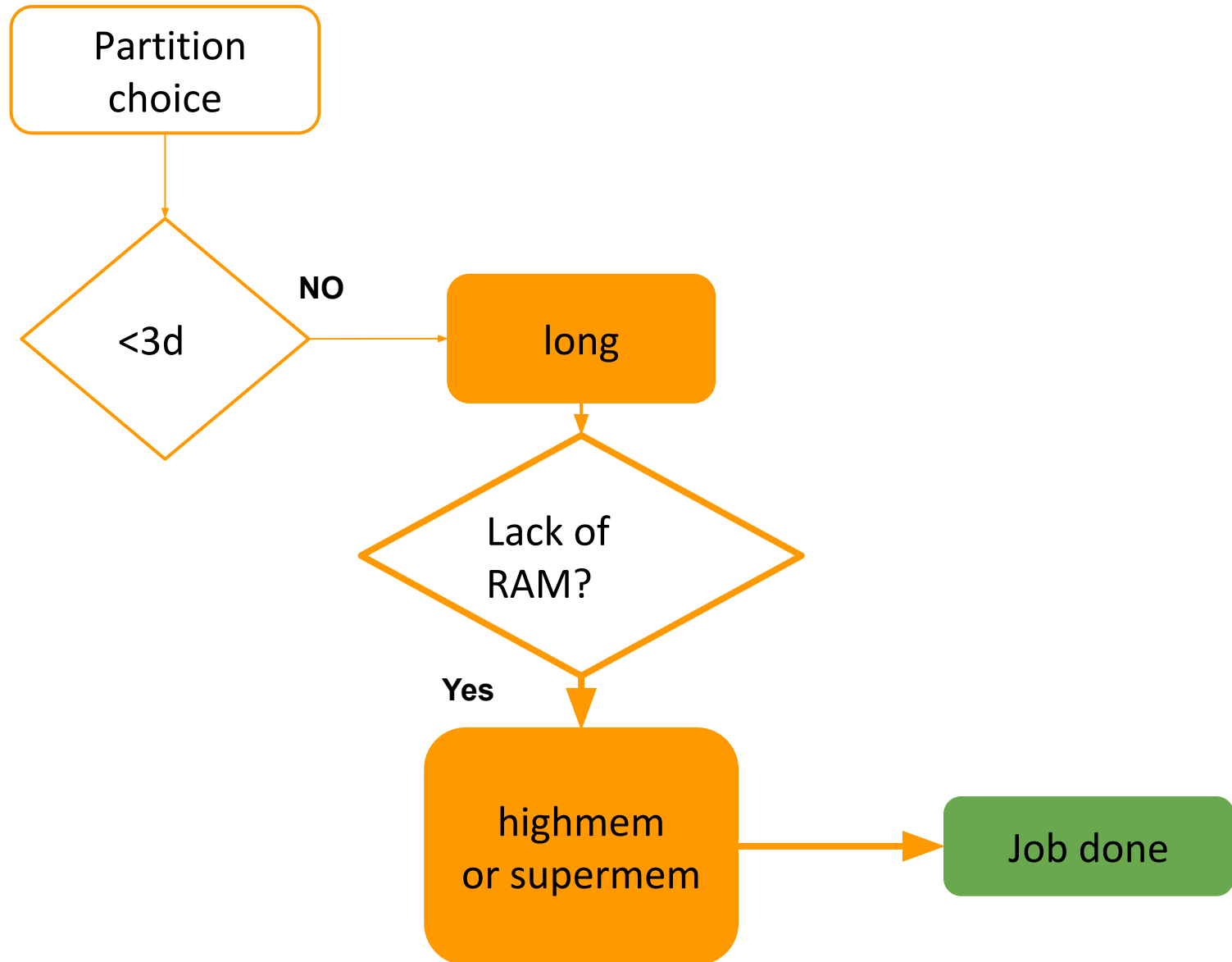
How do I choose the partition?



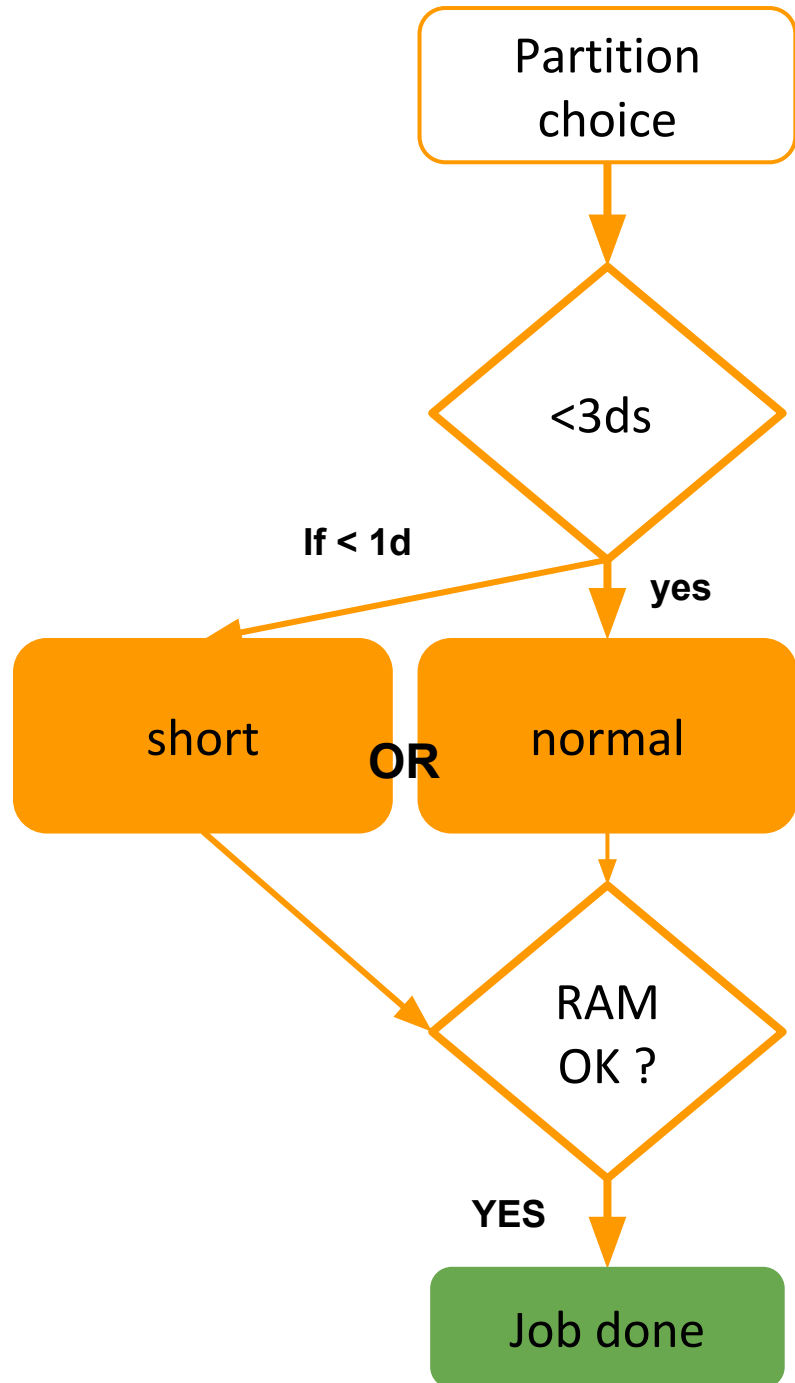
How do I choose the partition?



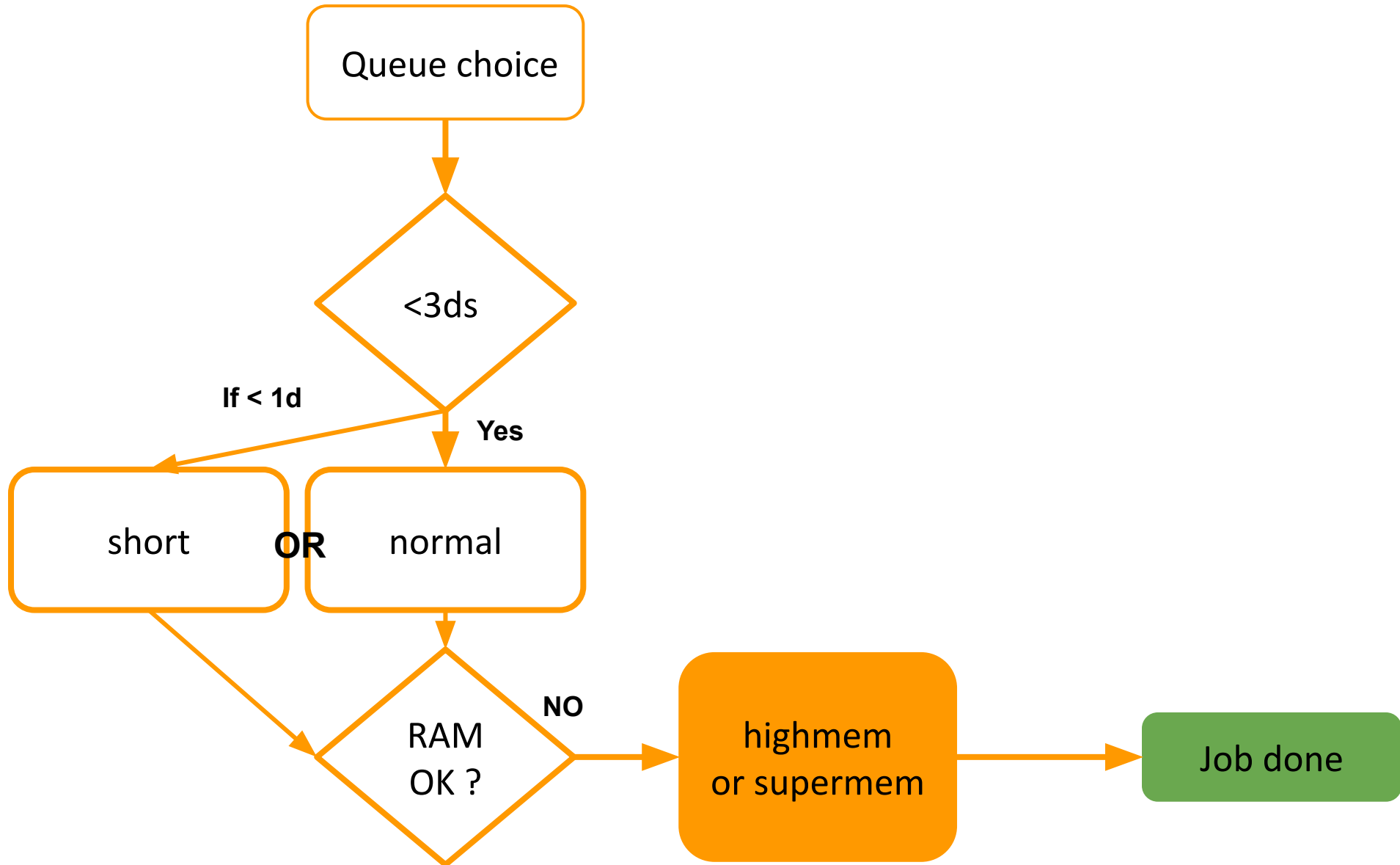
How do I choose the partition?



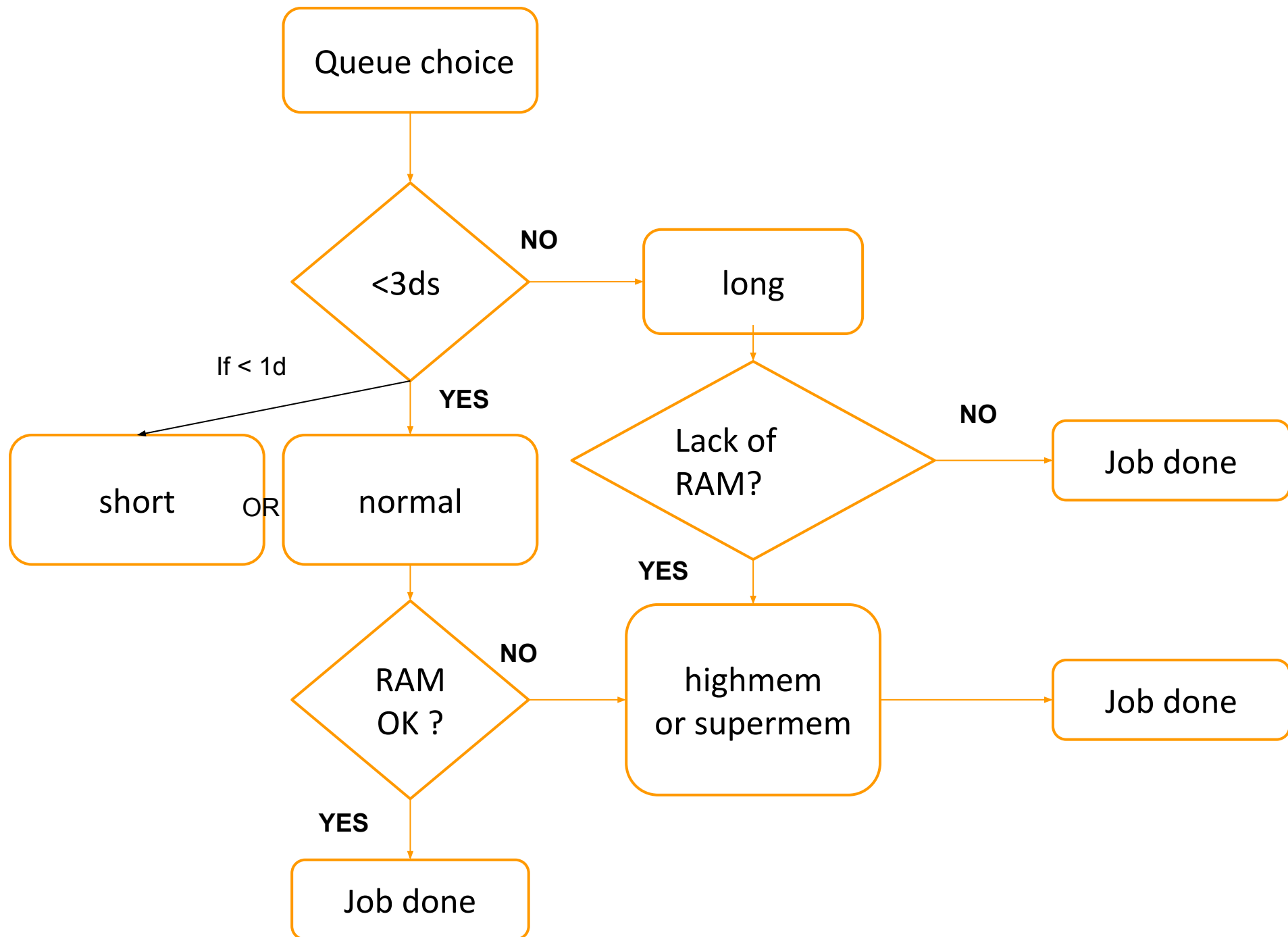
How do I choose the partition?



How do I choose the queue?



How do I choose the queue?



- **1 Master node**



bioinfo-master.ird.fr

Role :

- Launch and prioritize jobs on computing nodes
- Accessible from the Internet

- **27 computing nodes**



nodeX

X : 0..26



Role :

- Used by the master to execute jobs
- Not accessible from the Internet

- **3 NAS servers**



Bioinfo-nas.ird.fr
(nas)

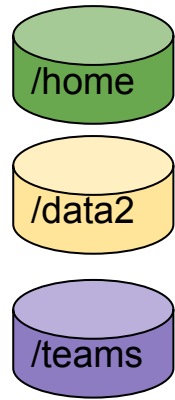
Bioinfo-nas2.ird.fr
(nas2)

Bioinfo-nas3.ird.fr
(nas3)

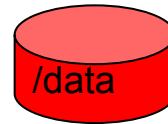
Role :

- Store users data
- Accessible from the Internet
- To transfer data : *via filezilla or scp*

cluster i-Trop disk partitions



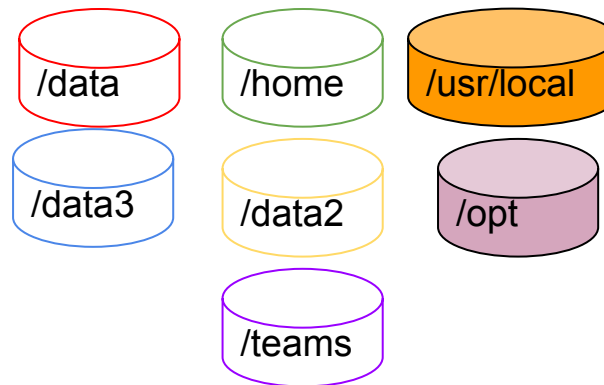
bioinfo-nas.ird.fr



bioinfo-nas2.ird.fr

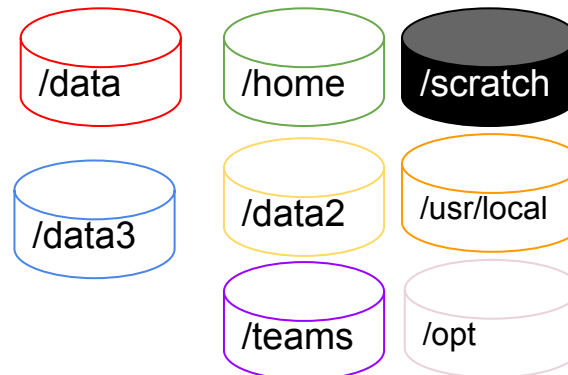


bioinfo-nas3.ird.fr



bioinfo-master.ird.fr

**Virtual links to the
other servers
partitions**



25 nodes



Connection
to
bioinfo-mas
ter.ird.fr
and
resources
reservation

Step 1



Creation of
the analyses
folder in the
/scratch of
the node

Step 2
mkdir



Practice

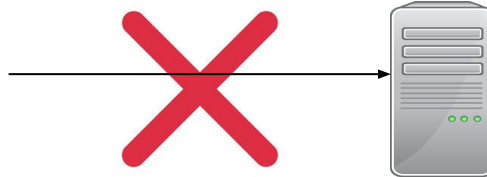
Step 2:qrsh, partition

2

Go to the [Practice2](#) of the github



PC/MAC

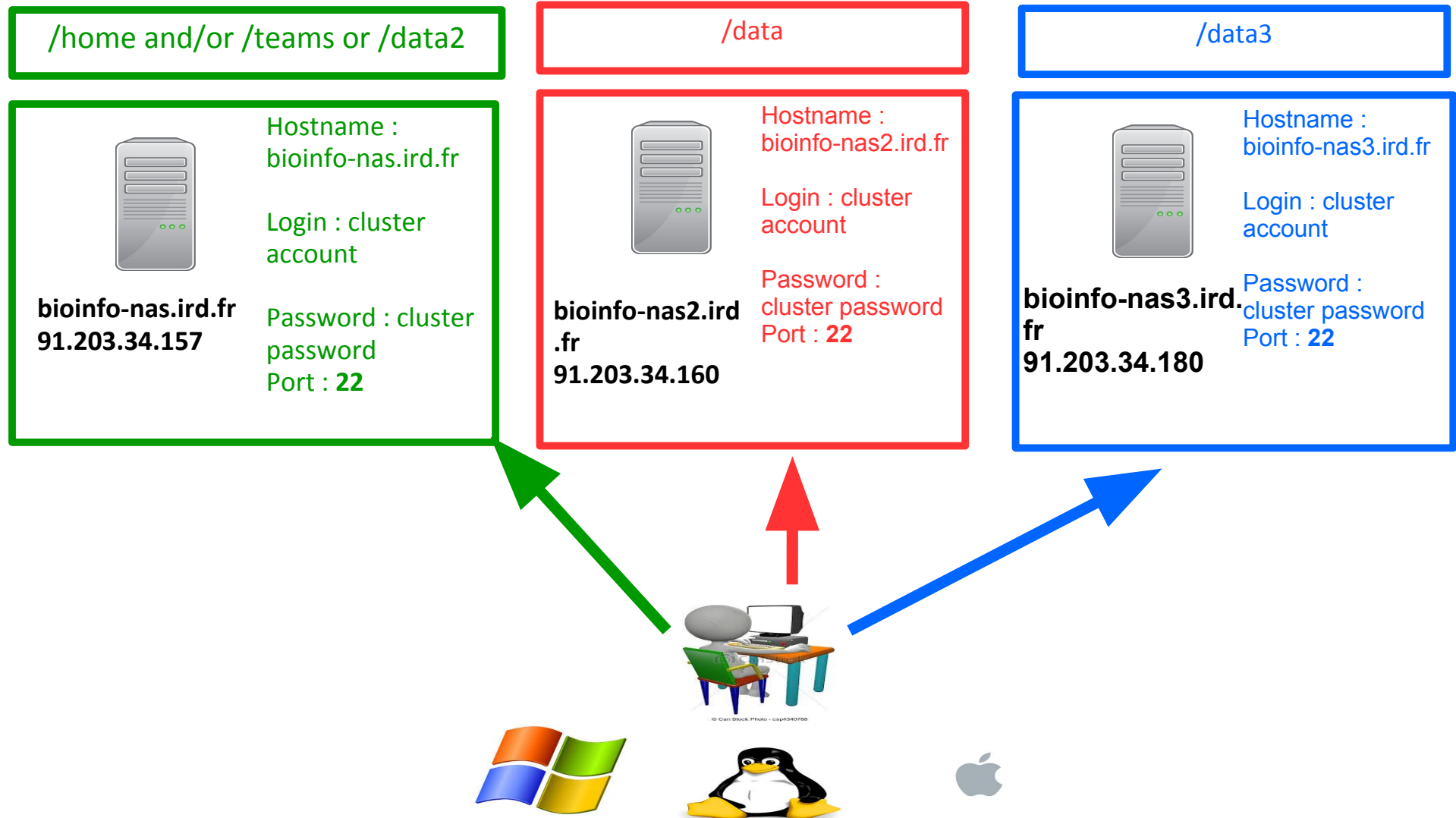


**direct transfer
via filezilla
forbidden**



**bioinfo-master.ird.fr
91.203.34.148**

Data transfer on i-Trop cluster



Analyses steps of the cluster

Connection
to
bioinfo-mas
ter.ird.fr
and
resources
reservation

Step 1



Creation of
the analyses
folder in the
/scratch of
the node

Step 2



Data
transfer
from your
PC/MAC to
the nas
servers

Step 3



Copy your data from your PC/MAC to the nas serve if they are not on the cluster



Practice

Step 3: filezilla

3

Go to the [Practice3](#) of the github

- Copy between 2 remote servers :

```
scp -r source destination
```

- Syntax if the source is remote :

```
scp -r server_name:/path/file_to_copy local_folder
```

- Syntax if the destination is remote :

```
scp -r /path/file_to_copy server_name:/path/remote_folder
```

Ex: `scp -r nas:/home/tando/folder/ /scratch/tando/`

Analyses steps of the cluster

Connection
to
bioinfo-mas
ter.ird.fr
and
resources
reservation

Step 1



Creation of
the analyses
folder in the
/scratch of
the node

Step 2



Data
transfer
from your
PC/MAC to
the nas
servers

Step 3



Data
transfer
from the
nas servers
to the
/scratch of
the node

Step 4
scp



Practice

Step 4: scp to nodes

4

Go to the [Practice4](#) of the github

- Allow to choose the version of software you want to use
- 2 types of softwares :
 - bioinfo : includes all the bioinformatics softwares (example BEAST)
 - system : includes all the system softwares(example JAVA)
- Overcome the environment variables

➤ 5 types of commands :

- See the available modules :
module avail
- Obtain infos on a particular module:
module whatis + module name
- Load a module :
module load + modulename
- List the loaded module :
module list
- Unload a module :
module unload + modulename
- Unload all the modules :
Module purge

Analyses steps of the cluster

Connection
to
bioinfo-mas
ter.ird.fr
and
resources
reservation

Step 1

Creation of
the analyses
folder in the
/scratch of
the node

Step 2

Data
transfer
from your
PC/MAC to
the nas
servers

Step 3

Data
transfer
from the
nas servers
to the
/scratch of
the node

Step 4

Load
softwares
with
modules
environment

Step 5
module



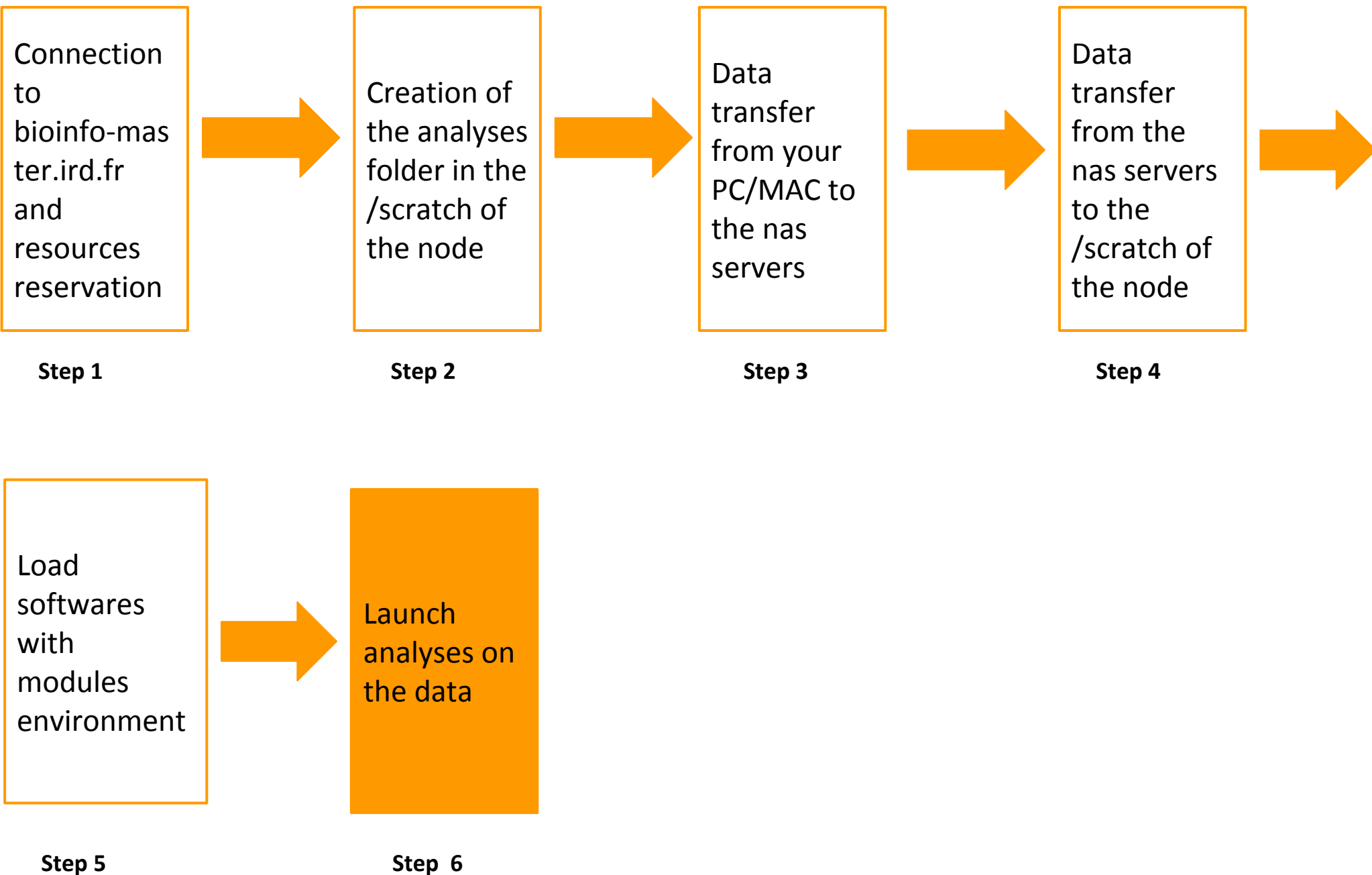
Practice

Step 5: module environment

5

Go to the [Practice5](#) of the github

Analyses steps of the cluster



Commande	Description	Exemple
<code>srun --time=0X:00 --pty bash -i</code>	Interactive way to connect to a node for X minutes	<code>srun --time=02:00:00 --pty bash -i</code> Connection for 2h
<code>salloc --time=0X:00</code>	Allocate one or several nodes for a later use	<code>Salloc -N 2 --p short --time=05:00</code>
<code>sbatch</code>	Launch a analyses in backkground via a script	<code>sbatch script.sh</code>
<code>sinfo</code>	Informations on partitions	<code>sinfo</code>
<code>sinfo -N l</code>	Informations on nodes of the partitions	<code>sinfo -N l</code>
<code>squeue</code>	Infos on all jobs	<code>squeue -u tando</code>
<code>scontrol show job <job_id></code>	Infos on the active job <job_id>	<code>scontrol show job 1029</code>

Options	Description	Exemple
<code>--job-name=<name></code>	Name the job	<code>sbatch --job-name=tando_blast</code>
<code>-p <partition></code>	Choose a partition	<code>sbatch -p highmem</code>
<code>--odelist=<nodeX></code>	Choisir a particular node	<code>Sbatch -p normal --odelist=node14</code>
<code>-n <nbre_cpus></code>	Launch with several cores	<code>srun -n 4</code>
<code>--mail-user=<emailaddress></code>	Send a email	<code>sbatch --mail-user=ndomassi.tando@ird.fr</code>
<code>--mail-type=<event></code>	Send a email when : END: end of the job FAIL: abortion BEGIN: beginning of job	<code>Sbatch ---mail-type=BEGIN</code>
<code>--workdir=[dir_name]</code>	Precise the working directory	<code>sbatch s--workdir=/scratch/tando script.sh</code>

- Load the software version to launch
- Launch the data analysis

```
$~ command <options> <arguments>
```

With *command*: the command to launch

- Execute a bash command via qsub
- Launch the command from a node
- We use:

```
$~ srun <options> <command>
```

With *command*: the command to launch



Practice

Step6: launch the analysis

6

Go to the [Practice6](#) of the github

- Copy between 2 remote servers :

```
scp source destination
```

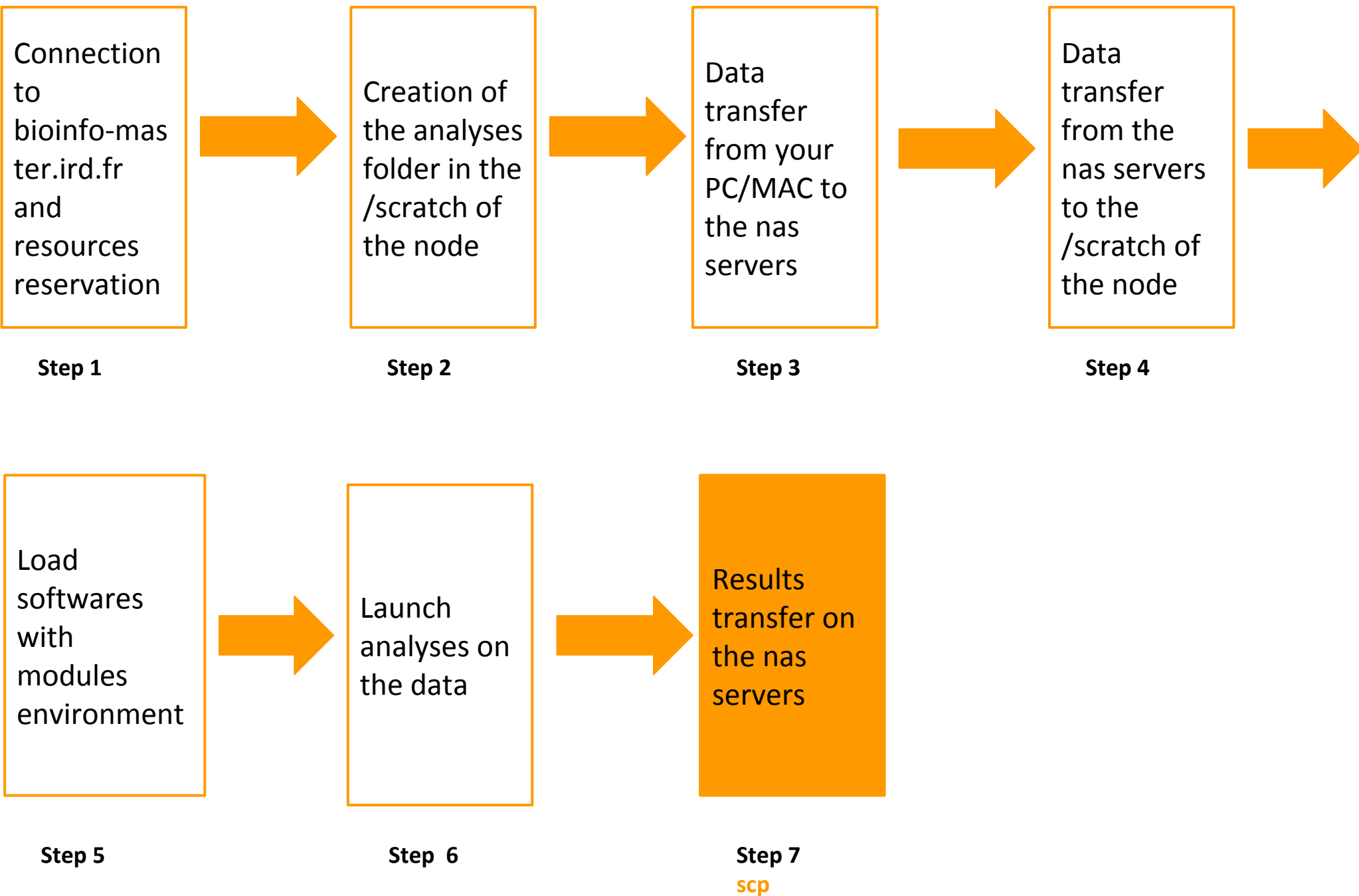
- Syntax if the source is remote :

```
scp server_name:/path/file_to_copy local_folder
```

- Syntax if the destination is remote :

```
scp /path/file_to_copy server_name:/path/remote_folder
```

Analyses steps of the cluster





Practice

Step 7: Retrieve the results

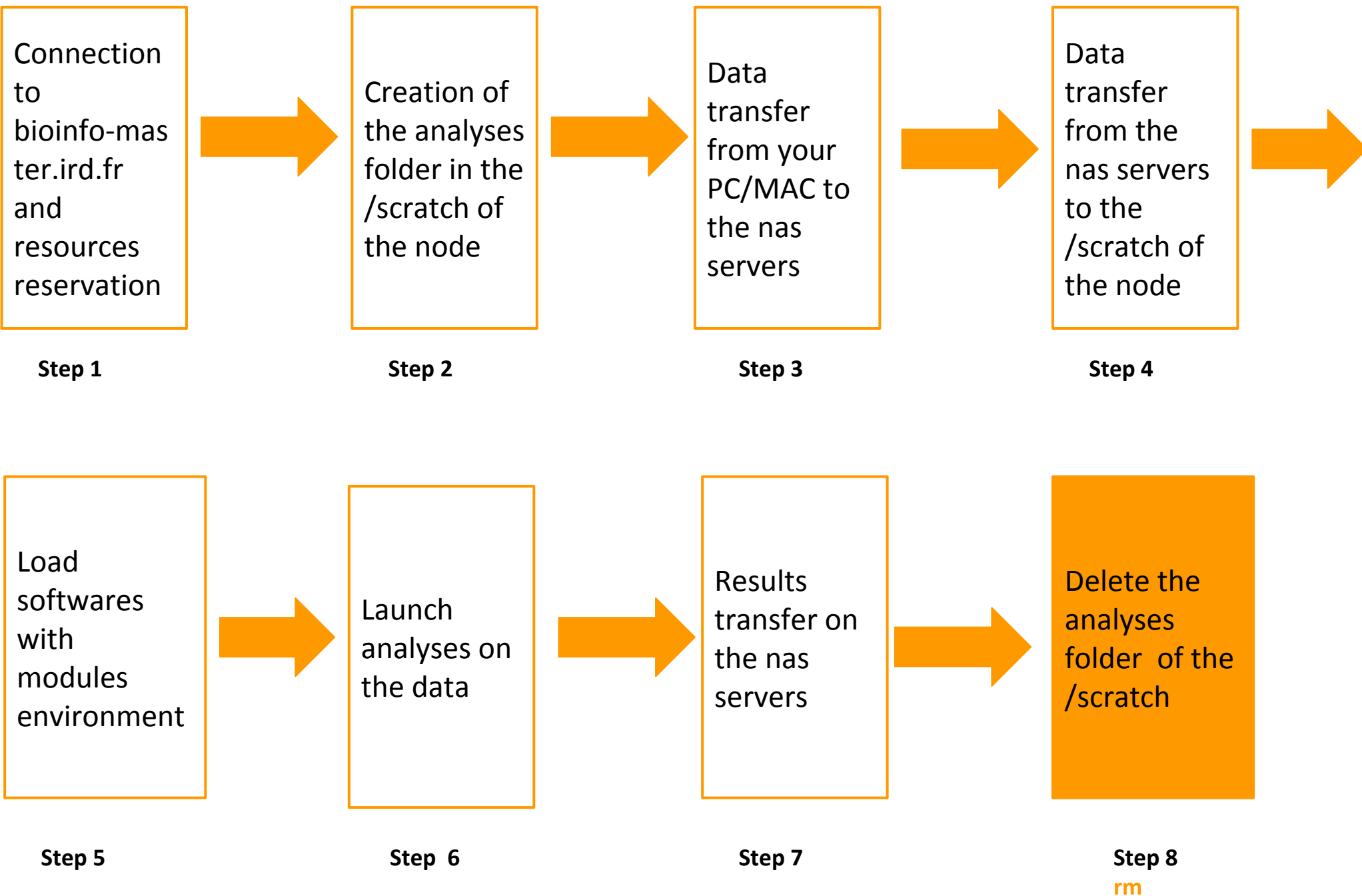
7

Go to the [Practice7](#) of the github

- Scratch= temporary spaces
- Verify that the copy is OK before
- Use rm command

```
cd /scratch  
rm -rf nom_rep
```


Analyses steps of the cluster





Practice

Step8: Data deletion

8

Go to the [Practice8](#) of the github

Scripts to visualize/delete données temporary data

- Scripts location: /opt/scripts/scratch-scripts
- Visualize data on scratches: scratch_use.sh

```
sh /opt/scripts/scratch-scripts/scratch_use.sh
```

- Delete data on scratches: clean_scratch.sh

```
sh /opt/scripts/scratch-scripts/clean_scratch.sh
```

BONUS

LAUNCH A JOB

- Scheduler choose resources automatically
- Use up to 24 cores at the same time
- Possibility to configure this choice
- Jobs launch in background
 - possibility to turn off your PC/MAC
 - automatic results retrieving

- Execute a script via rm
- Use:

```
$~ sbatch script.sh
```

with `script.sh` : the name of the script

Options	Description	Exemple
<code>--job-name=<name></code>	Name the job	<code>sbatch --job-name=tando_blast</code>
<code>-p <partition></code>	Choose a partition	<code>sbatch -p highmem</code>
<code>--odelist=<nodeX></code>	Choisir a particular node	<code>Sbatch -p normal --odelist=node14</code>
<code>-n <nbre_cpus></code>	Launch with several cores	<code>srun -n 4</code>
<code>--mail-user=<emailaddress></code>	Send a email	<code>sbatch --mail-user=ndomassi.tando@ird.fr</code>
<code>--mail-type=<event></code>	Send a email when : END: end of the job FAIL: abortion BEGIN: beginning of job	<code>Sbatch ---mail-type=BEGIN</code>
<code>--workdir=[dir_name]</code>	Precise the working directory	<code>sbatch s--workdir=/scratch/tando script.sh</code>

First part of the script (in green): sge execution options with the key word #SBATCH

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

```
##### Configuration SLURM#####  
## Name of the job:  
#SBATCH --job-name=test  
## Name of the output file:  
#SBATCH --output=res.txt  
## Number of tasks  
#SBATCH --ntasks=1  
## Execution Time Limit  
#SBATCH --time=10:00  
#####
```

In the 2nd part of the script: the command to execute

```
#####Partie exécution des commandes #####
```

```
nom_variable1="valeur_variable1"  
nom_variable2="valeur_variable2"
```

```
sleep 30  
hostname
```



Practice

Launch a script with sge

9

Go to the [Practice9](#) of the github

If you use i-Trop Bioinformatics resources.

Thank you for citing with:

“The authors acknowledge the IRD itrop HPC (South Green Platform) at IRD montpellier
for providing HPC resources that have contributed to the
research results reported within this paper.

URL: <https://bioinfo.ird.fr/>- <http://www.southgreen.fr>”

- Include a budget for bioinformatics resources in your answer to projects funding
- A need in hard drives, renewal machines etc...
- Available quotations
- Contact bioinfo@ird.fr : help, needs definition, quotations...

Thank you for your attention !



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