HPC cluster Initiation

www.southgreen.fr

https://southgreenplatform.github.io/trainings

i-Trop Presentation

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i-Trop Presentation

Provisioning of softwares and HPC ressources

Analysis software and IS development

Plateau bioinformatique

Help and support to IRD teams

Training to north and South

Requests/incidents/Howtos

- Request forms: https://bioinfo.ird.fr/index.php/en/cluster-2/
  - Accounts
  - Softwares
  - Projects
- Incidents: contact bioinfo@ird.fr
- Howtos: https://bioinfo.ird.fr/index.php/en/tutorials-howtos-i-trop-cluster/
- Slurm Tutorials: https://bioinfo.ird.fr/index.php/en/tutorials-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 ressources availabilty

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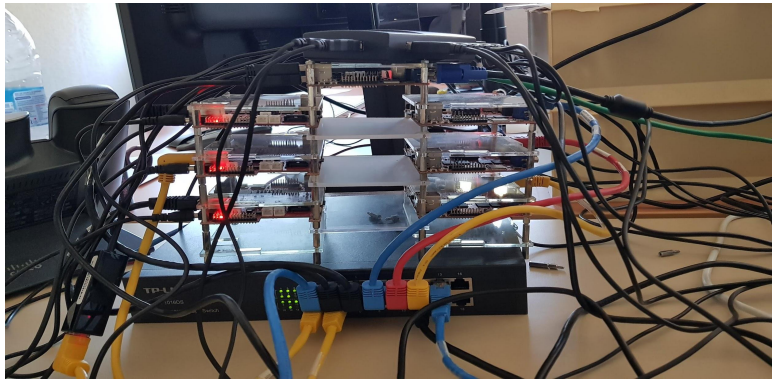

Cluster components

COMPUTING

- **Master Node**
  Handle resources and jobs priorities

- **Computing nodes**
  Resources (CPU or RAM memory)

Cluster components

COMPUTING

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- **Computing nodes**
  Resources (CPU or RAM memory)

STORAGE

- **NAS Server(s)**
  Storage

Architecture: components role

- **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
```

Architecture: components role

- **1 Master Node**

bioinfo-master.ird.fr

Role :

- Launch and prioritize jobs on computating 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-master.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

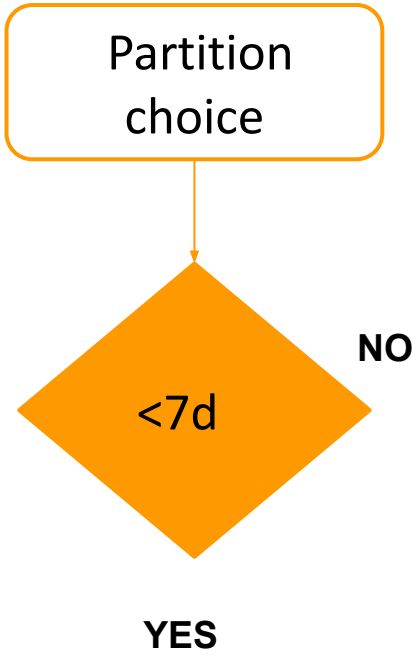
*Request to do with arguments

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?



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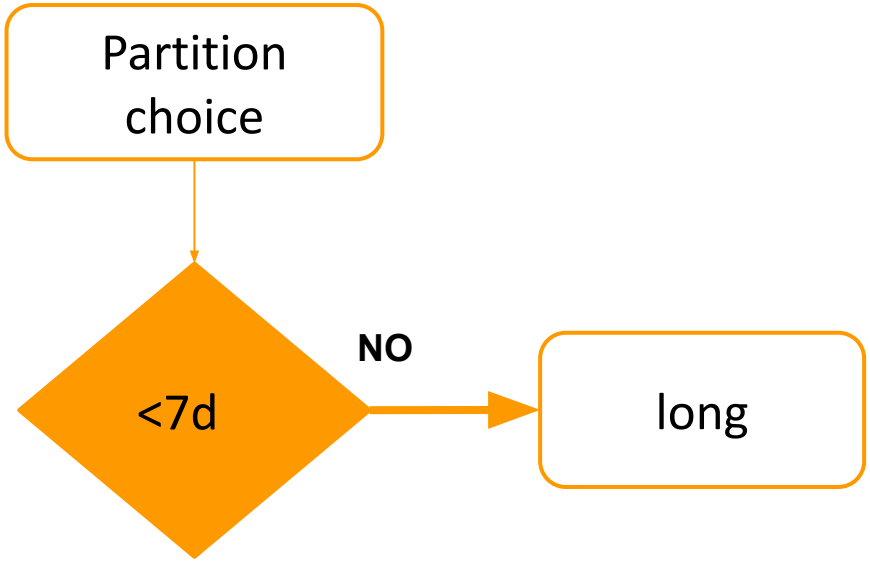

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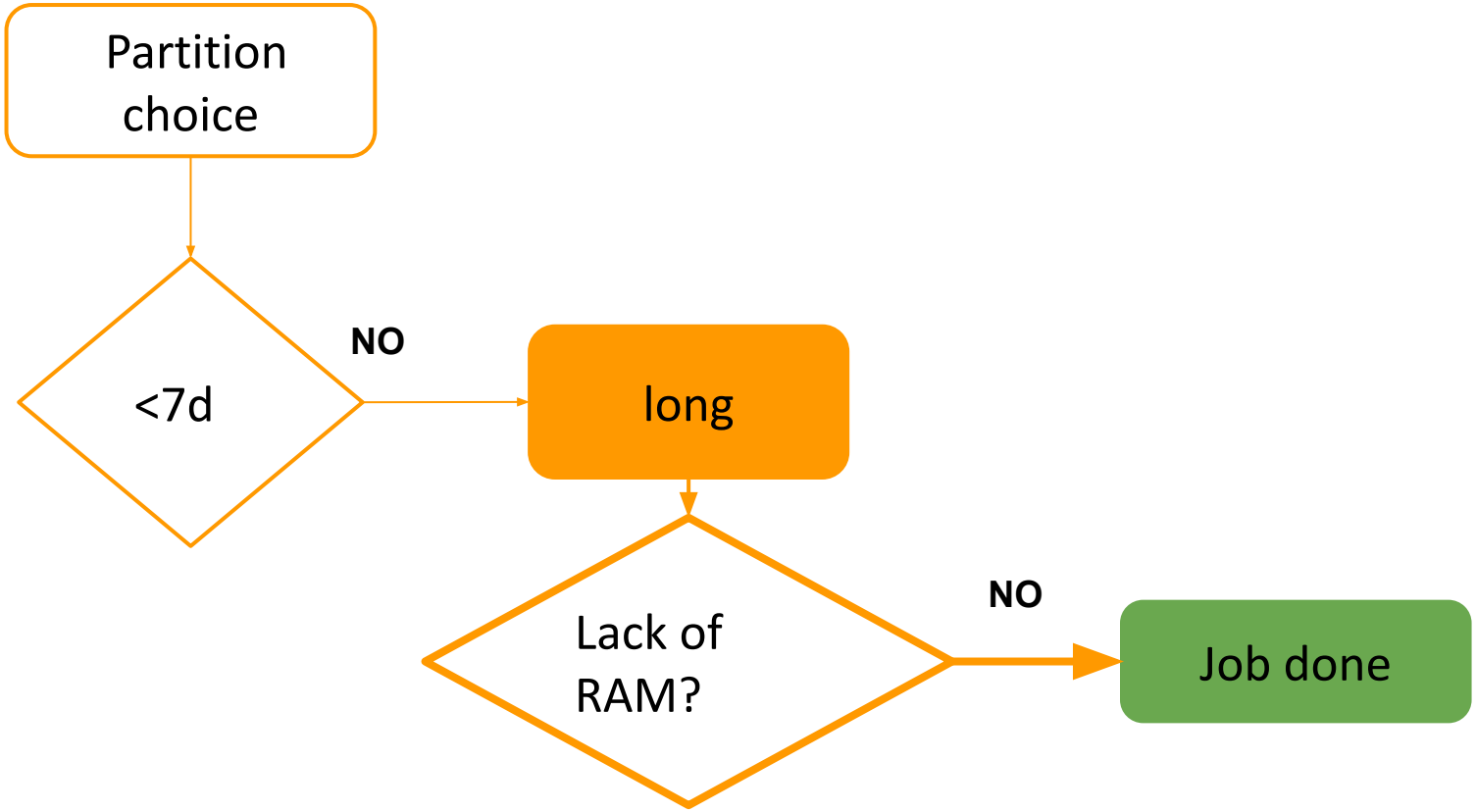
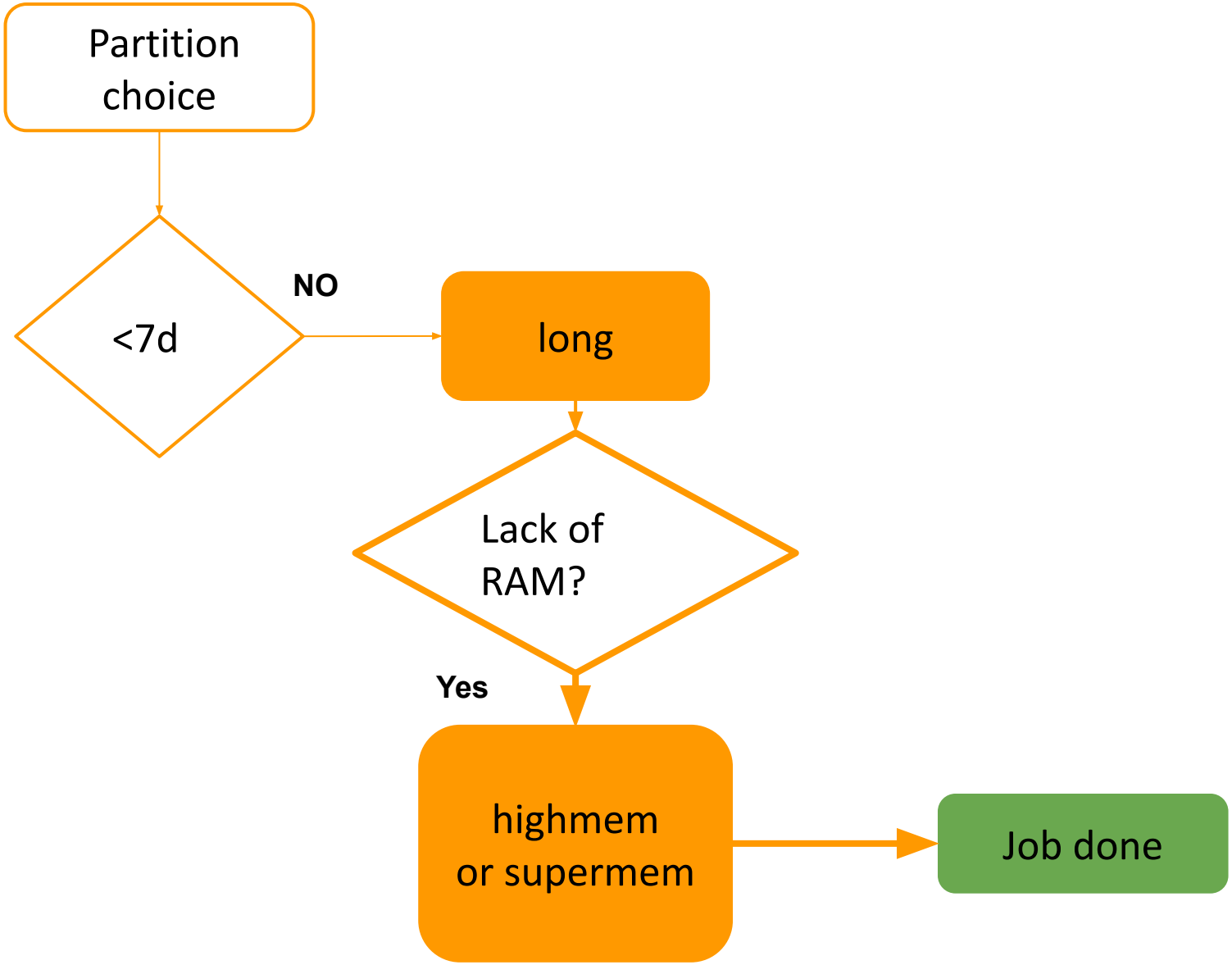


How do I choose the partition?



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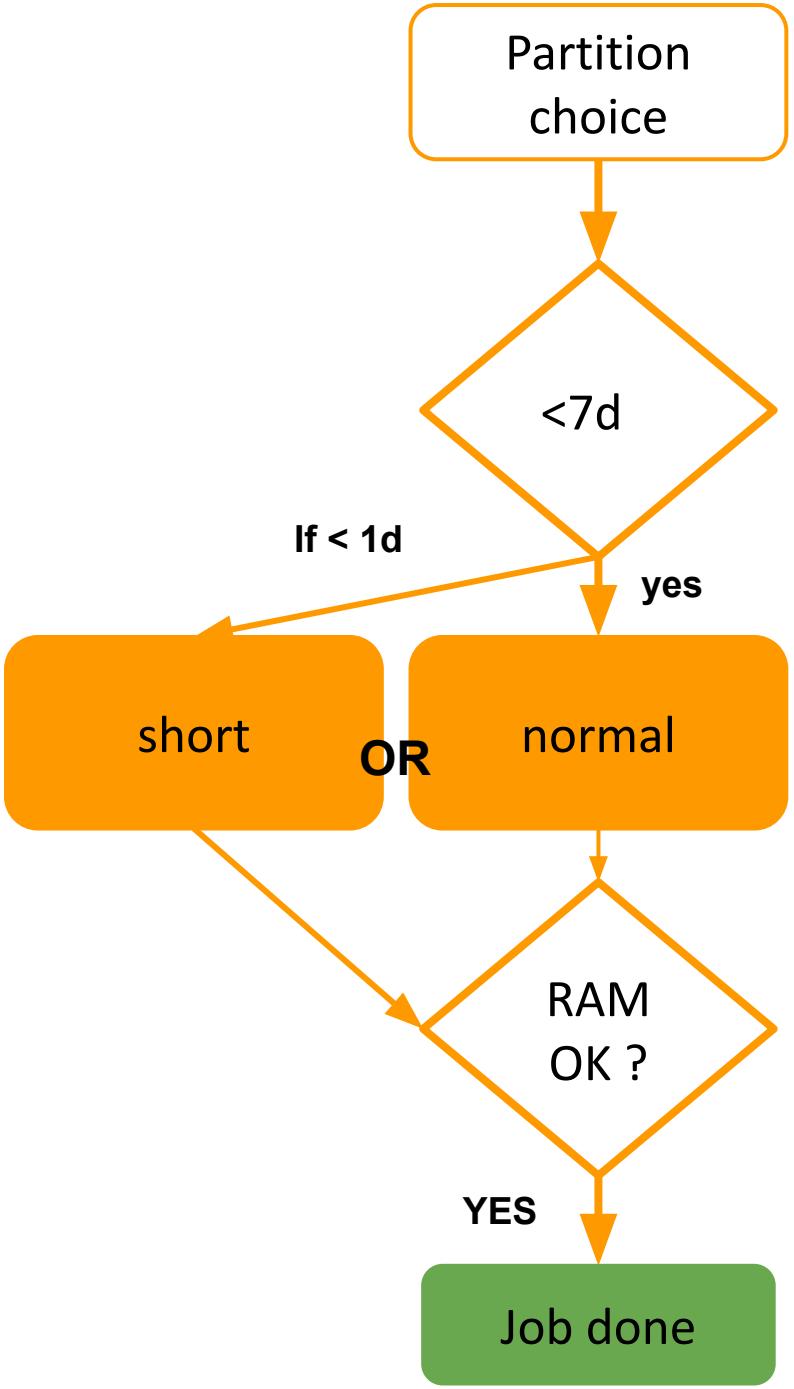

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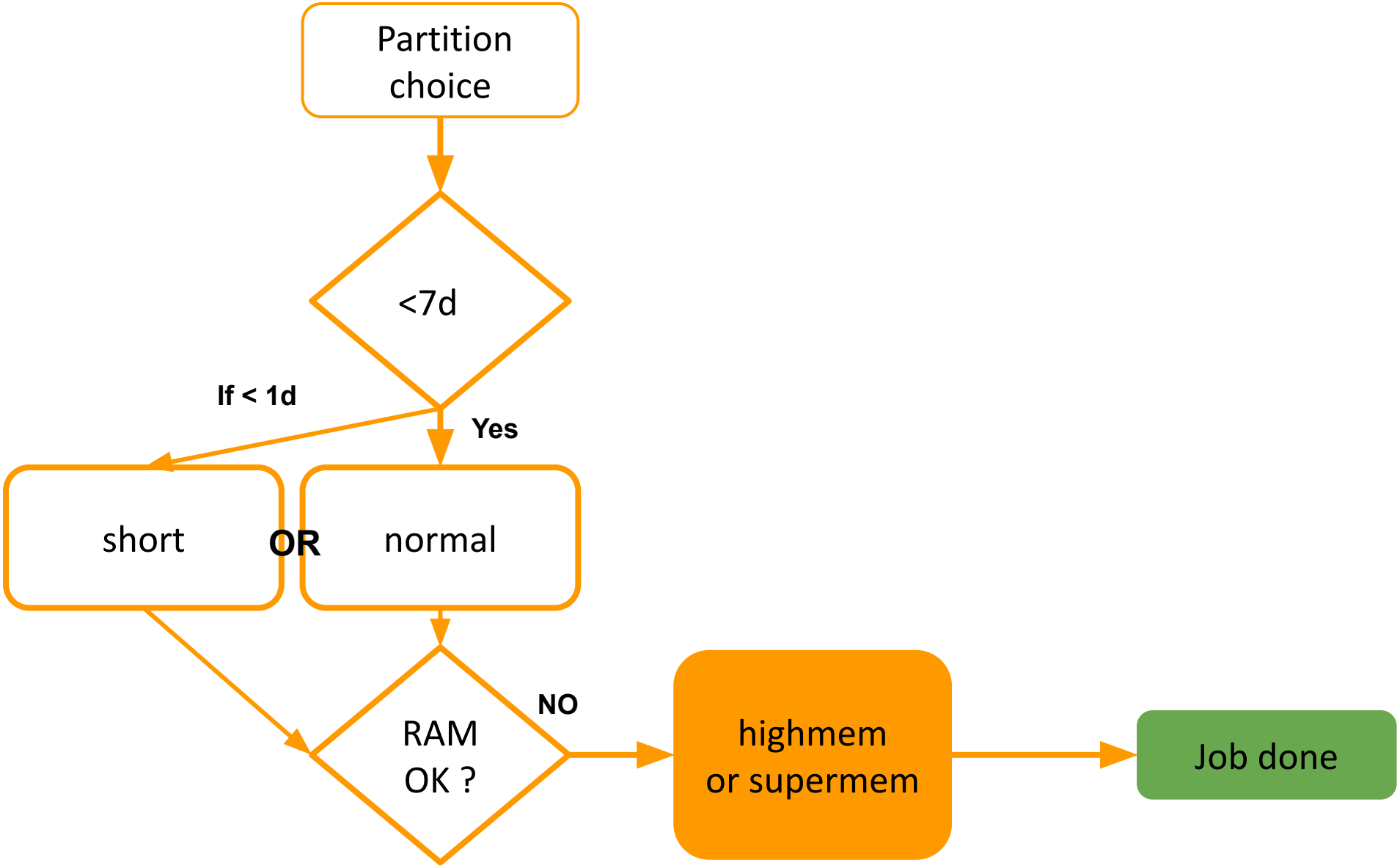

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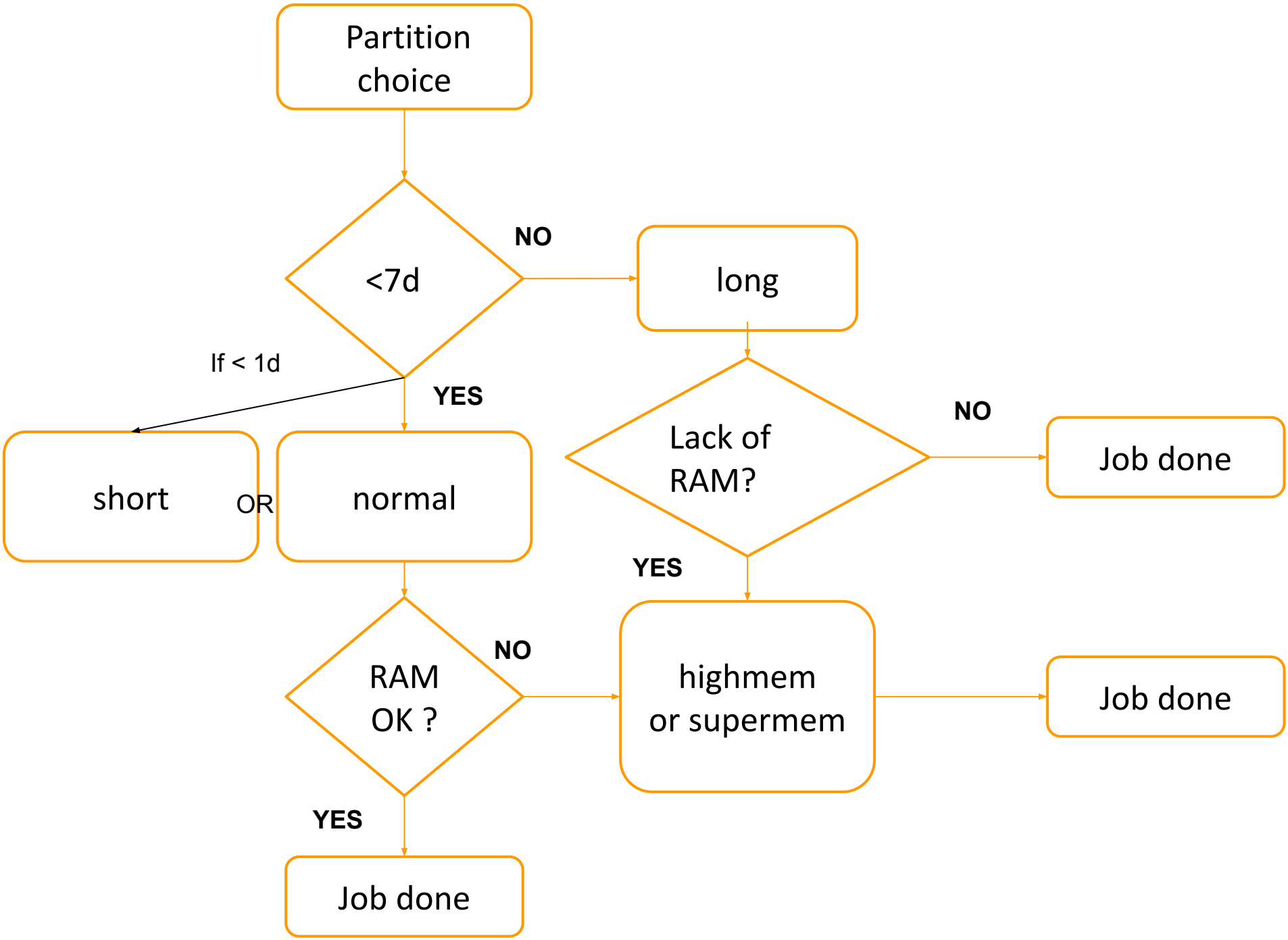


Which partition to choose?

Rules	Partition	Tools example	comments
basecalling, demultiplexing, correction	***gpu***	medaka, guppy, machine learning tools	Restricted access
assembling >100G RAM	***supermem***	miniasm, flye, raven, smartdenovo	Target genome > 400 Mb (rice genome doesn't need 100 GB)
genomicsbd (gatk) > 100G RAM	***supermem***	GATK genomicsDB	Target genome for more than 400 Mb (>10 samples)
assembling => 35G et < 120G RAM	***highmemplus***	miniasm, flye, raven, smartdenovo	Target genome between 100 and 400 Mb
assembling => 35G et < 100G RAM	***highmem***	miniasm, flye, raven, smartdenovo	Target genome between 100 and 400 Mb
Pops structure	***long***		
simulations	***long***		
metagenomic	***normal***	quiime2, frogs	
mapping	***normal***	bwa, minimap2, hisat2	Need a lot of cores not too many RAM **Tool number of cores = number of cores to reserve**
genotypage	***normal***	GATK haplotypecaller, samtools mpileup, bcftools	Need a lot of cores not too many RAM **Tool number of cores = number of cores to reserve**
stats	***normal***	R	
Scripts tests	***short***	bash, python, R	

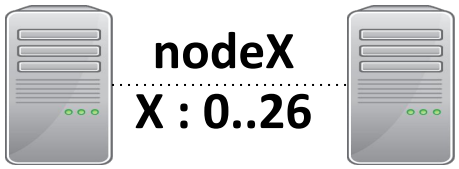
Architecture: components role

- **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**

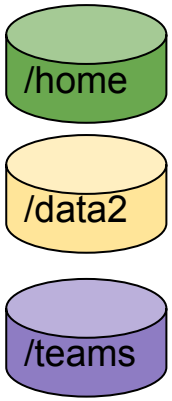
bioinfo-nas.ird.fr
(nas)

bioinfo-nas2.ird.fr
(nas2)

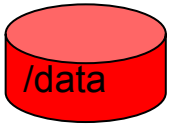
bioinfo-nas3.ird.fr
(nas3)

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

cluster i-Trop disk partitions

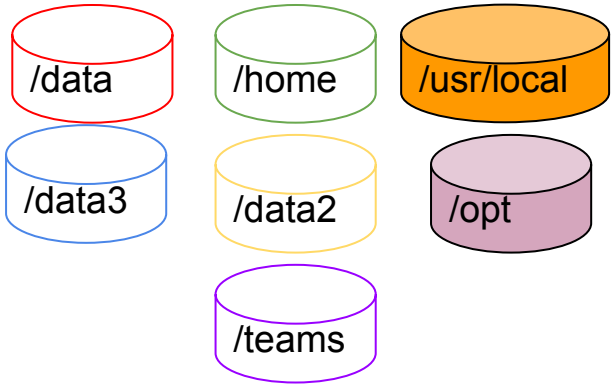


bioinfo-nas.ird.fr

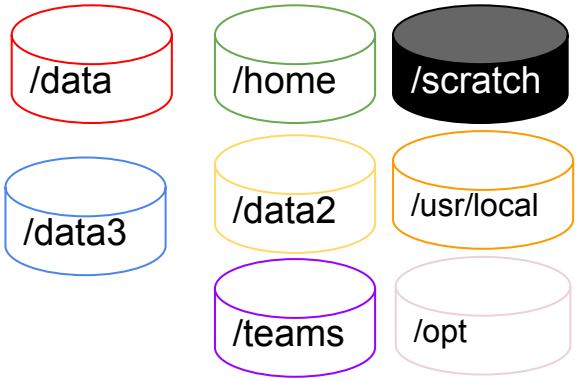


bioinfo-nas2.ird.fr

bioinfo-nas3.ird.fr



bioinfo-master.ird.fr



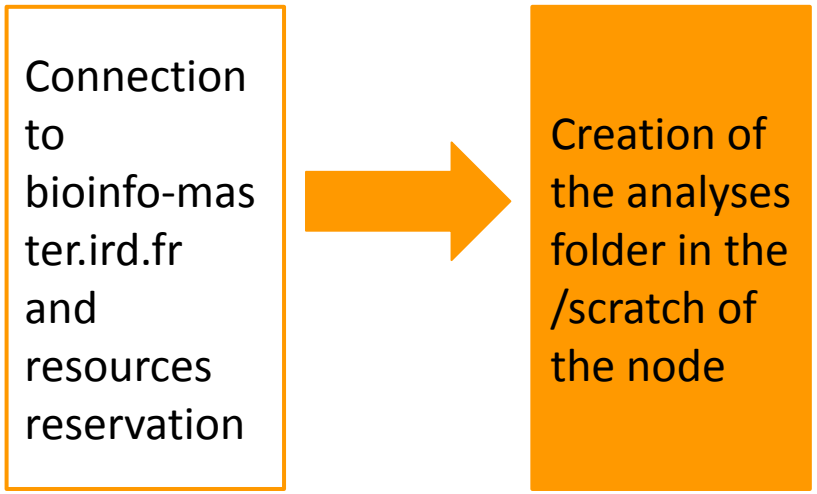
27 nodes

Illustration legend:

Local Hard drives in full cylinders

Virtual links to physical hard drives (empty cylinders)

Analyses steps of the cluster



Step 1

Step 2
mkdir

Practice

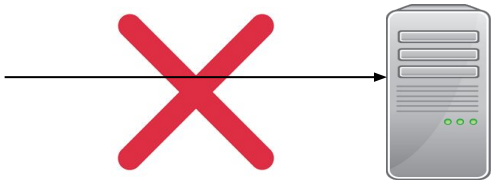
Step 2:qrsh, partition

2

Go to the Practice2 *of the github*

Data transfer on i-Trop cluster

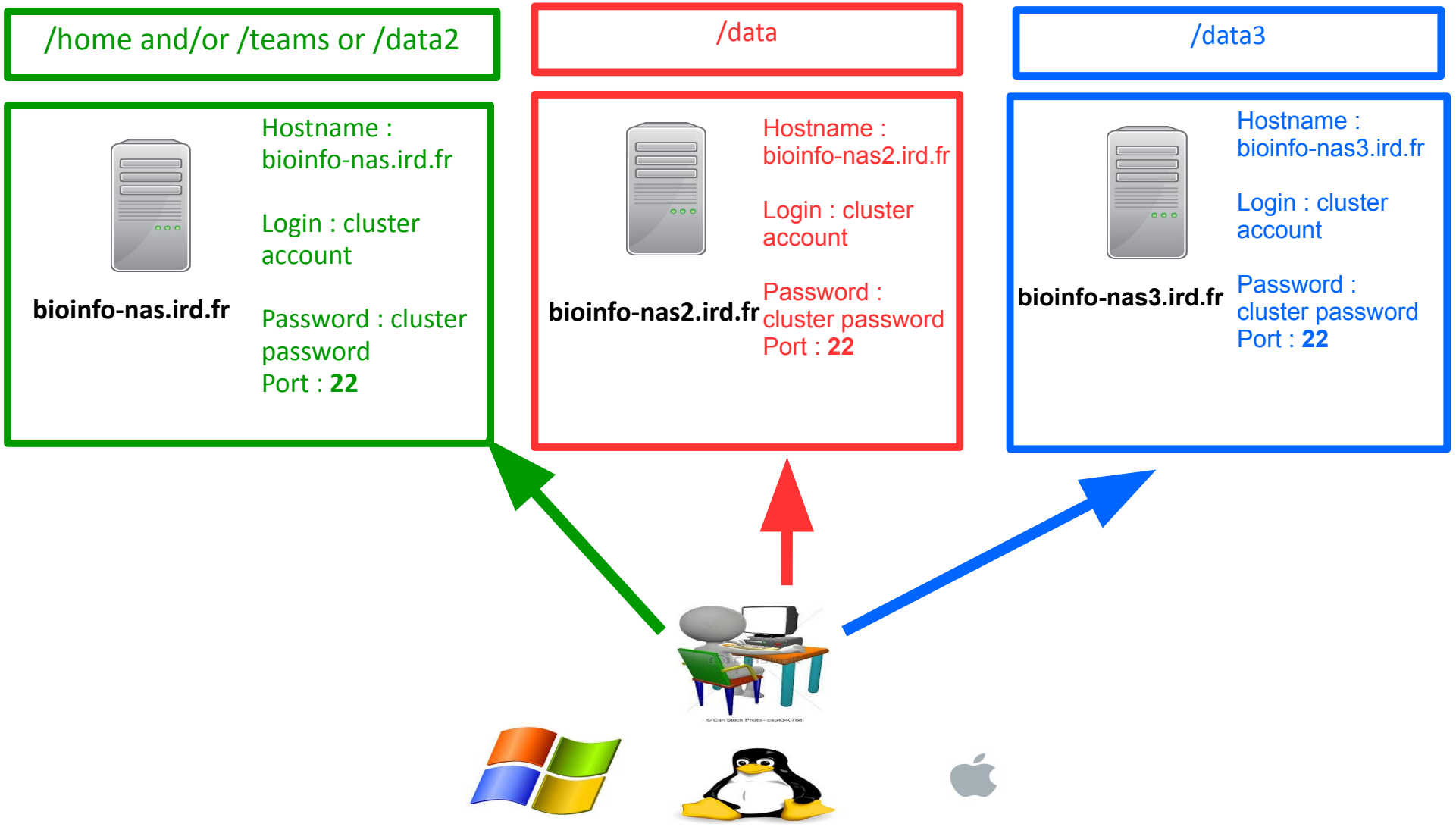
PC/MAC



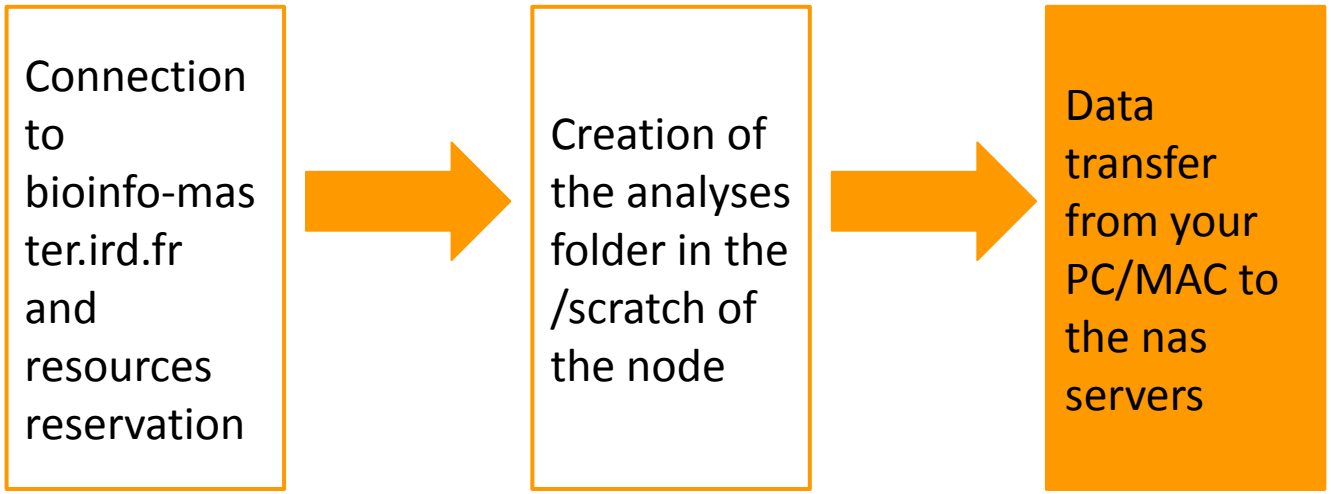
bioinfo-master.ird.fr

direct transfer via filezilla forbidden

Data transfer on i-Trop cluster



Analyses steps of the cluster



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 :

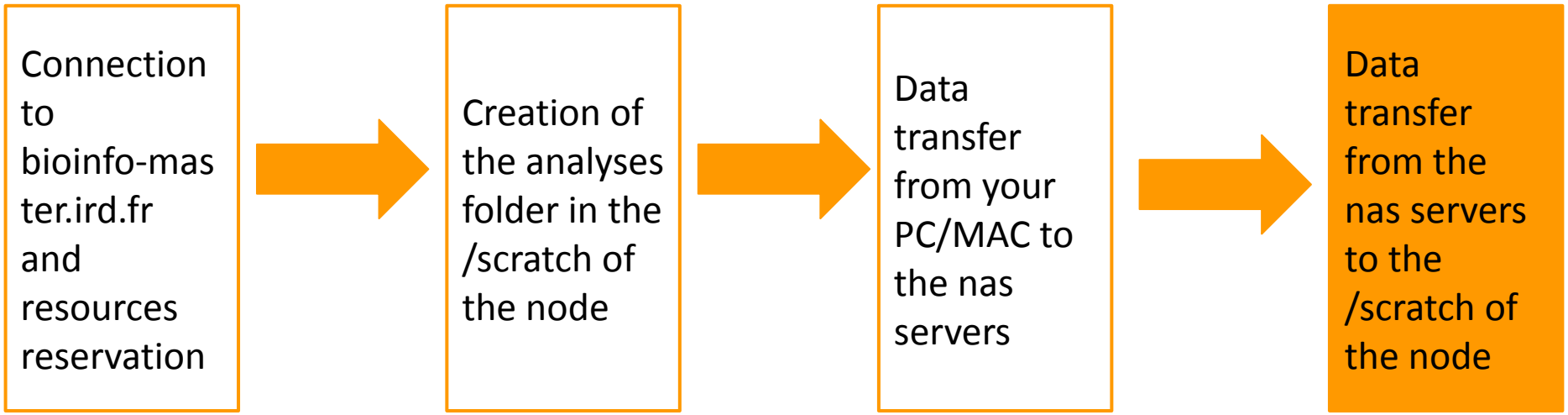
  scp -r server_name:/path/file_to_copy local_folder

- 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



Step 1

Step 2

Step 3

Step 4

scp

Practice

Step 4: scp to nodes

4

Go to the Practice4 *of the github*

Module Environment

- 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

Module Environment

➢ 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

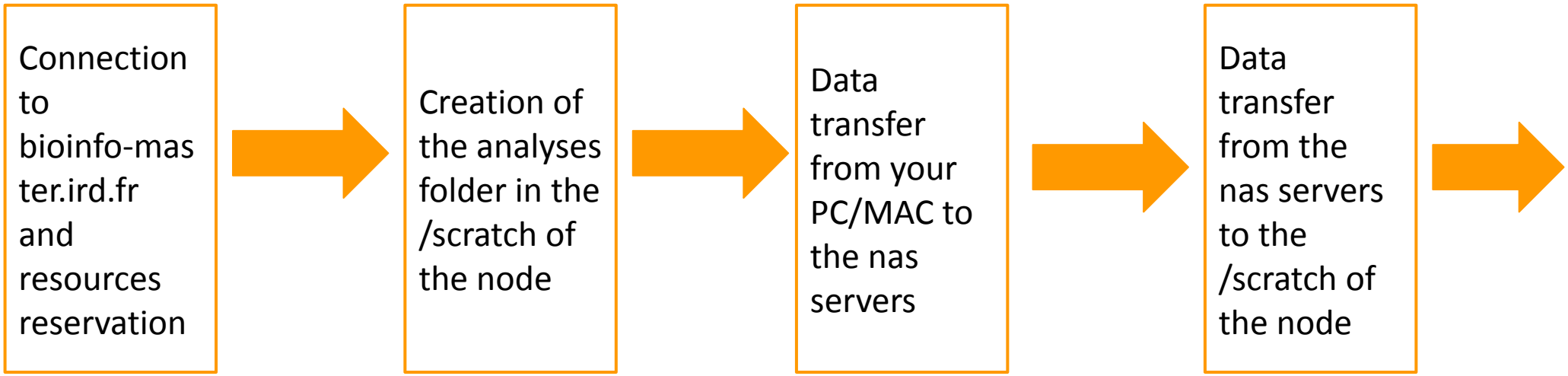
- Unload a module :

  module unload + modulename

- Unload all the modules :

  module purge

Analyses steps of the cluster



Load softwares with modules environment

Step 5
module

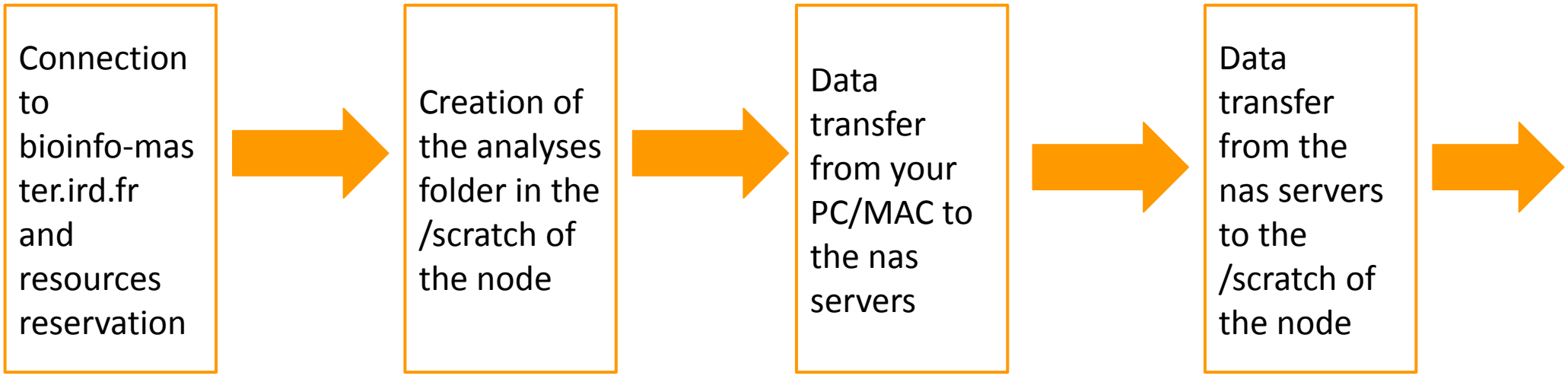
Practice

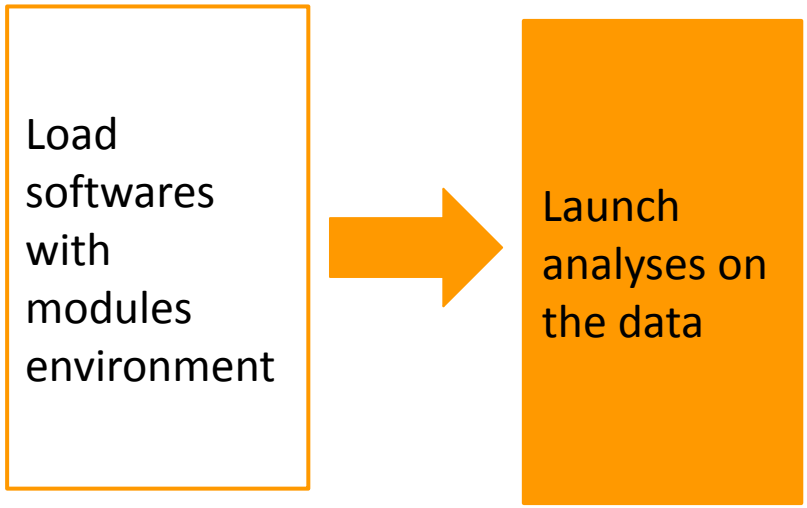
Step 5: module environment

5

Go to the Practice5 *of the github*

Analyses steps of the cluster





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

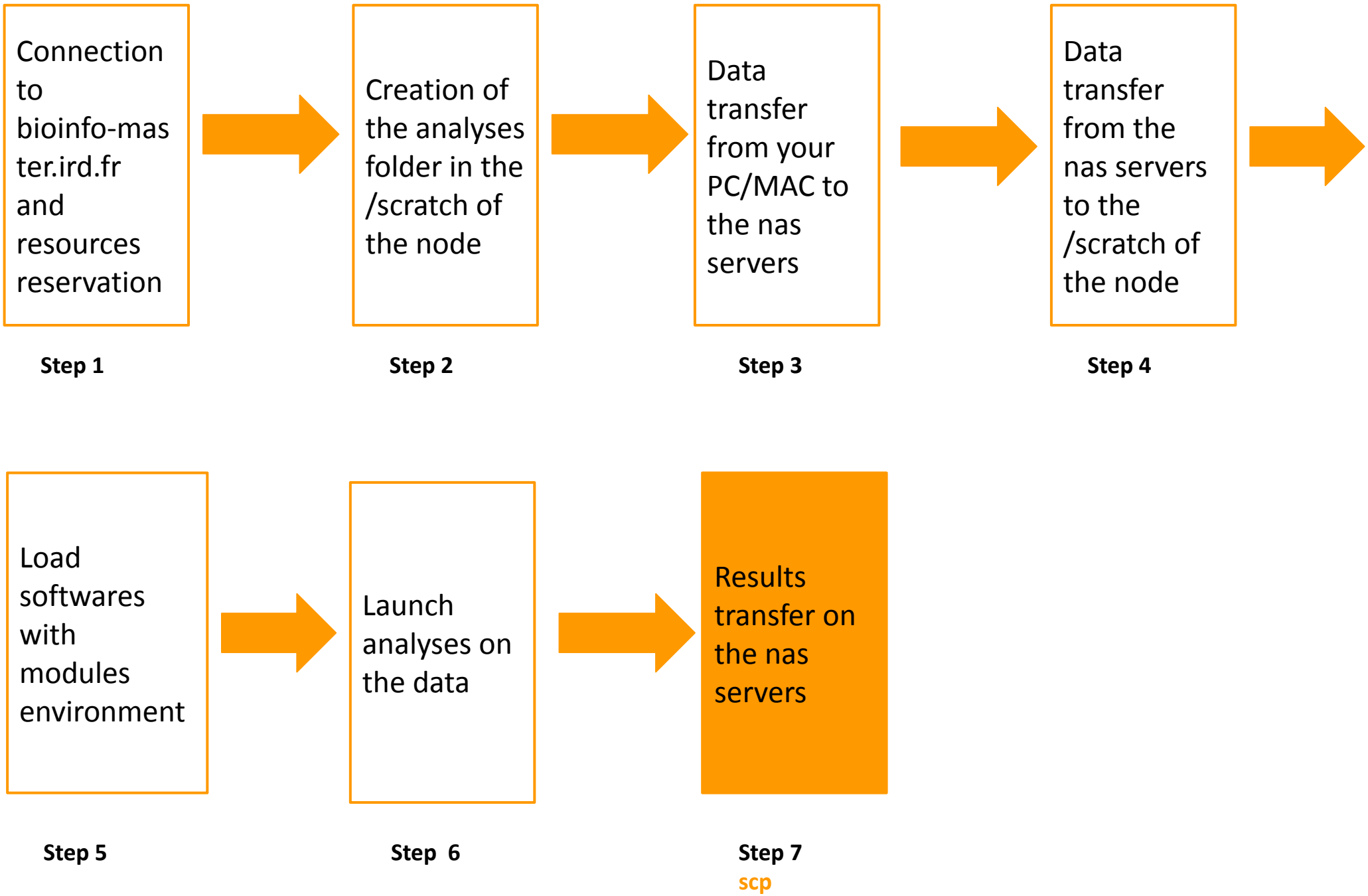
- Syntax if the source is remote :

  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

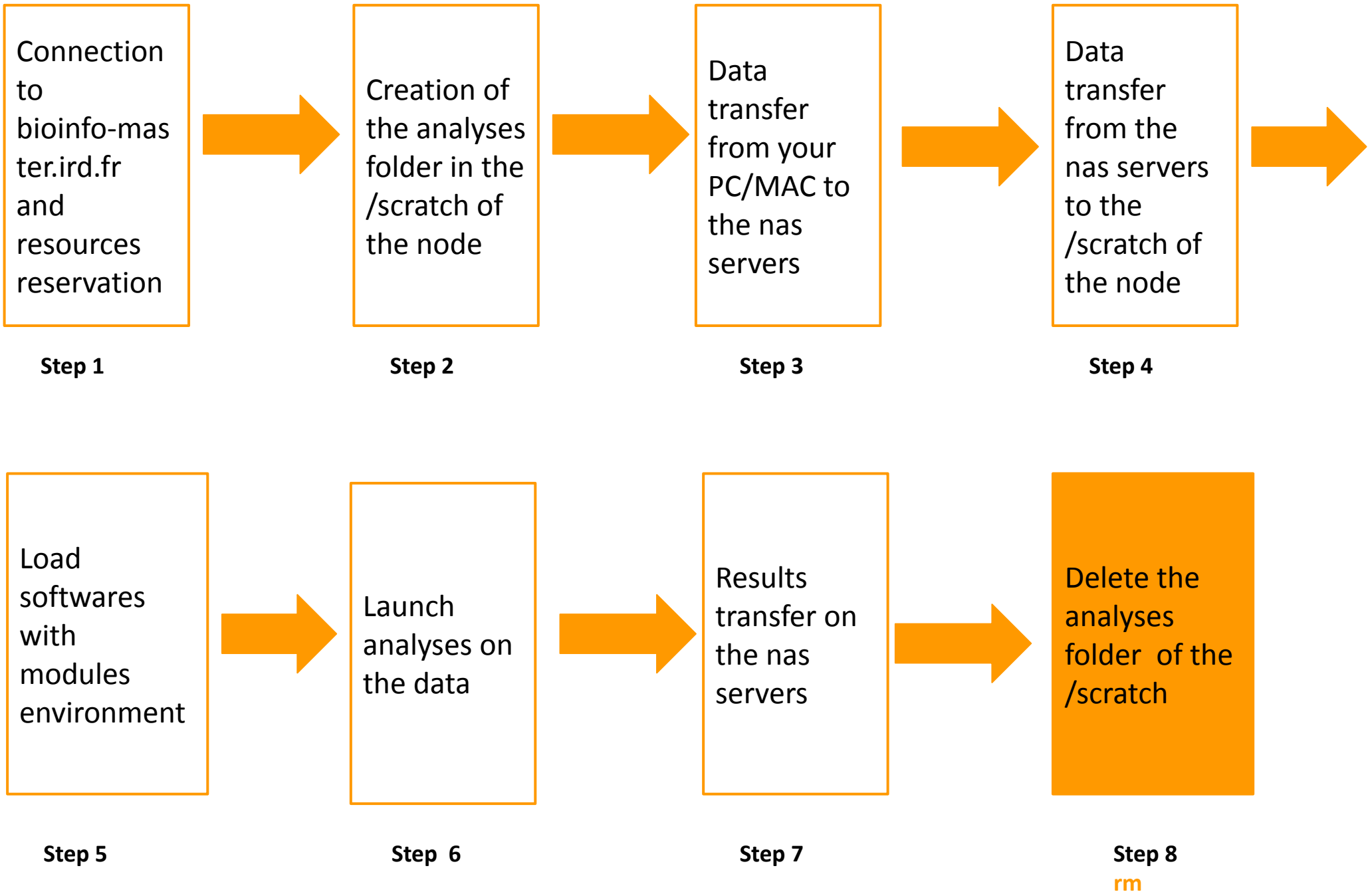
Go to the Practice7 *of the github*

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 a 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
#############################################################
```

Bash scripts syntax

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

```
###############Command execution part ###################

nom_variable1=”value_variable1”
nom_variable2=”value_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”

Projects

- 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 !