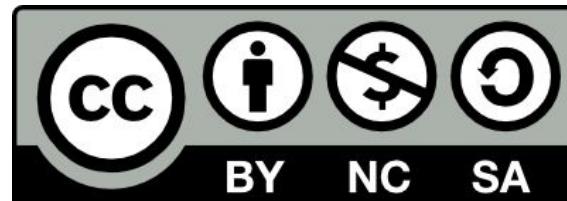




HPC cluster Initiation

www.southgreen.fr

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





Julie ORJUELA-
BOUNIOL¹, IE
Bioinformaticienne
25%

Ndomassi TANDO, IE
Administrateur système
100%
Animateur plateau

Aurore COMTE, IE
Bioinformaticienne
20%

Valérie NOEL, TCS
Bioinformaticienne
25%

Bruno GRANOUILLAG³, IE
Systèmes d'information
20%

Christine TRANCHANT-
DUBREUIL, IE
Bioinformaticienne
20%

Alexis DEREEPER², IE
Bioinformaticien
20%

**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/trainings/hpc/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

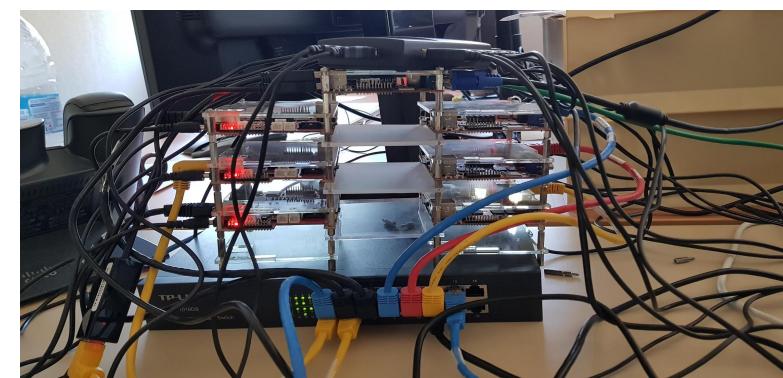
A cluster?

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



- **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**



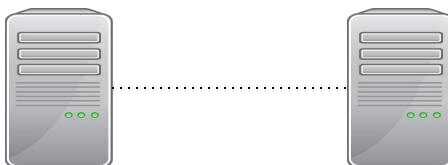
bioinfo-master.ird.fr

Role :

- Launch and prioritize jobs on computing nodes
- 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

- **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

Analyses steps of the cluster

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



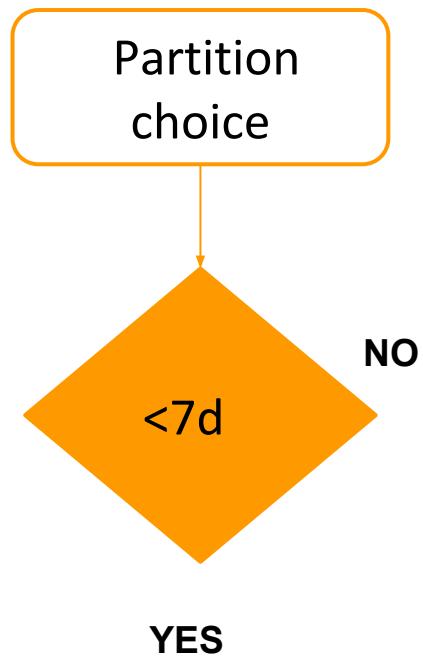
Step 1
salloc/srun
ou sbatch

Partitions

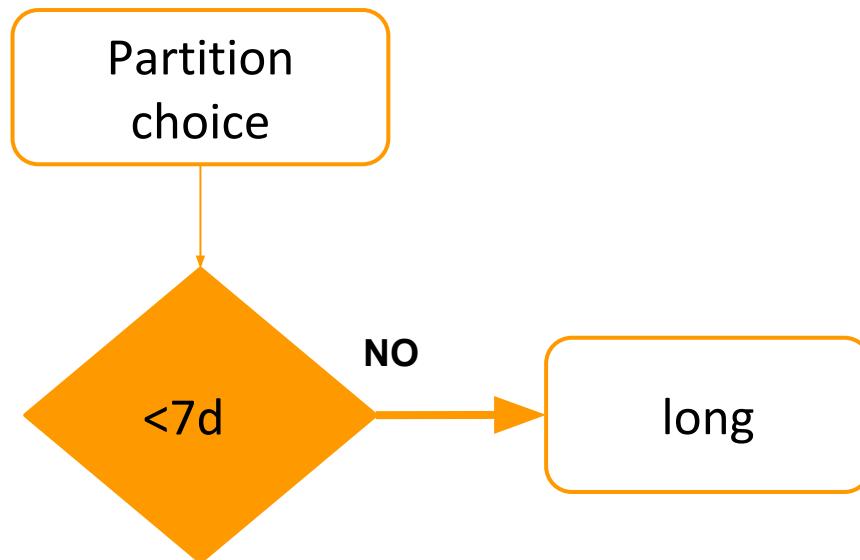
Partitions	Use	RAM on nodes	Core on nodes
short	Short Jobs < 1 day (higher priority, interactive jobs)	48 to 64 GB	12 cores
normal	Short Jobs max 7 days	64 Go to 96 GB	12 to 24 cores
long	45 days >long jobs > 3 days	48 GB	12 to 24 cores
highmem	Jobs with more memory needs	144 GB	12 to 24 cores
supermem	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

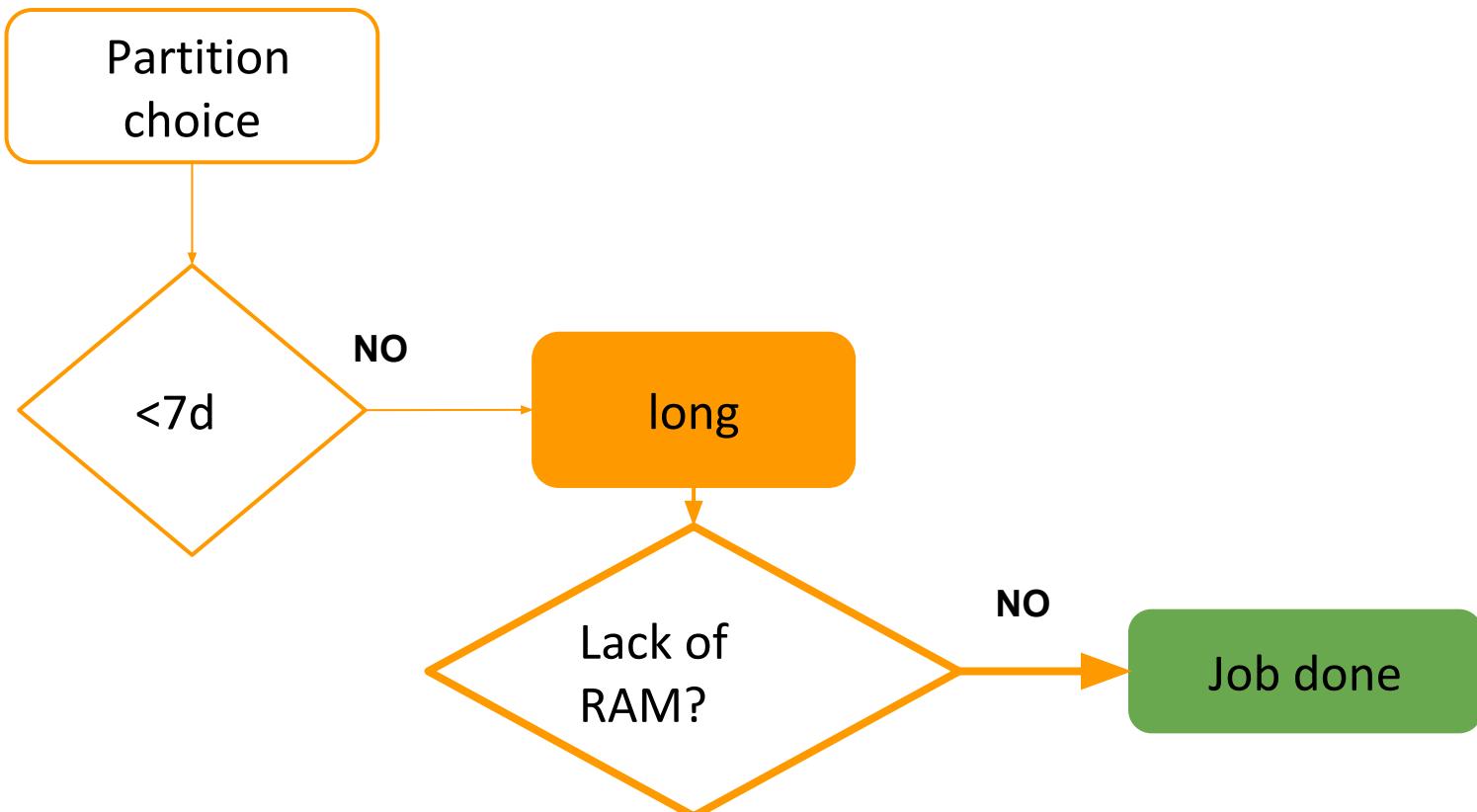
How do I choose the partition?



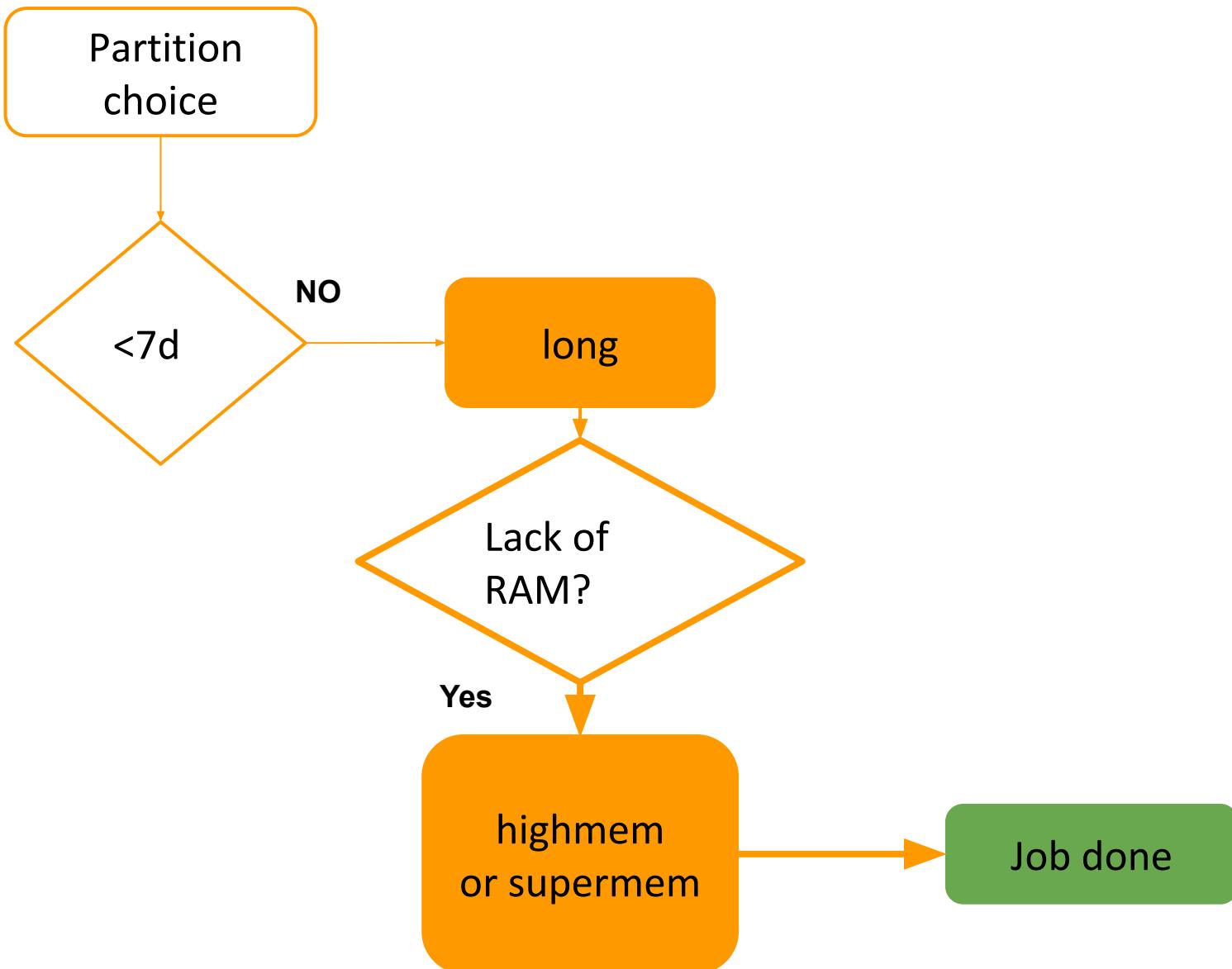
How do I choose the partition?



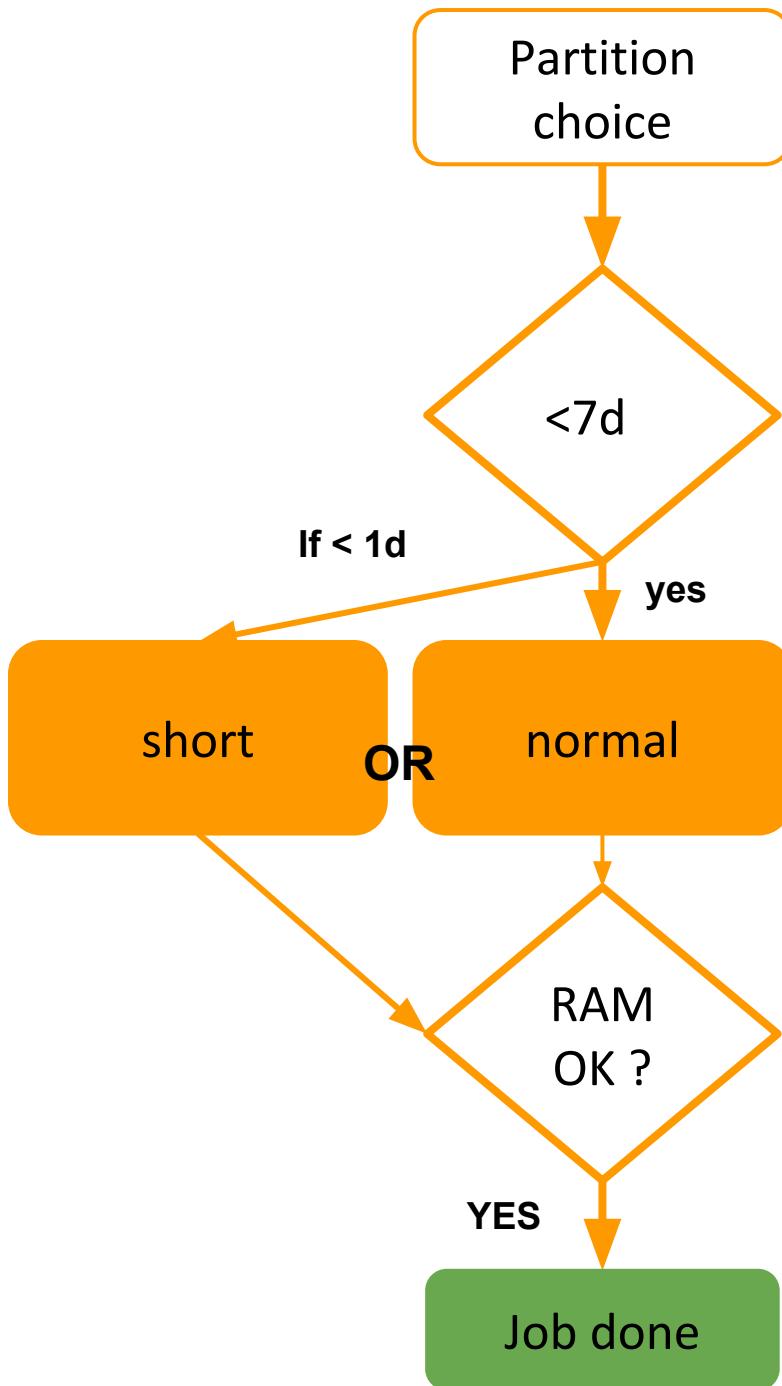
How do I choose the partition?



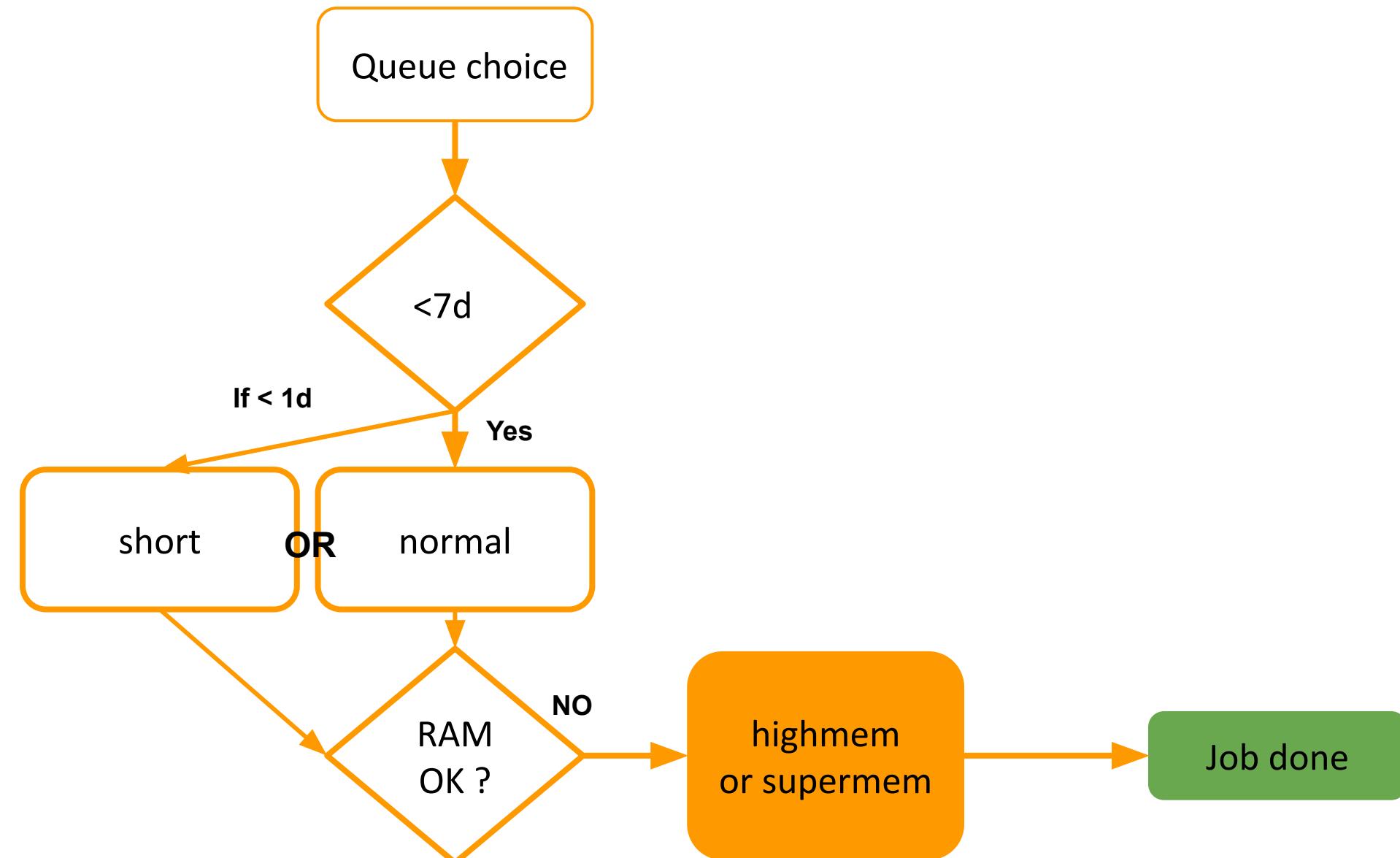
How do I choose the partition?



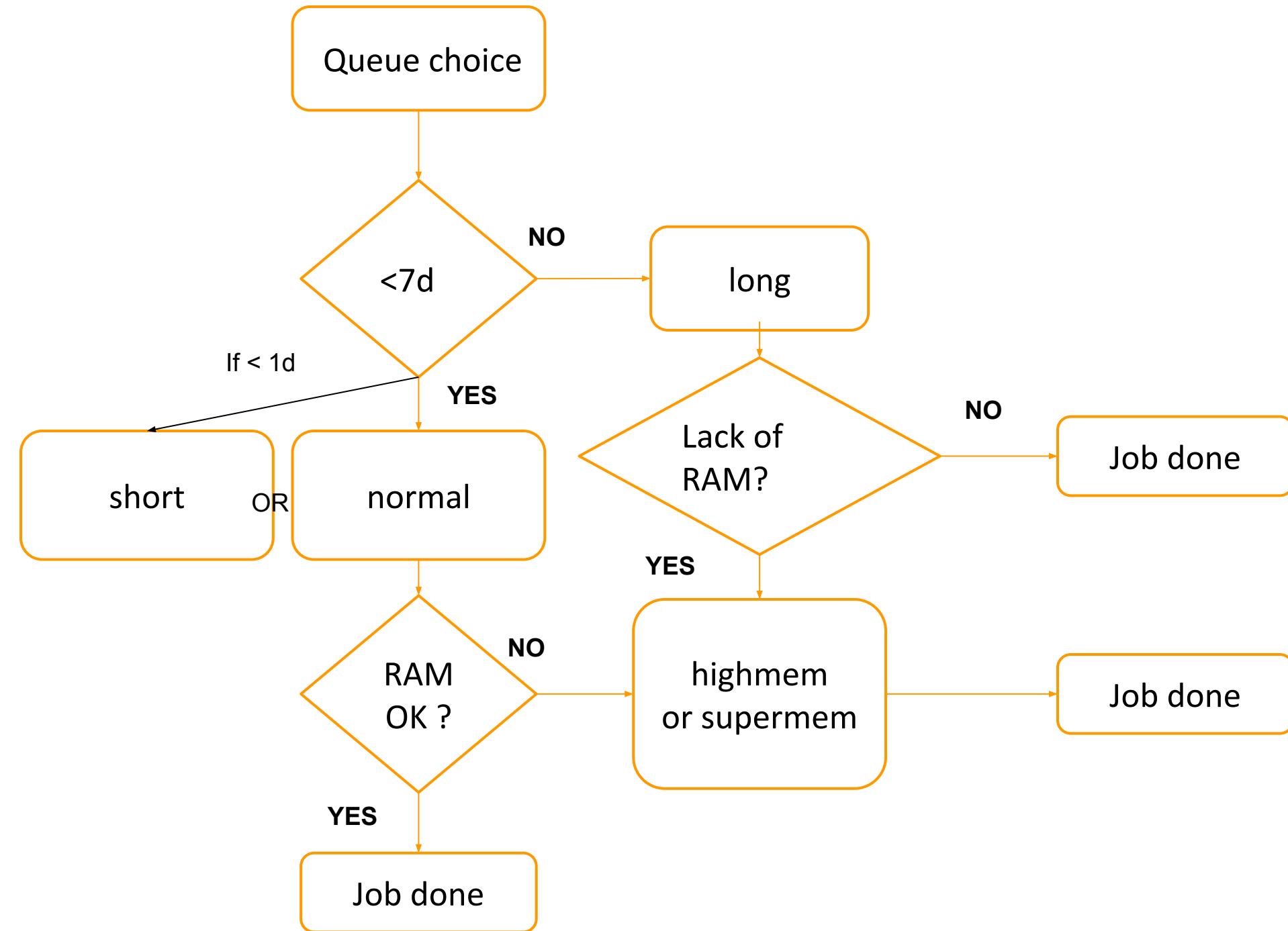
How do I choose the partition?



How do I choose the queue?



How do I choose the queue?



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>

- **1 Master node**

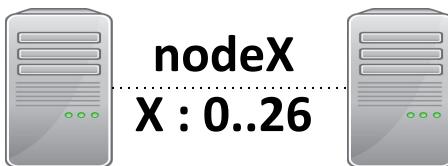


bioinfo-master.ird.fr

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**

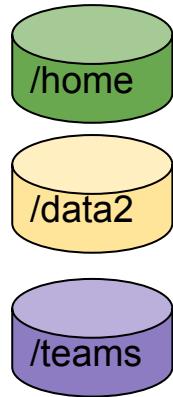


Bioinfo-nas.ird.fr
(nas)
Bioinfo-nas2.ird.fr
(nas2)
Bioinfo-nas3.ird.fr
(nas3)

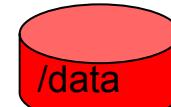
Role :

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

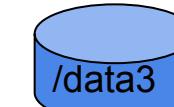
cluster i-Trop disk partitions



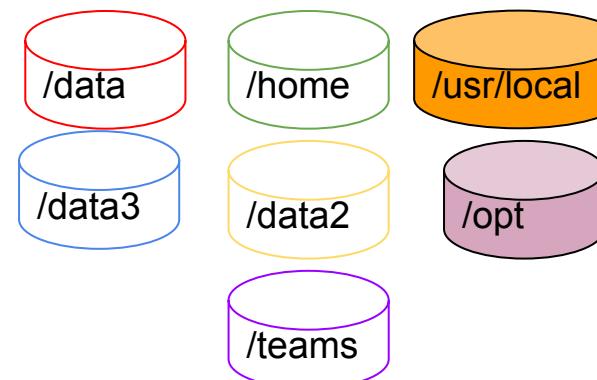
bioinfo-nas.ird.fr



bioinfo-nas2.ird.fr

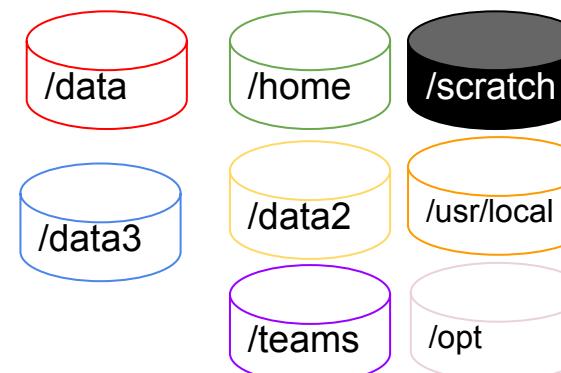


bioinfo-nas3.ird.fr



bioinfo-master.ird.fr

Virtual links to the other servers partitions



25 nodes



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

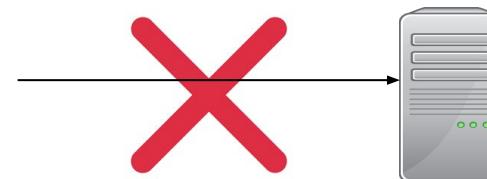
2

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

Data transfer on i-Trop cluster



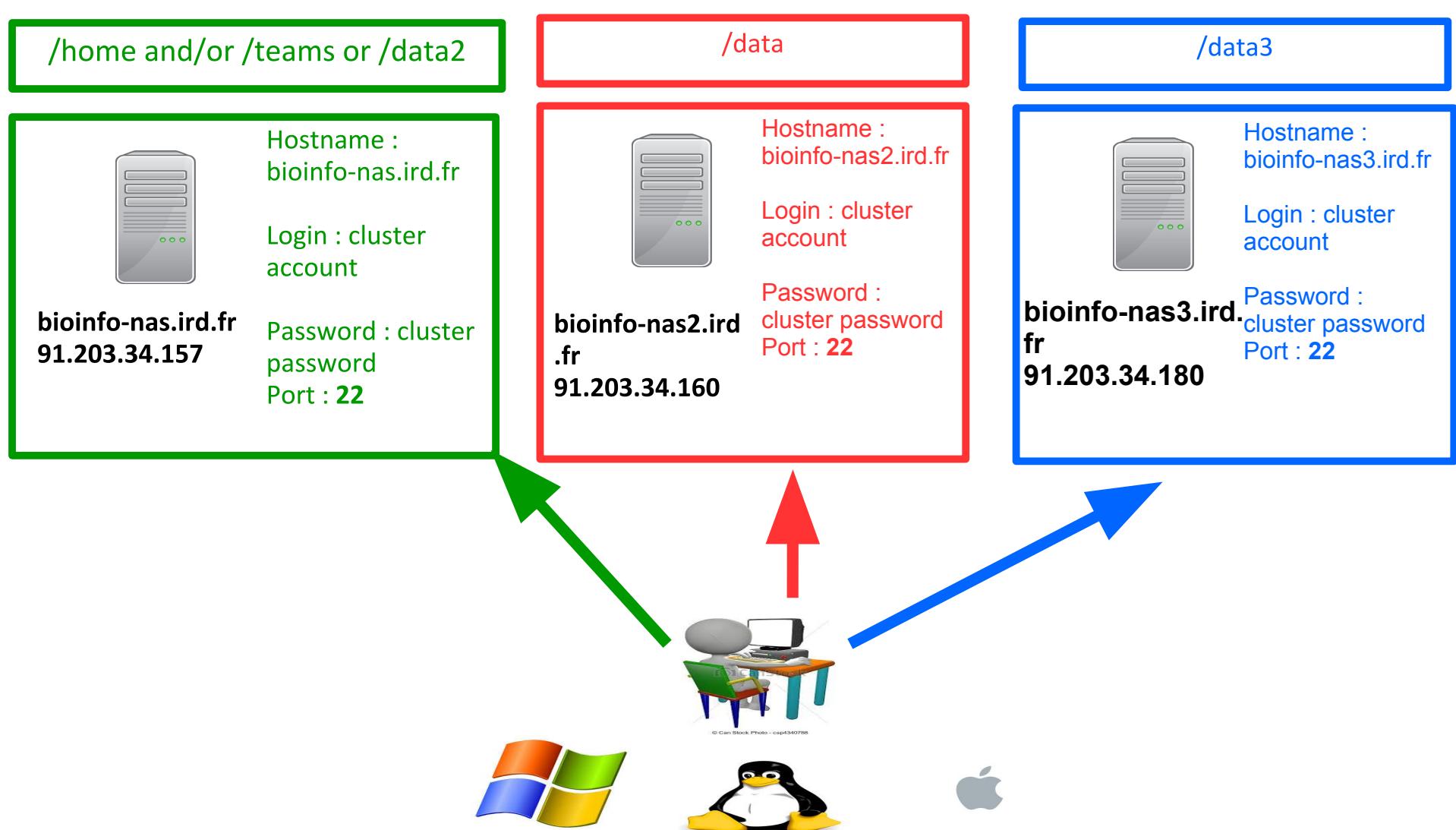
PC/MAC



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



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 :

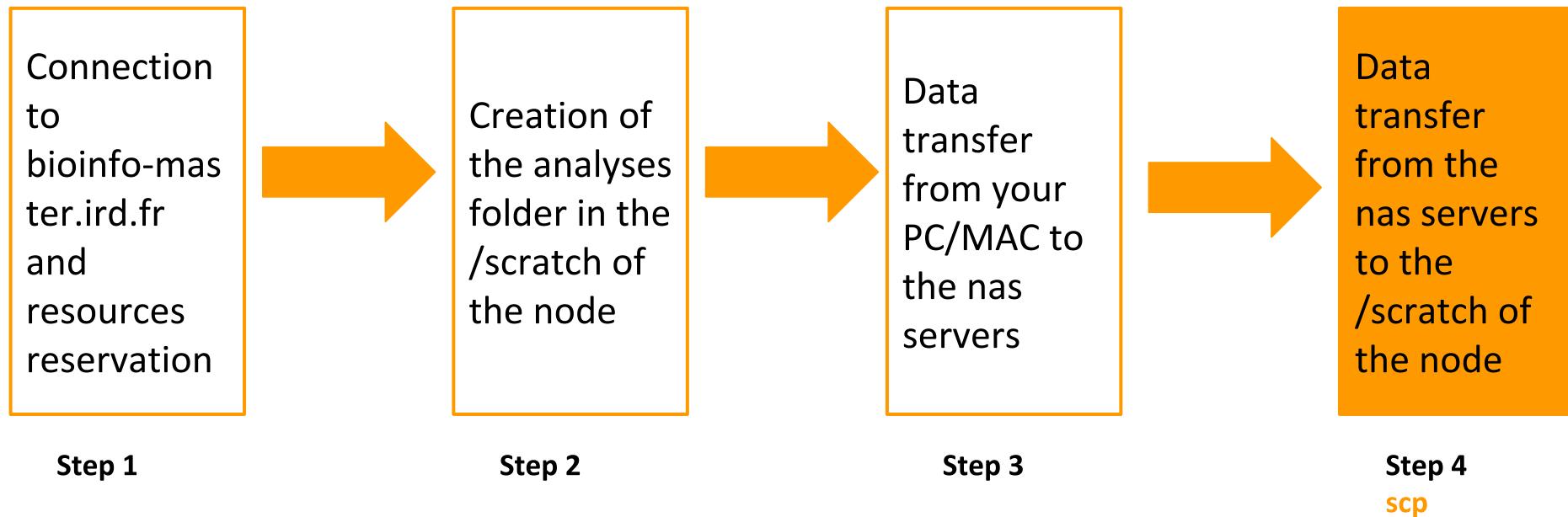
```
scp -r server_name:/path/file_to_copy local_folder
```

- 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

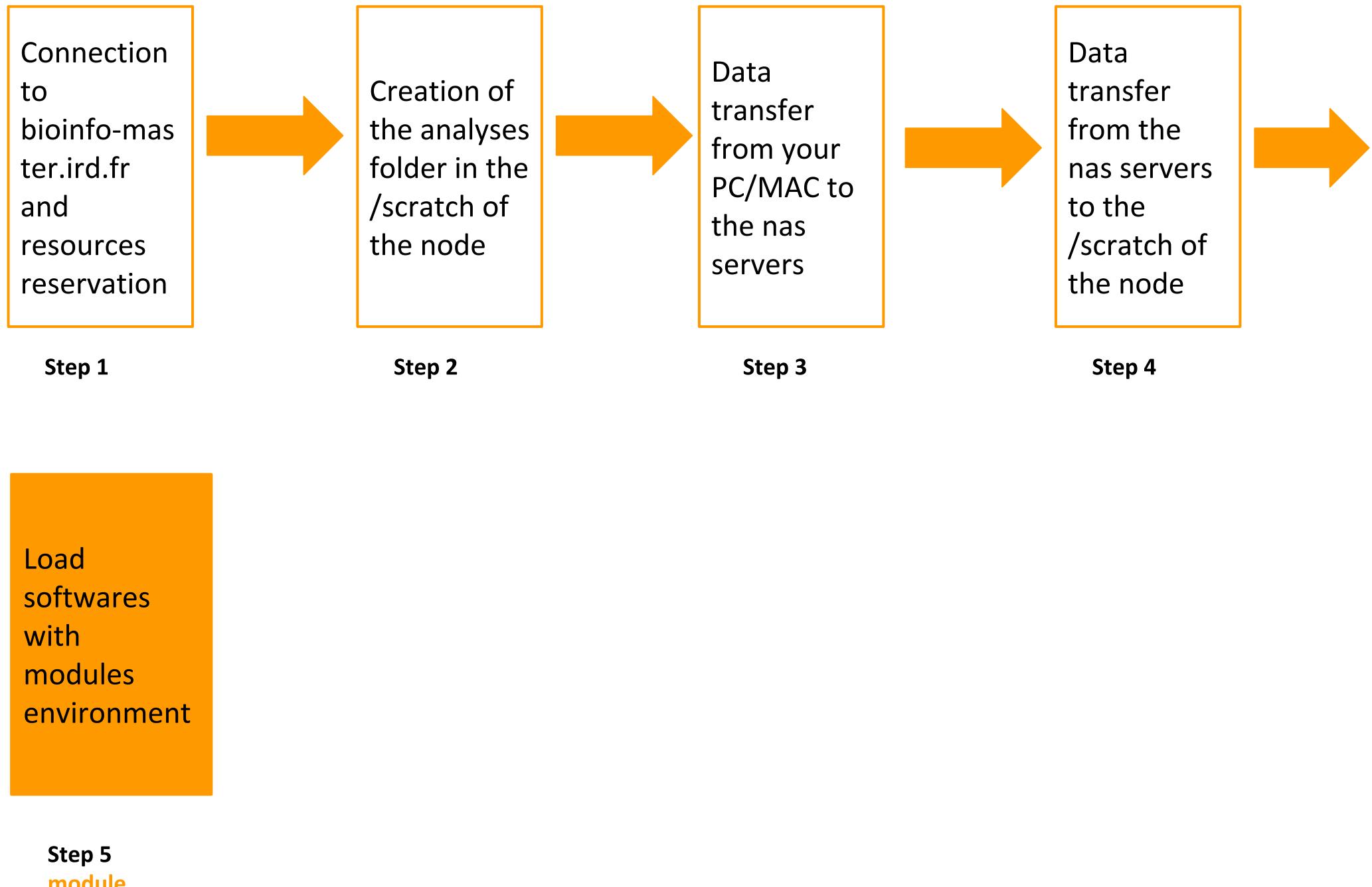
4

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





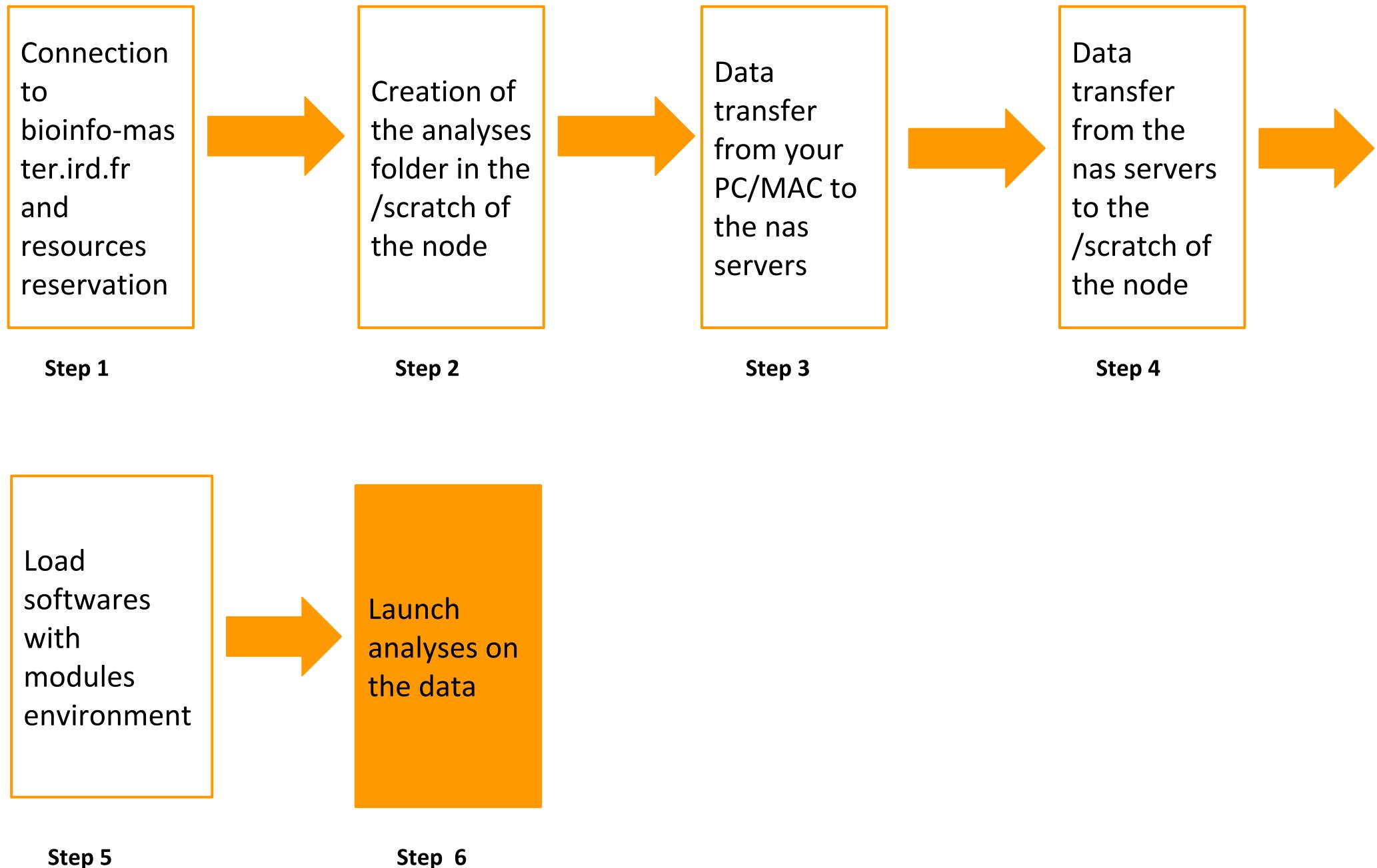
Practice

Step 5: module environment

5

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

Analyses steps of the cluster



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
salloc --time=0X:00	Allocate one or several nodes for a later use	Salloc -N 2 --p short --time=05:00
sbatch	Launch analyses in background via a script	sbatch script.sh
sinfo	Informations on partitions	sinfo
sinfo -N l	Informations on nodes of the partitions	sinfo -N l
squeue	Infos on all jobs	squeue -u tando
scontrol show job <job_id>	Infos on the active job <job_id>	scontrol show job 1029

Options des commandes sbatch, srun, salloc

Options	Description	Exemple
--job-name=<name>	Name the job	sbatch --job-name=tando_blast
-p <partition>	Choose a partition	sbatch -p highmem
--nodelist=<nodeX>	Choisir a particular node	Sbatch -p normal --nodelist=node14
-n <nbre_cpus>	Launch with several cores	srun -n 4
--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	Sbatch ---mail-type=BEGIN
--workdir=[dir_name]	Precise the working directory	sbatch s--workdir=/scratch/tando script.sh

Plus d'infos sur Slurm ici: <https://southgreenplatform.github.io/tutorials//cluster-itrop/Slurm/#part-2>

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

Launch a command line job

- Execute a bash command via srun
- 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

Transfer your results to the nas servers

- Copy between 2 remote servers :

```
scp source destination
```

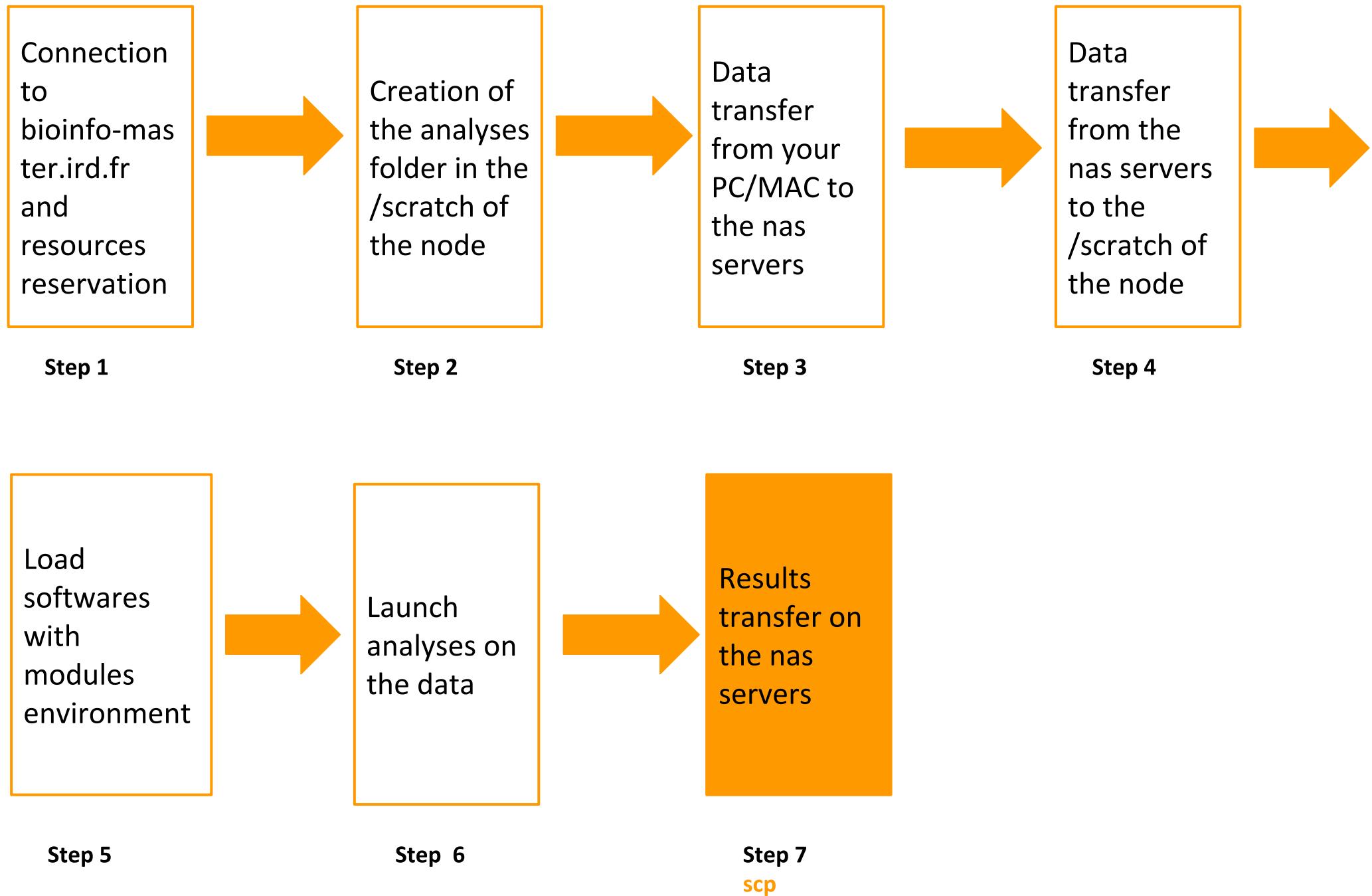
- Syntax if the source is remote :

```
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

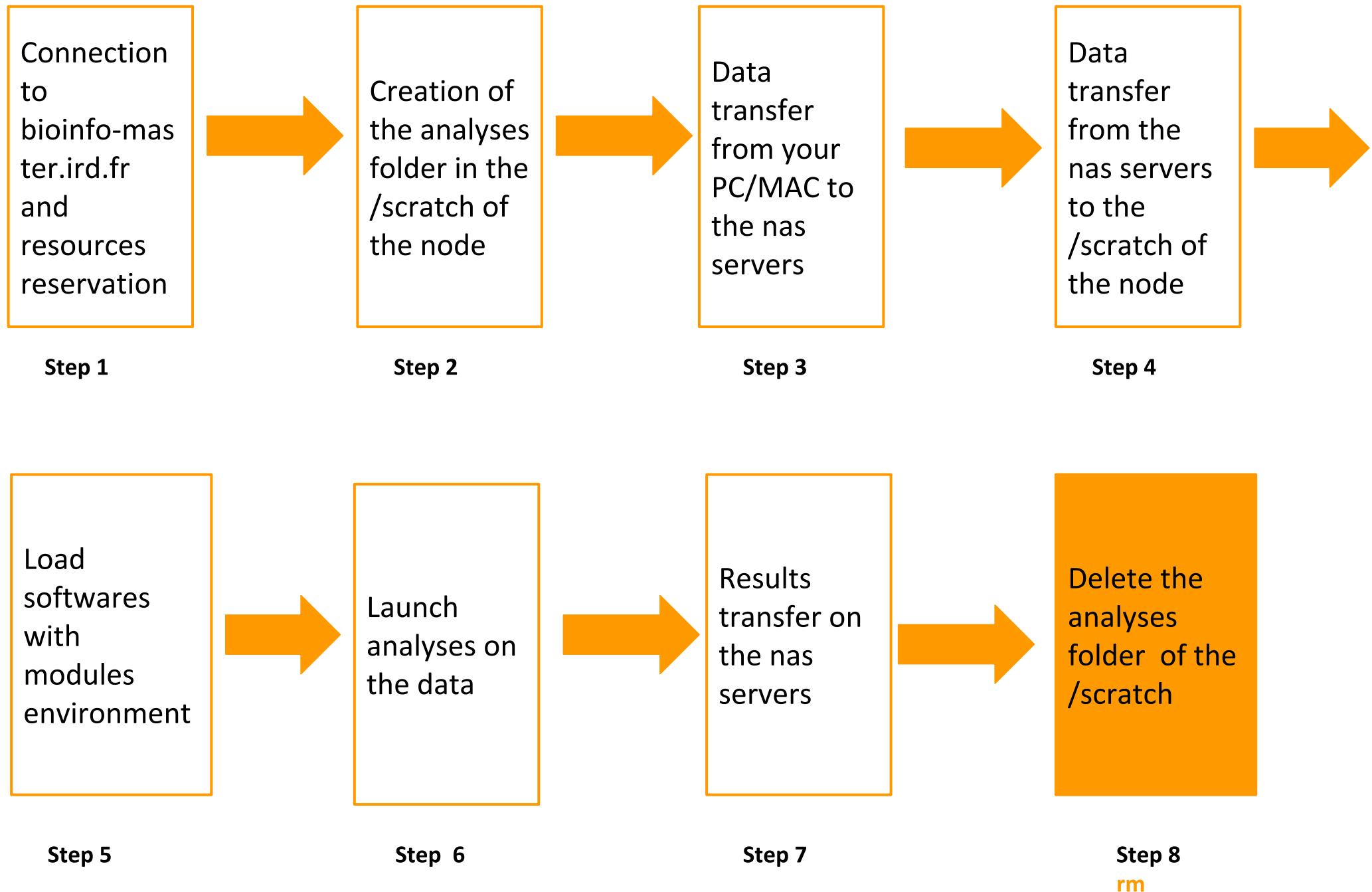
Go to the [Practice7](#) of the github

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
```

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 rm
- Use:

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

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

Options des commandes sbatch, srun, salloc

Options	Description	Exemple
--job-name=<name>	Name the job	sbatch --job-name=tando_blast
-p <partition>	Choose a partition	sbatch -p highmem
--nodelist=<nodeX>	Choisir a particular node	Sbatch -p normal --nodelist=node14
-n <nbre_cpus>	Launch with several cores	srun -n 4
--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	Sbatch ---mail-type=BEGIN
--workdir=[dir_name]	Precise the working directory	sbatch s--workdir=/scratch/tando script.sh

Plus d'infos sur Slurm ici: <https://southgreenplatform.github.io/tutorials//cluster-itrop/Slurm/#part-2>

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 sge

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:

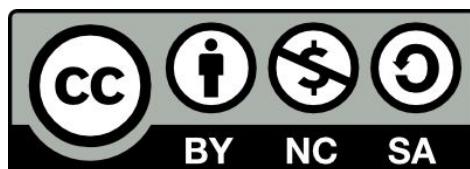
“The authors acknowledge the IRD itrop HPC (South Green Platform) at IRD montpellier

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, renewal machinesetc...
- Available quotations
- Contact bioinfo@ird.fr : help, needs definition, quotations...

Thank you for your attention !



Le matériel pédagogique utilisé pour ces enseignements est mis à disposition selon les termes de la licence Creative Commons Attribution - Pas d'Utilisation Commerciale - Partage dans les Mêmes Conditions (BY-NC-SA) 4.0 International:

<http://creativecommons.org/licenses/by-nc-sa/4.0/>