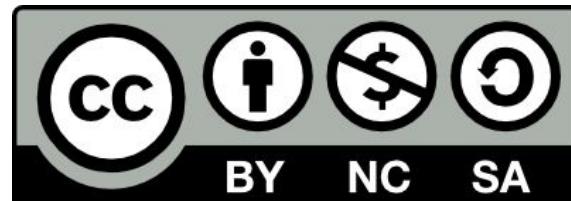




HPC cluster Initiation

www.southgreen.fr

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





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Systèmes d'information



Cluster certification in process

Provisioning of softwares and HPC ressources

Analysis software and IS development

Plateau bioinformatique

Help and support to IRD teams

Training to north and South

- 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/tutorials//cluster-itrop/hpchowto/>

- Slurm Tutorials:

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

ARCHITECTURE

A Cluster?

- 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

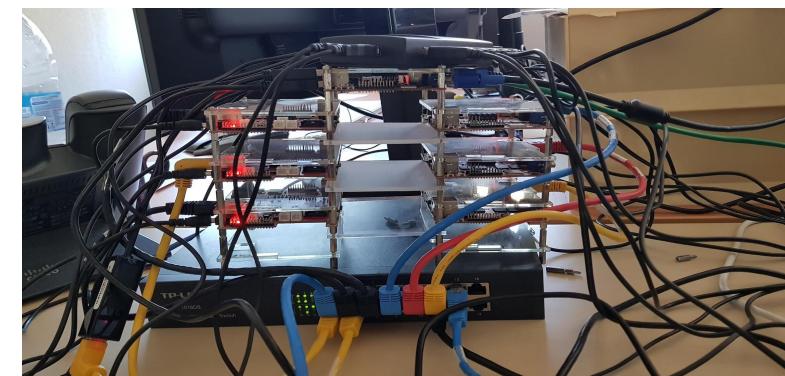
A cluster?

- A logical unit composed of several servers
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- A better ressources availability



A cluster?

- 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 ressources availability



Cluster components

COMPUTING



- **Master Node**

Handle resources and jobs priorities

- **Computing nodes**

Resources (CPU or RAM memory)

Cluster components

COMPUTING



STORAGE



- **Master Node**

Handle resources and jobs priorities

- **Computing nodes**

Resources (CPU or RAM memory)

- **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
- 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



Practice

Step 1: Connection, qhost

1

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

Analyses steps of the cluster

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



Step 1
salloc/srun ou
sbatch

Partitions

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 7 days	64 Go to 96 GB	12 to 24 cores
r900	Short Jobs max 7 days	32GB	16 cores /scratch 117GB
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

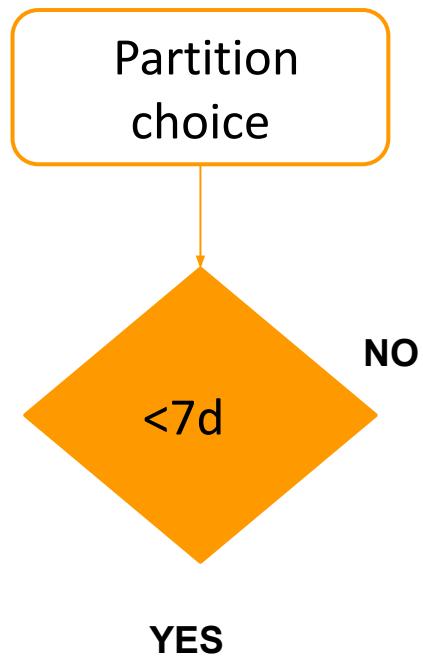
*Request to do with arguments

Particular case : gpu partition

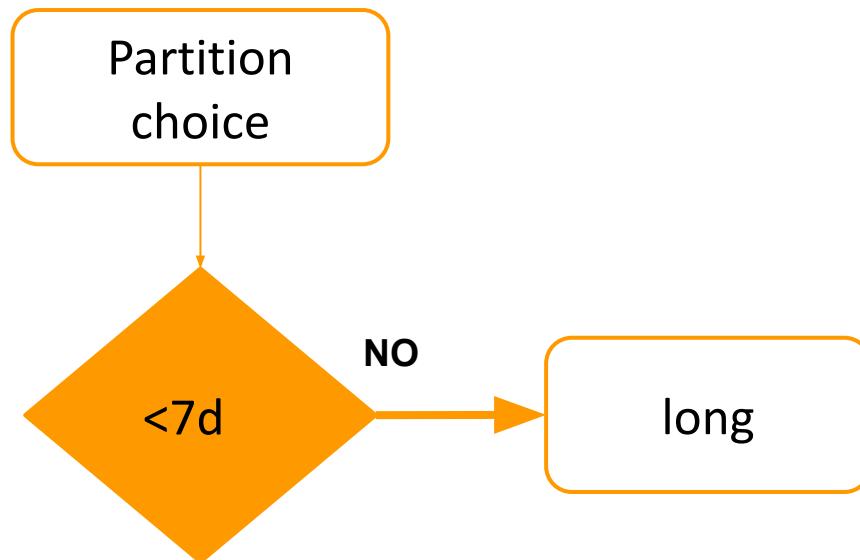
- Partition to work on GPUs processors : basecalling, MiniOn etc..
- Restricted access to gpu_account group
- Request access with arguments to do here:

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

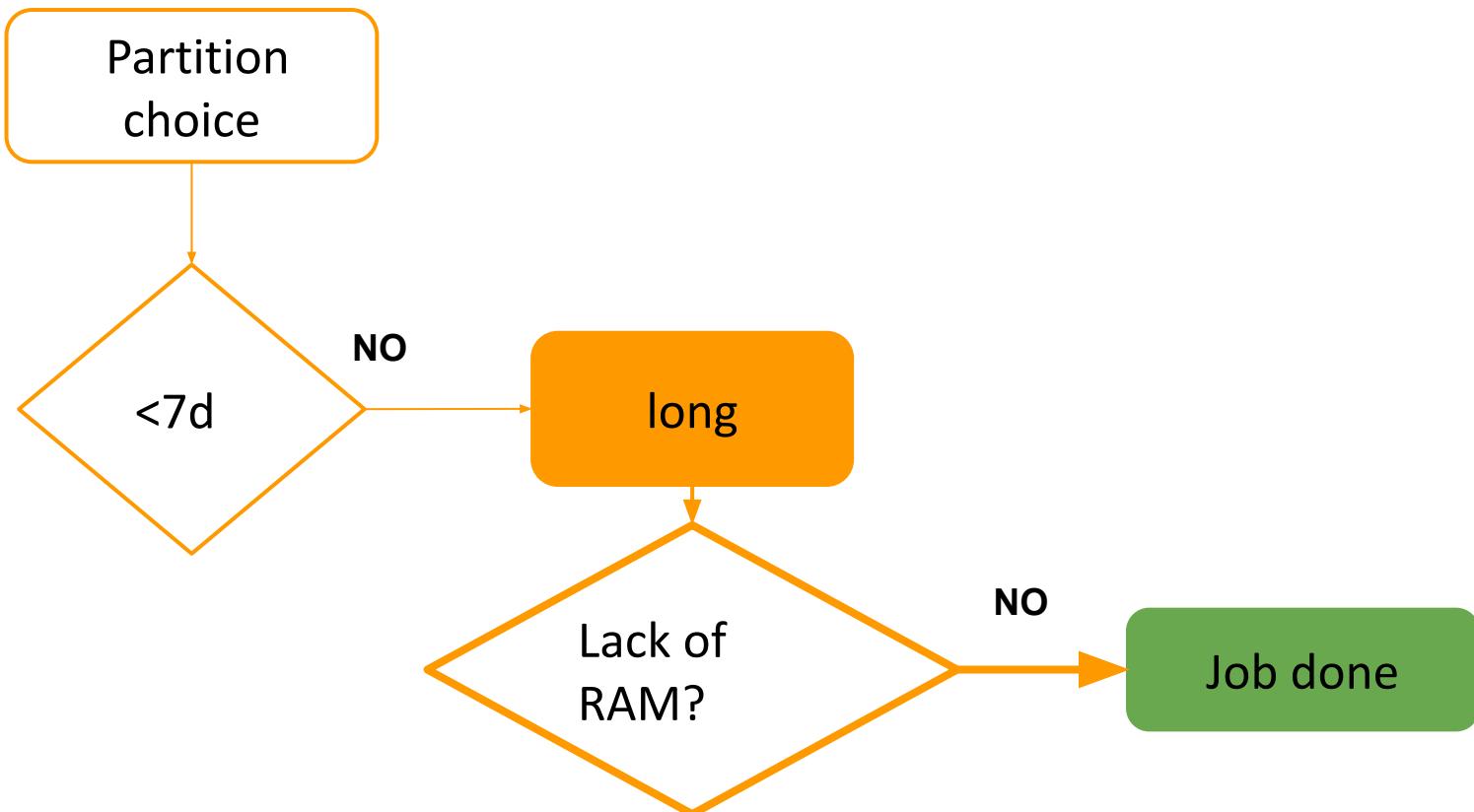
How do I choose the partition?



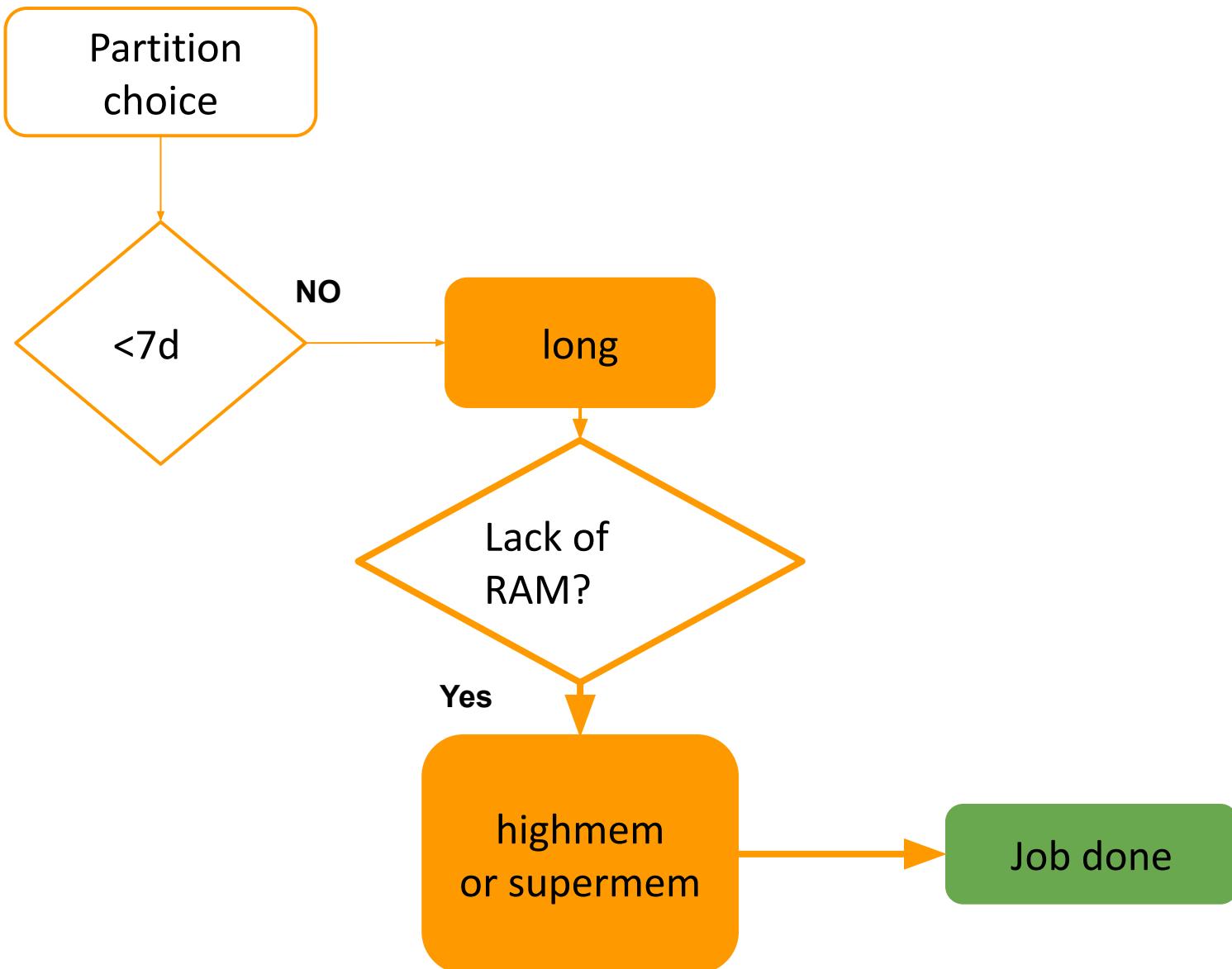
How do I choose the partition?



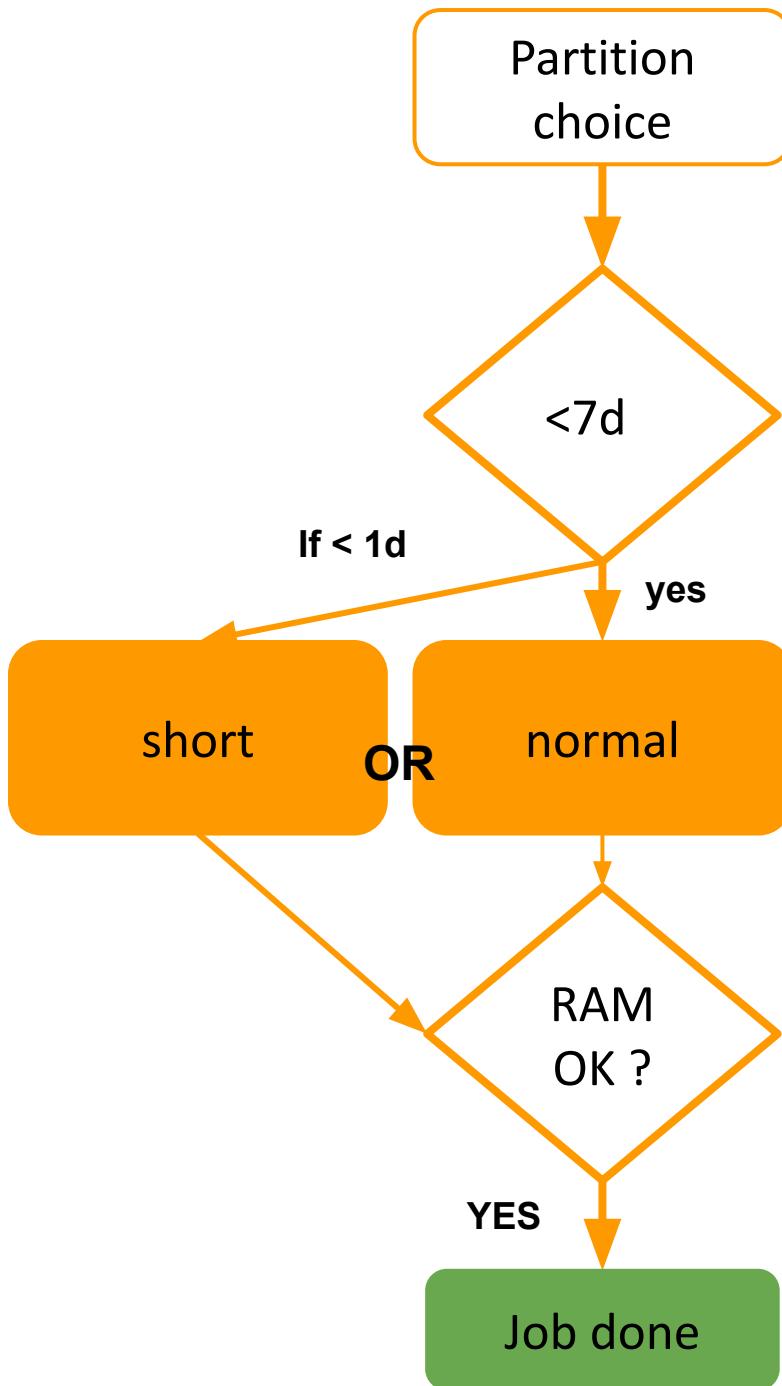
How do I choose the partition?



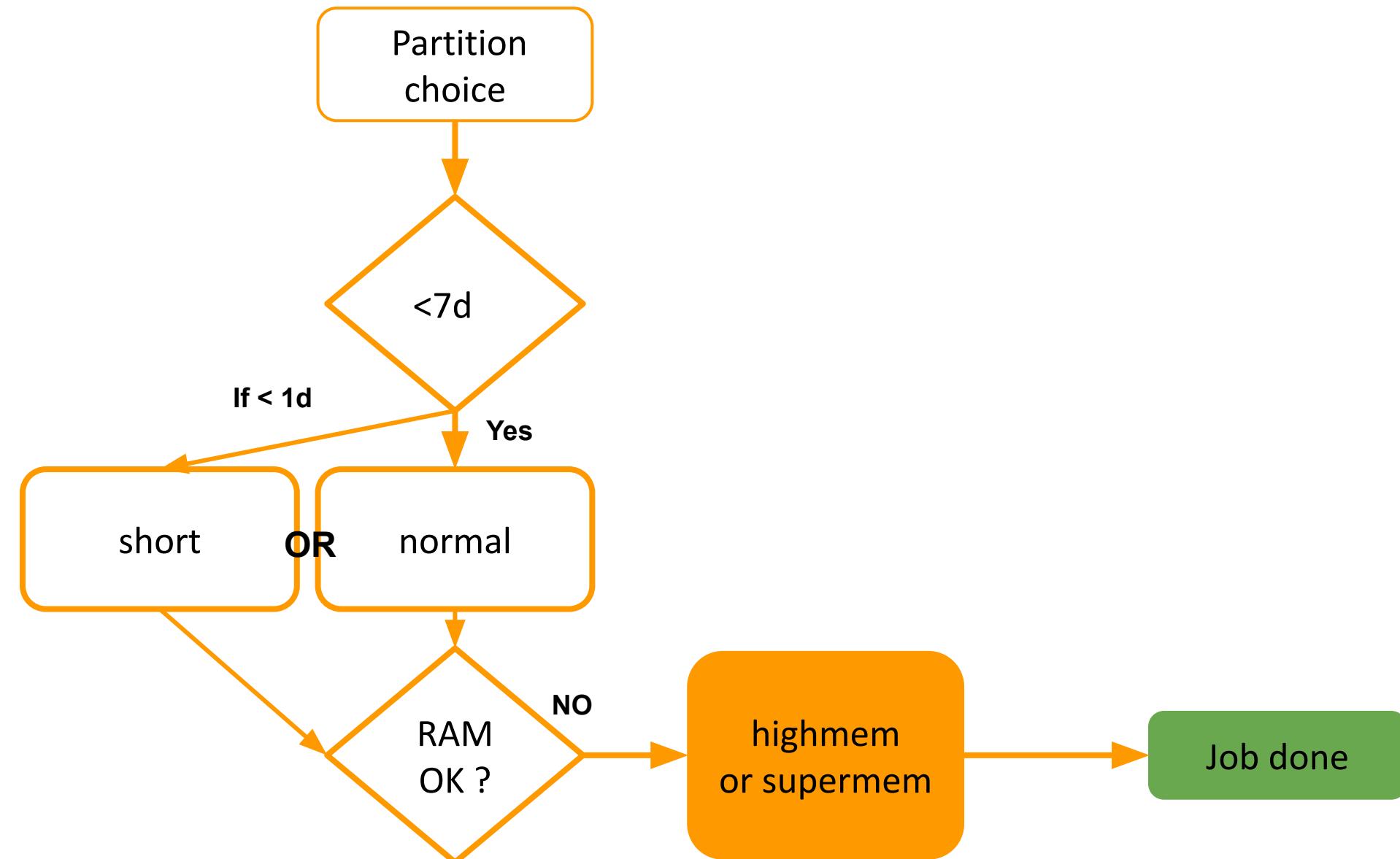
How do I choose the partition?



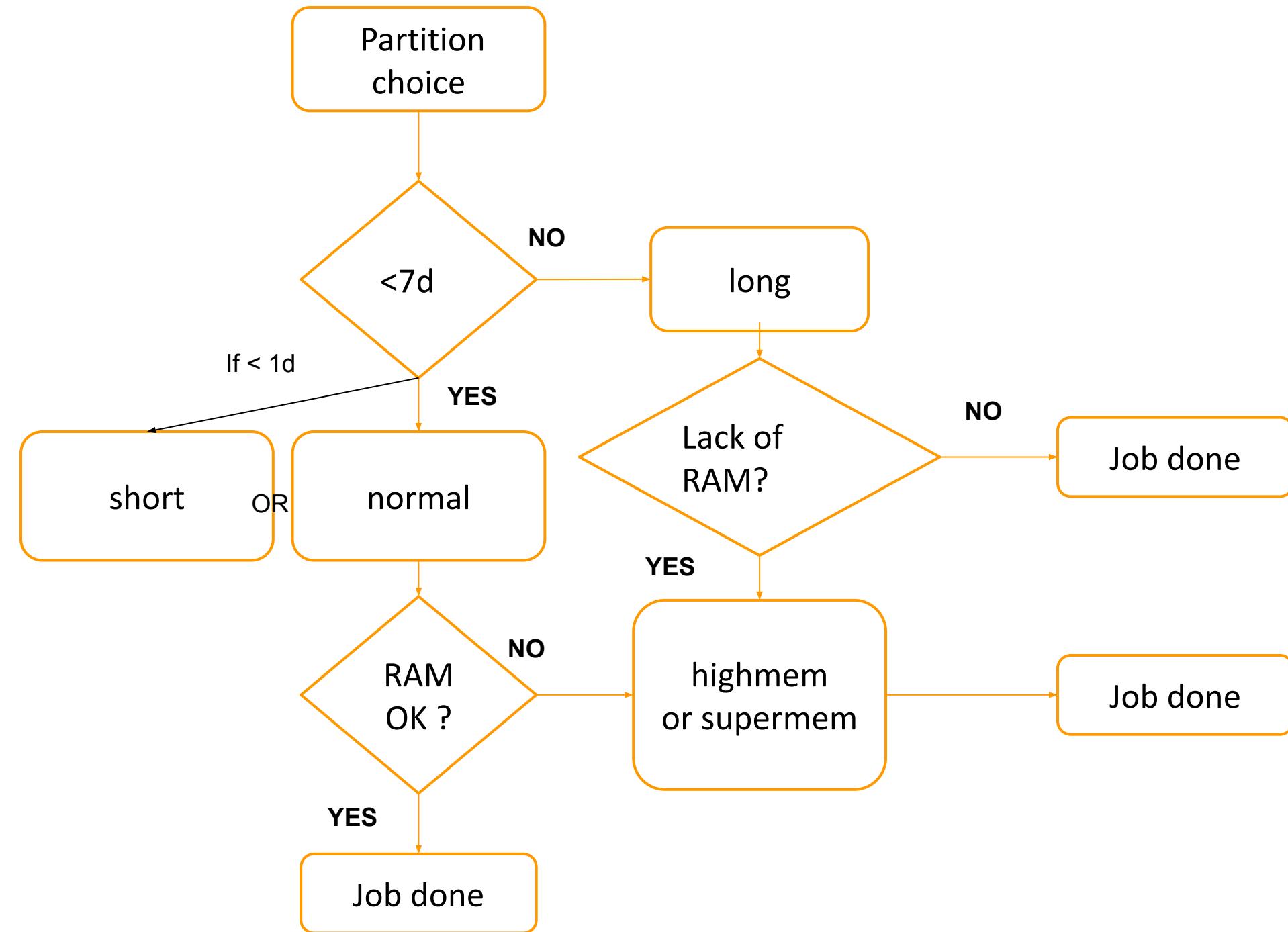
How do I choose the partition?



How do I choose the partition?



How do I choose the partition?



- **1 Master node**

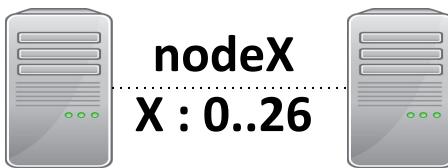


bioinfo-master.ird.fr

Role :

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

- **27 computing nodes**



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

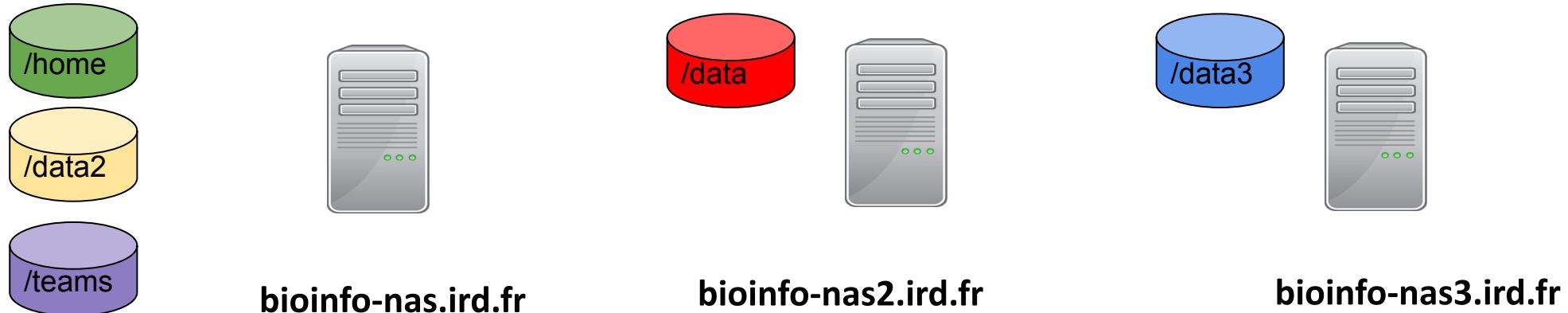
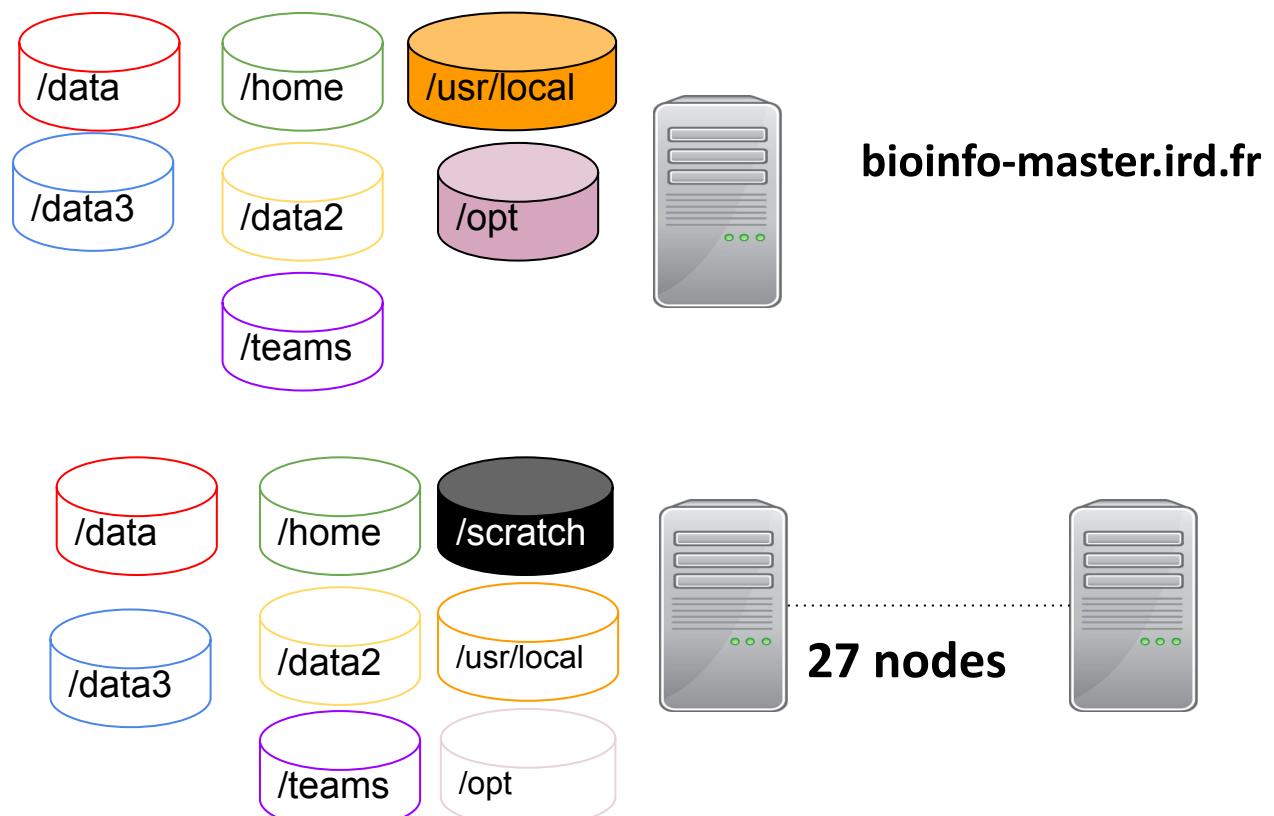


Illustration legend:

Local Hard drives in full cylinders

**Virtual links to physical hard drives
(empty cylinders)**



Analyses steps of the cluster

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



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

Step 1

Step 2
mkdir



Practice

Step 2:qrsh, partition

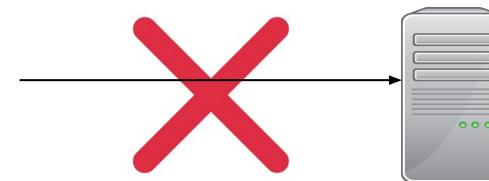
2

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

Data transfer on i-Trop cluster



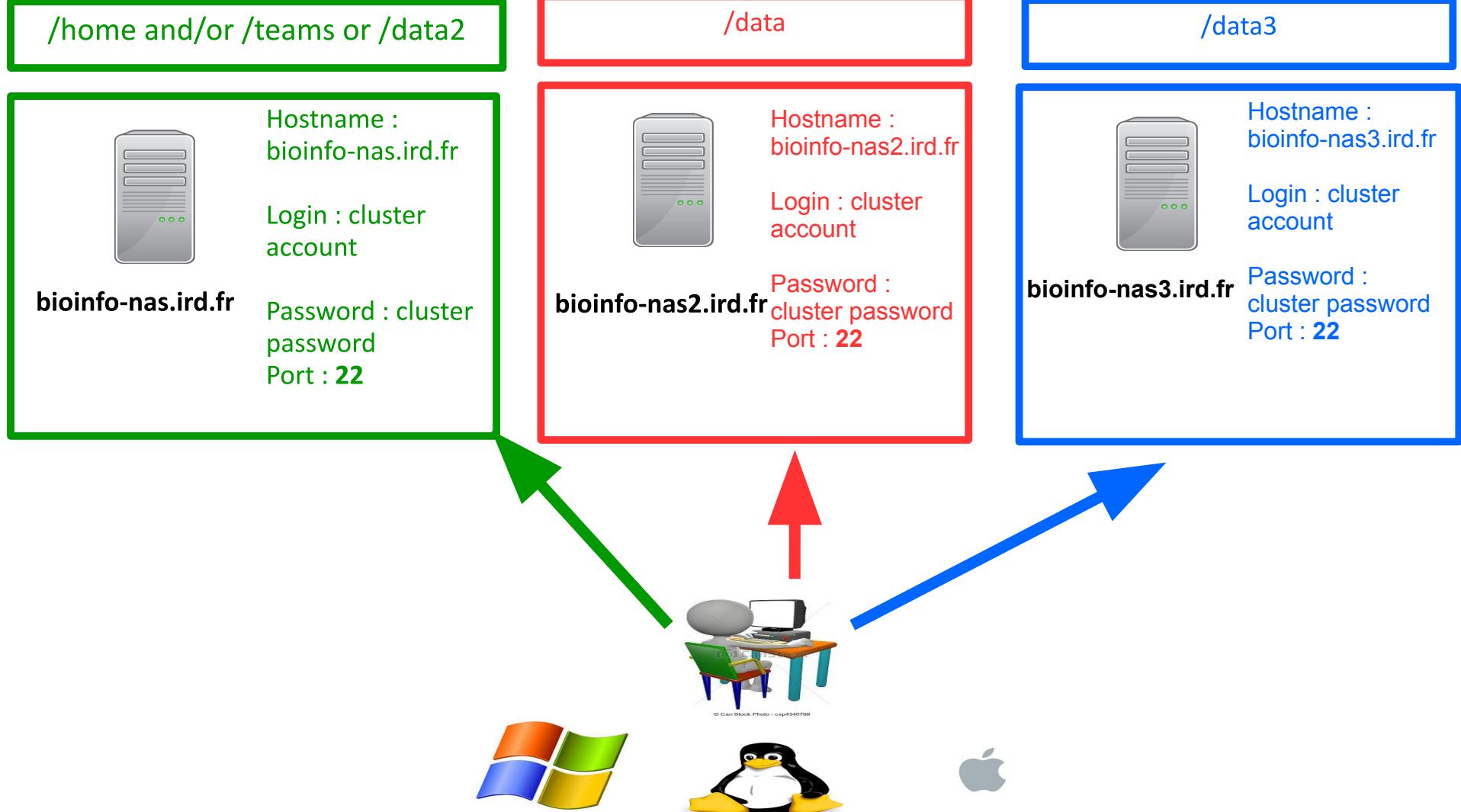
PC/MAC



bioinfo-master.ird.fr

**direct transfer
via filezilla
forbidden**

Data transfer on i-Trop cluster



Analyses steps of the cluster

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



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



Data
transfer
from your
PC/MAC to
the nas
servers

Step 1

Step 2

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 with scp

- Copy between 2 remote servers :

```
scp -r source destination
```

- Syntax if the source is remote :

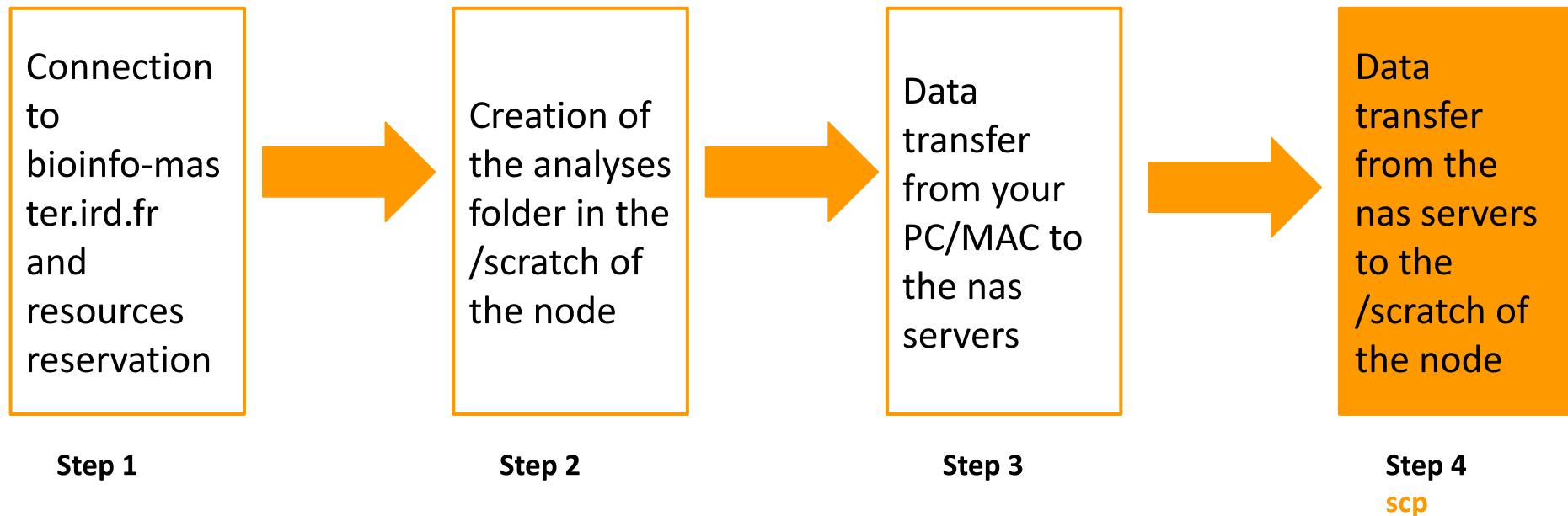
```
scp -r server_name:/path/file_to_copy local_folder
```

- 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





Practice

Step 4: scp to nodes

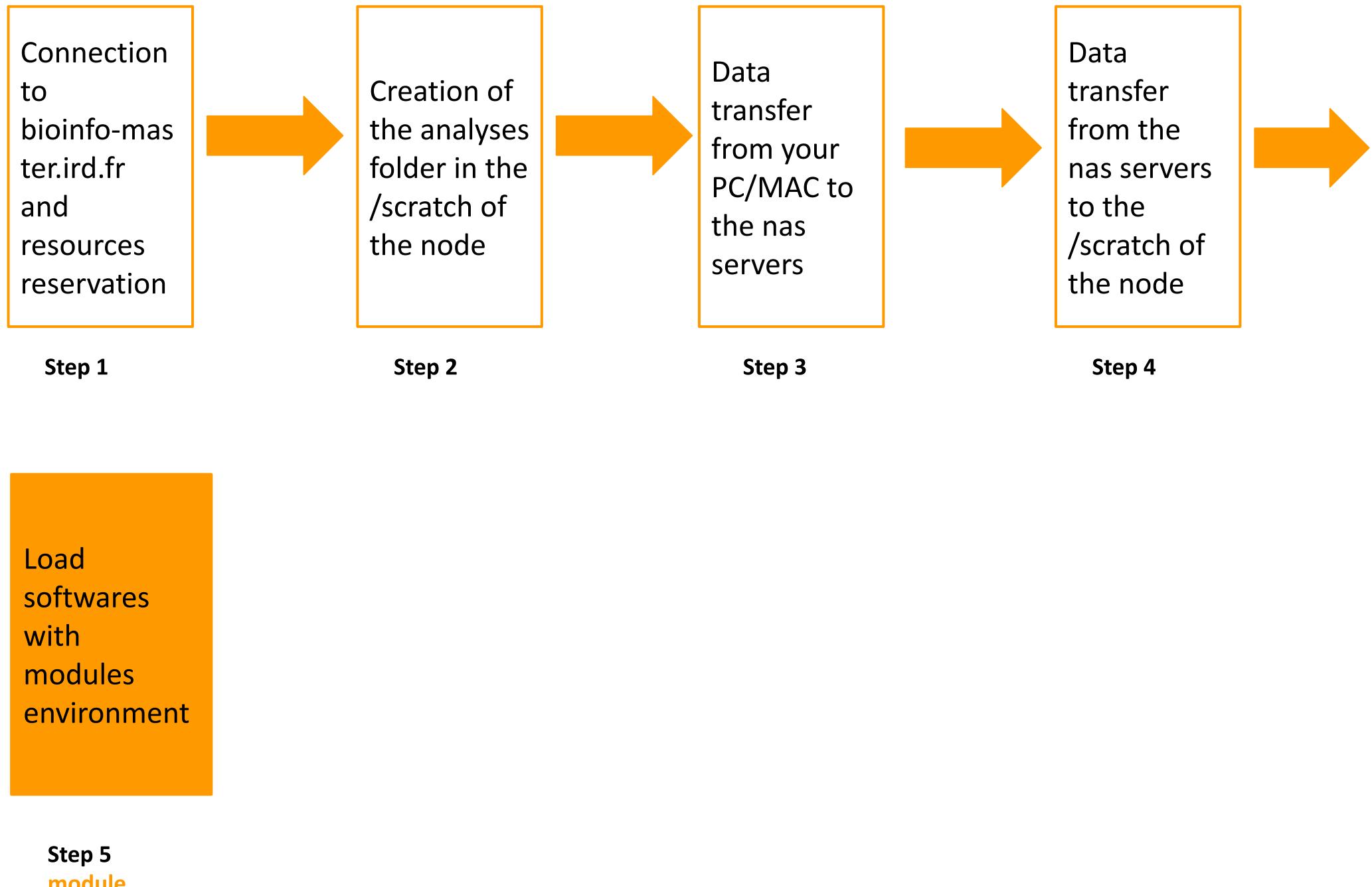
4

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





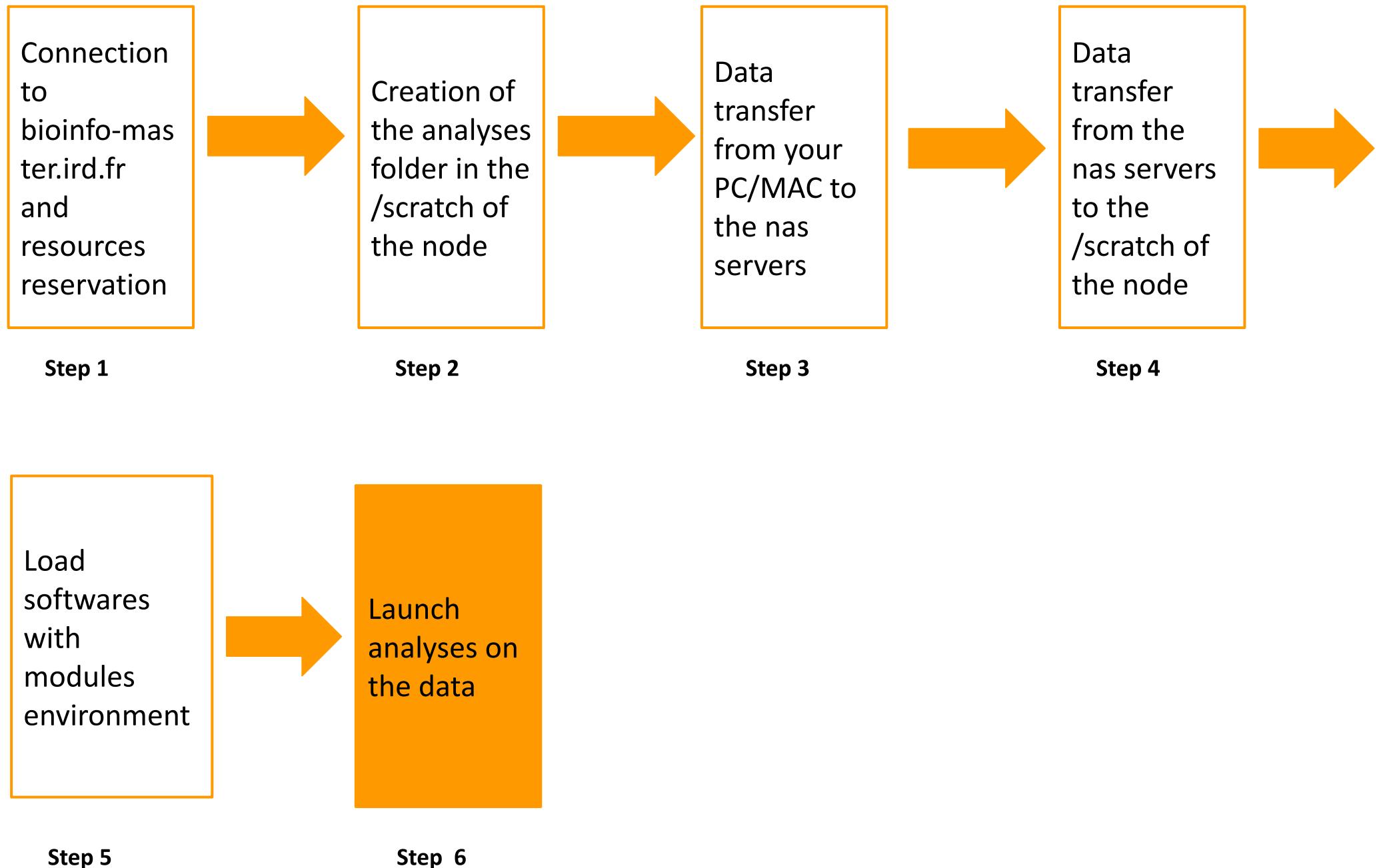
Practice

Step 5: module environment

5

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

Analyses steps of the cluster



Launch a command from the prompt

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

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

With *command*: the command to launch



Practice

Step6: launch the analysis

6

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

Transfer your results to the nas servers

- Copy between 2 remote servers :

```
scp -r source destination
```

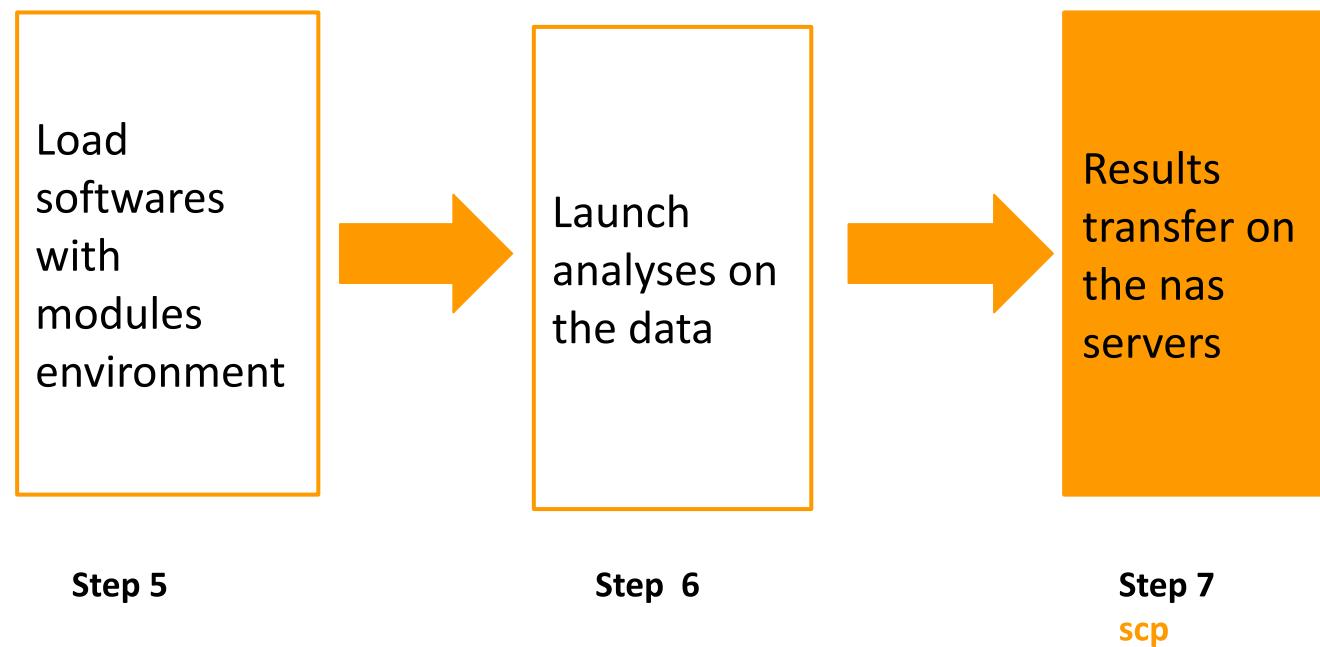
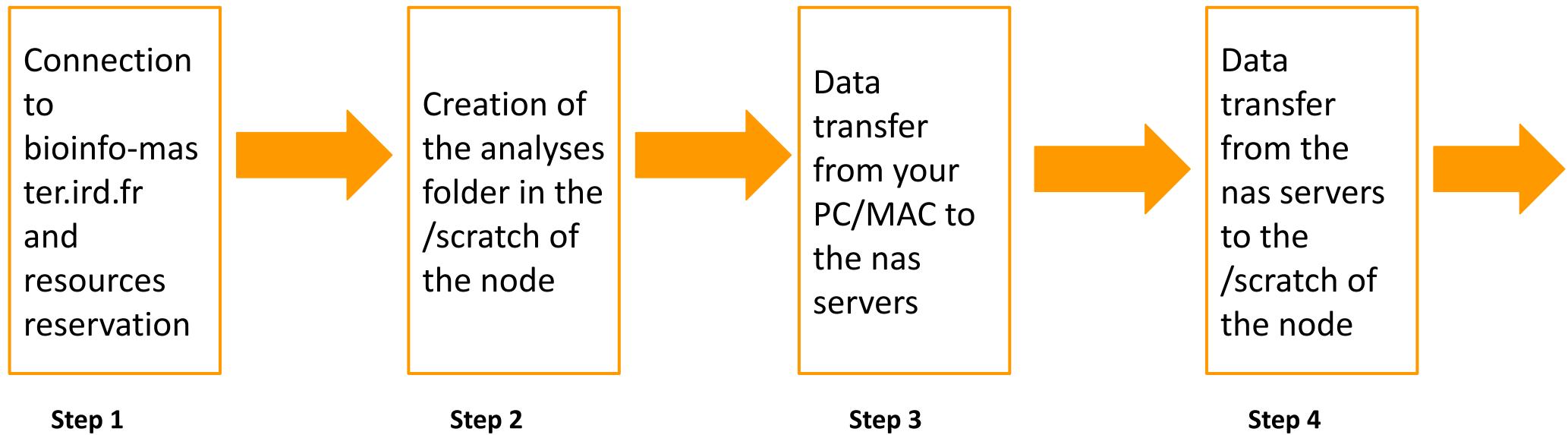
- Syntax if the source is remote :

```
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
```

Analyses steps of the cluster





Practice

Step 7: Retrieve the results

7

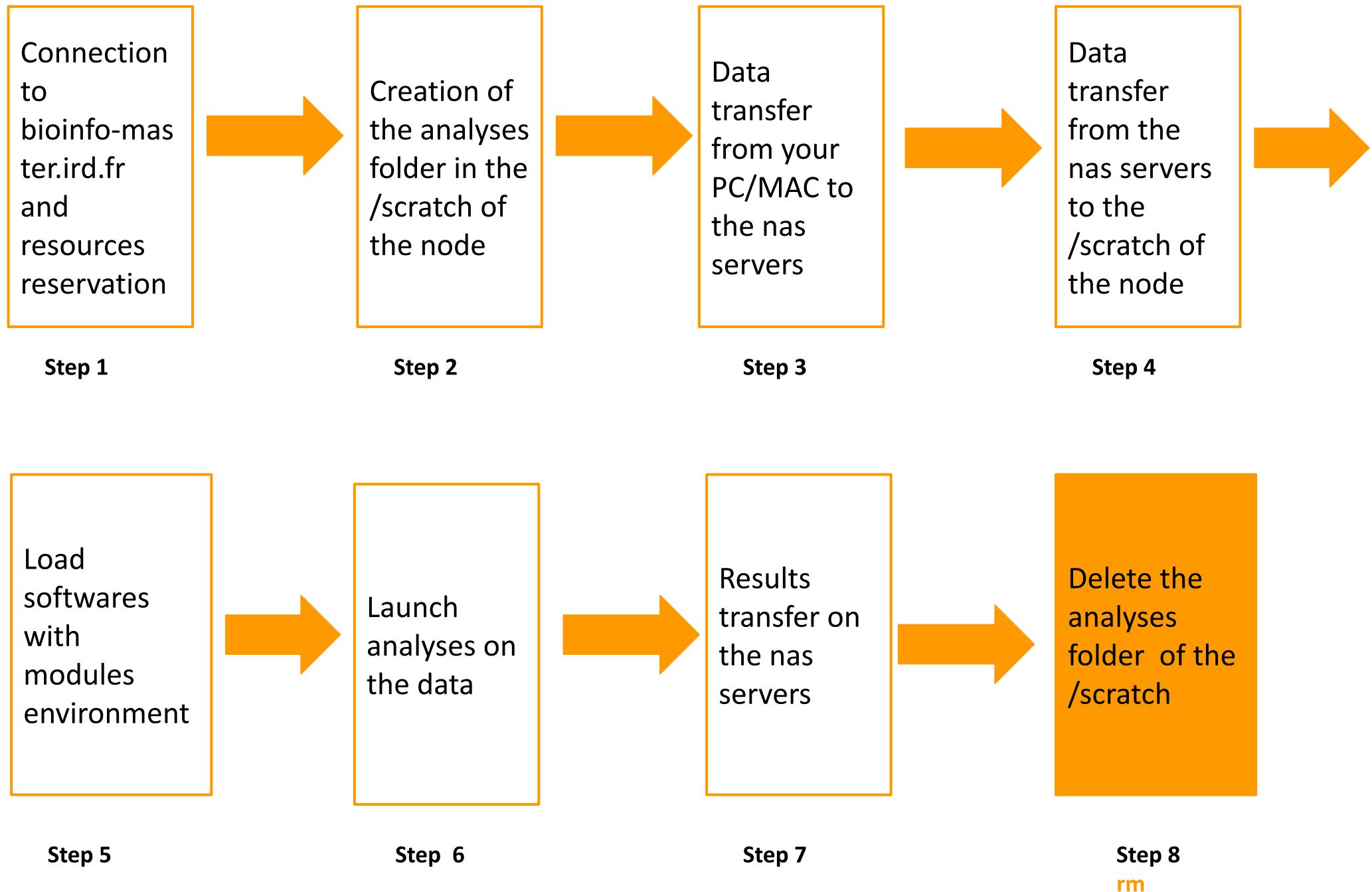
Go to the [Practice7](#) of the github

Delete results from scratchs

- 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 scratchs: scratch_use.sh

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

- Delete data on scratchs: clean_scratch.sh

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

Main Slurm commands

Commande	Description	Exemple
srun --time=0X:00 --pty bash -i	Interactive way to connect to a node for X minutes	srun --time=02:00:00 --pty bash -i Connection for 2h
sbatch	Launch analyses in background via a script	sbatch script.sh
sinfo	Informations on partitions	sinfo
scancel	Deletion of job with <job_id>	scancel 1029
squeue	Infos on all jobs	squeue -u tando
scontrol show job <job_id>	Infos on the active job <job_id>	scontrol show job 1029
sacct -j <job_id>	Infos on the finished job <job_id>	sacct -j 1029

More infos here: <https://southgreenplatform.github.io/tutorials//cluster-itrop/Slurm/#part-2>

Options of sbatch, srun, salloc commands

Options	Description	Exemple
--job-name=<name>	Name the job	sbatch --job-name=tando_blast
-p <partition>	Choose a partition	sbatch -p highmem
--nodelist=<nodeX>	Choose a particular node	sbatch -p normal --nodelist=node14
-n <nb_tasks>	Launch several instance of a command	srun -n 4
-c <nb_cpu_per_task>	Allocate the number of cpus per task	srun -n 4 -c 2 hostname
--mail-user=<emailaddress>	Send a email	sbatch --mail-user=ndomassi.tando@ird.fr
--mail-type=<event>	Send a email when : END: end of the job FAIL: abortion BEGIN: beginning of job ALL: all events	sbatch ---mail-type=BEGIN

BONUS

LAUNCH A JOB

Advantages

- 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

Launch a batch job

- Execute a script via Slurm
- Use:

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

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

Options of sbatch, srun, salloc commands

Options	Description	Exemple
--job-name=<name>	Name the job	sbatch --job-name=tando_blast
-p <partition>	Choose a partition	sbatch -p highmem
--nodelist=<nodeX>	Choose a particular node	sbatch -p normal --nodelist=node14
-n <nb_tasks>	Launch several instance of a command	srun -n 4
-c <nb_cpu_per_task>	Allocate the number of cpus per task	srun -n 4 -c 2 hostname
--mail-user=<emailaddress>	Send a email	sbatch --mail-user=ndomassi.tando@ird.fr
--mail-type=<event>	Send a email when : END: end of the job FAIL: abortion BEGIN: beginning of job ALL: all events	sbatch ---mail-type=BEGIN

Bash scripts syntax

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 sbatch

9

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

Satisfaction survey

Thank you to fill up the form at this URL:

<https://itrop-survey.ird.fr/index.php/562934?lang=fr>

Citations

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, renew machines etc...
- Available quotations
- Contact bioinfo@ird.fr : help, needs definition, quotations...

Thank you for your attention !



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