HPC cluster Initiation

www.southgreen.fr

https://southgreenplatform.github.io/trainings

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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/
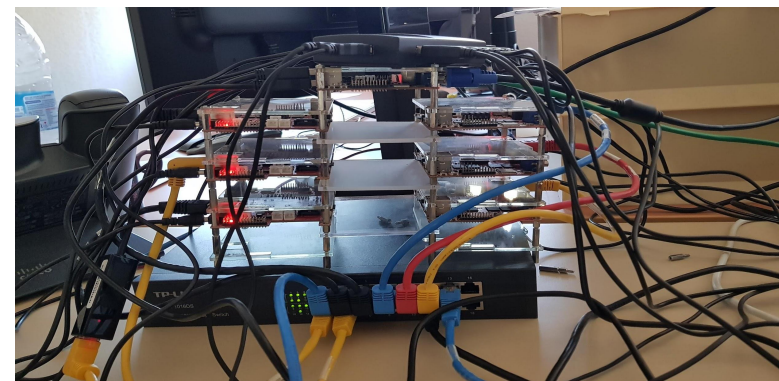
ARCHITECTURE

- A 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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COMPUTING

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

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

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- **Master Node**
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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
```
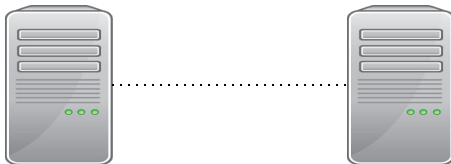
1 Master Node

bioinfo-master.ird.fr

Role :
- Launch and prioritize jobs on 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

1

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

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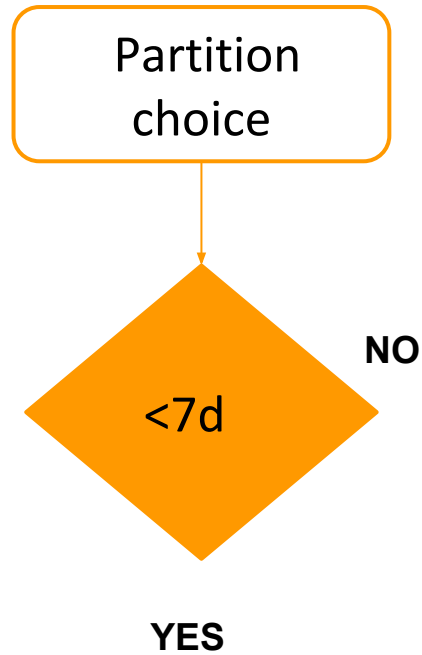reservation

Step 1
salloc/srun
ou sbatch

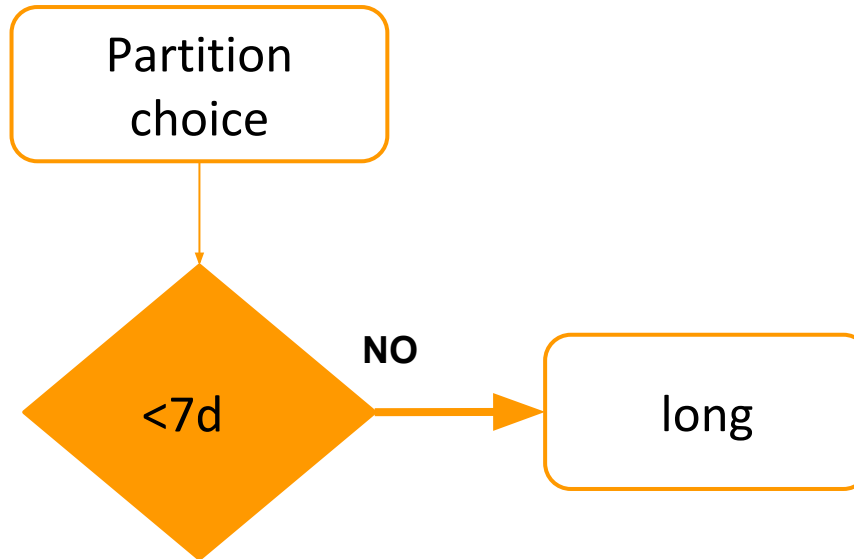| Partitions	Use	RAM on nodes	Core on nodes
short	Short Jobs < 1 day (higher priority, interactive jobs)	48 to 64 GB	12 cores
normal	Short Jobs max 7 days	64 Go to 96 GB	12 to 24 cores
r900	Short Jobs max 7 days	32GB	16 cores /scratch 117GB
long	45 days >long jobs > 3 days	48 GB	12 to 24 cores
highmem	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

- Partition to work on GPUs processors : basecalling, MiniOn etc..

- Restricted access to gpu_account group
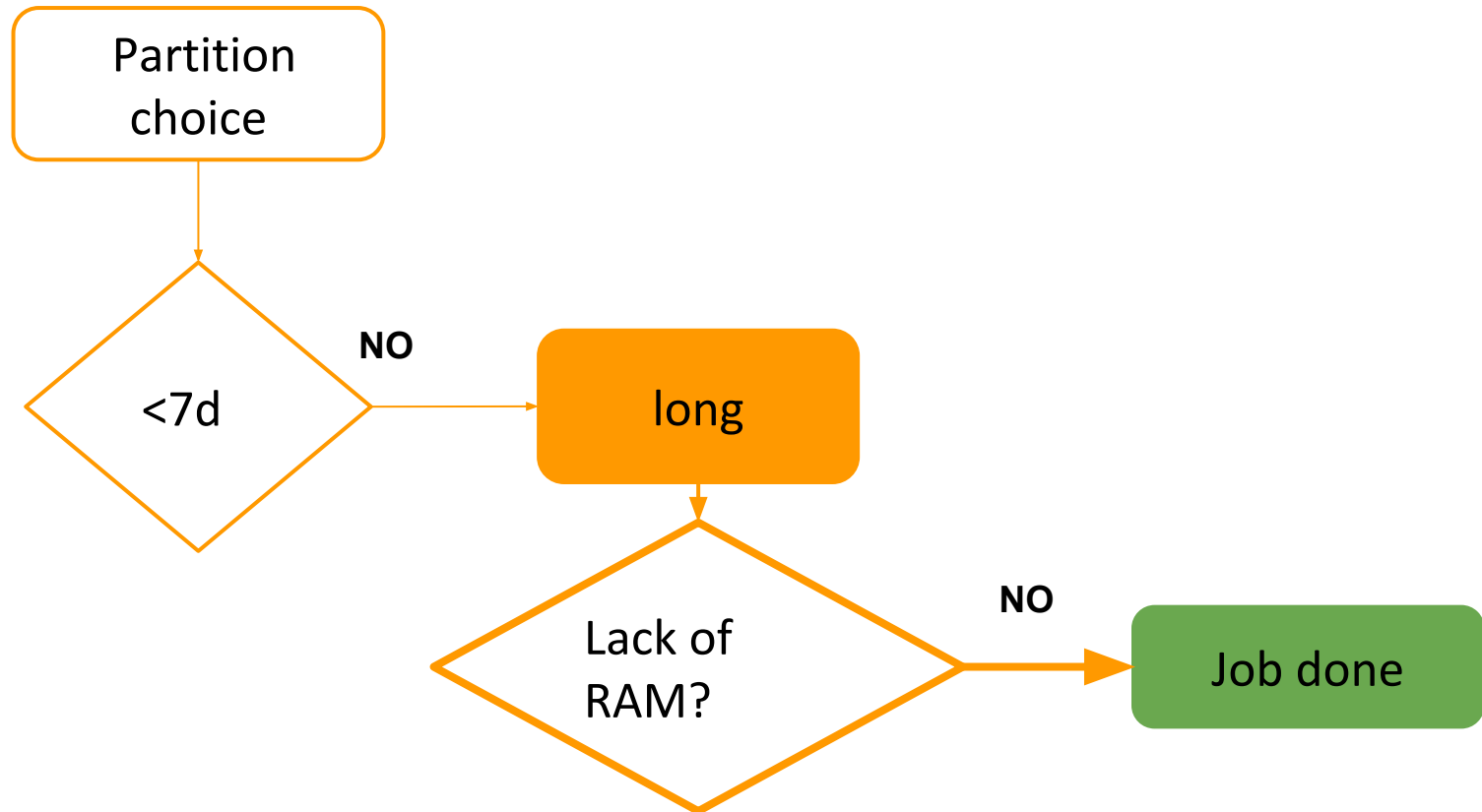
- Request access with arguments to do here:

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

Partition choice

<7d

NO

YES

Partition choice

<7d

NO

long

Partition choice

<7d

NO → long

Lack of RAM?

NO → Job done

Partition choice

<7d

NO → long

Lack of RAM?

Yes

highmem or supermem → Job done

How do I choose the partition?
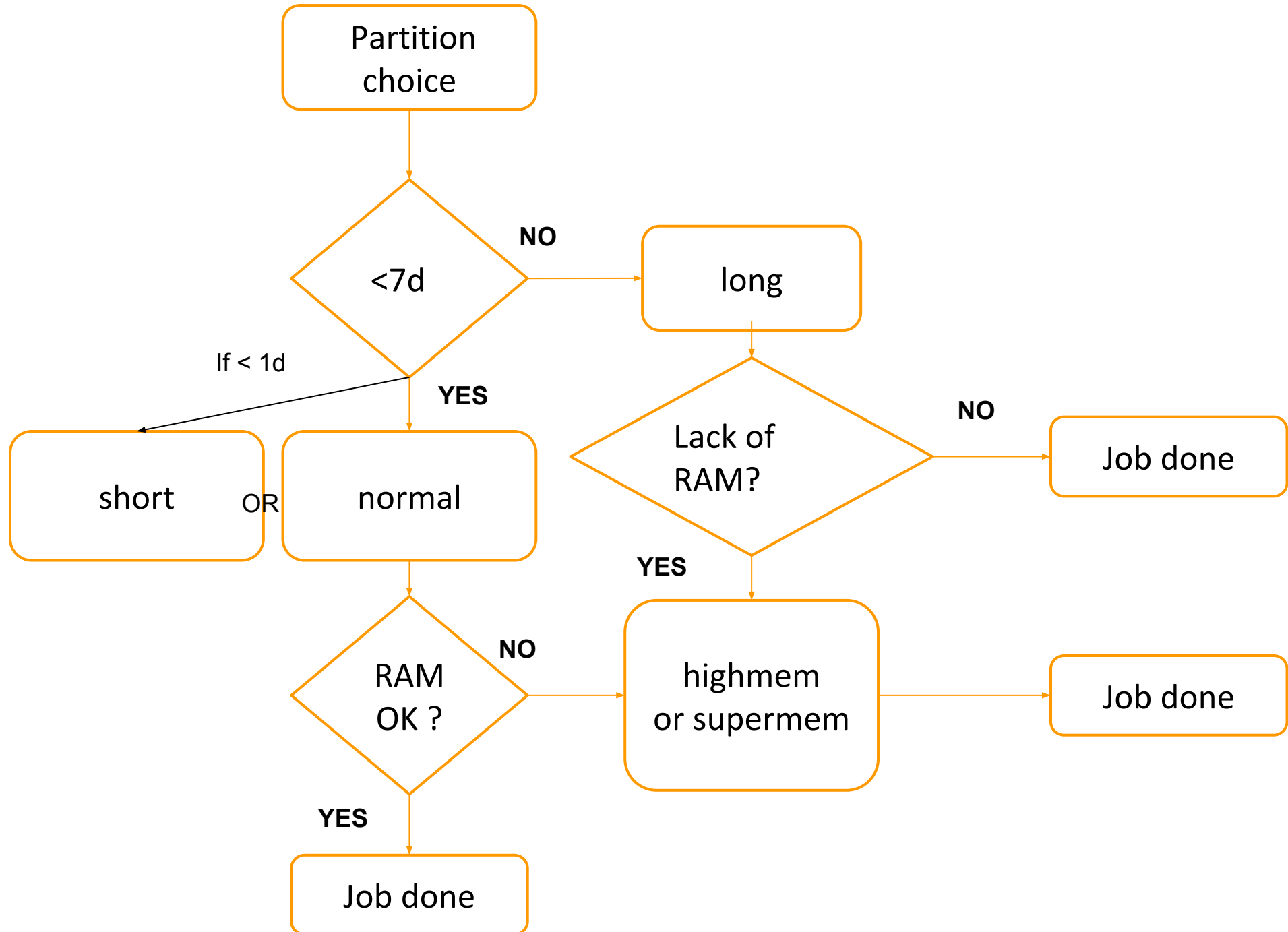
Partition choice

<7d — NO → long

If < 1d

short OR normal — YES

Lack of RAM? — NO → Job done

YES → highmem or supermem → Job done

RAM OK ? — NO → highmem or supermem

YES → Job done

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- **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`

SouthGreen bioinformatics platform

/home
/data2
/teams

bioinfo-nas.ird.fr

/data

bioinfo-nas2.ird.fr

/data3

bioinfo-nas3.ird.fr

/data /home /usr/local
/data3 /data2 /opt
/teams
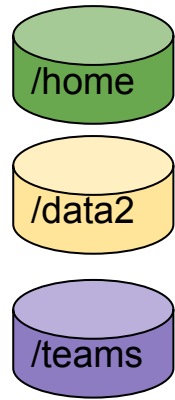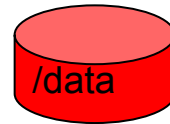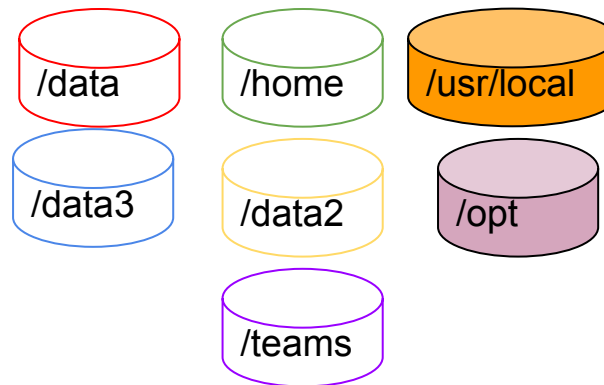
bioinfo-master.ird.fr

Virtual links to the other servers partitions

/data /home /scratch
/data3 /data2 /usr/local
/teams /opt
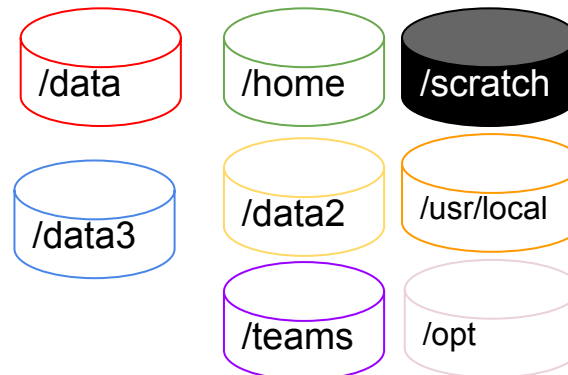
27 nodes

Connection to bioinfo-master.ird.fr and resources reservation

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

Step 1

Step 2
mkdir

Practice

2

Go to the Practice2 of the github

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PC/MAC

direct transfer via filezilla forbidden

bioinfo-master.ird.fr 91.203.34.148

/home and/or /teams or /data2

Hostname : bioinfo-nas.ird.fr

Login : cluster account

Password : cluster password
Port : **22**

bioinfo-nas.ird.fr
91.203.34.157

/data

Hostname : bioinfo-nas2.ird.fr

Login : cluster account

Password : cluster password
Port : **22**

bioinfo-nas2.ird.fr
91.203.34.160

/data3

Hostname : bioinfo-nas3.ird.fr

Login : cluster account

Password : cluster password
Port : **22**

bioinfo-nas3.ird.fr
91.203.34.180

© Can Stock Photo - csp4340788

SouthGreen bioinformatics platform

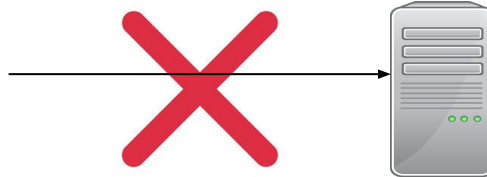| Connection to bioinfo-master.ird.fr and resources reservation	→	Creation of the analyses folder in the /scratch of the node	→	Data transfer from your PC/MAC to the nas servers
Step 1		**Step 2**		**Step 3**

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

Practice

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/

Practice

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-master.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

5

Go to the Practice5 *of the github*

Analyses steps of the cluster

Step 1 — Connection to bioinfo-master.ird.fr and resources reservation

Step 2 — Creation of the analyses folder in the /scratch of the node

Step 3 — Data transfer from your PC/MAC to the nas servers

Step 4 — Data transfer from the nas servers to the /scratch of the node

Step 5 — Load softwares with modules environment

Step 6 — Launch analyses on the data
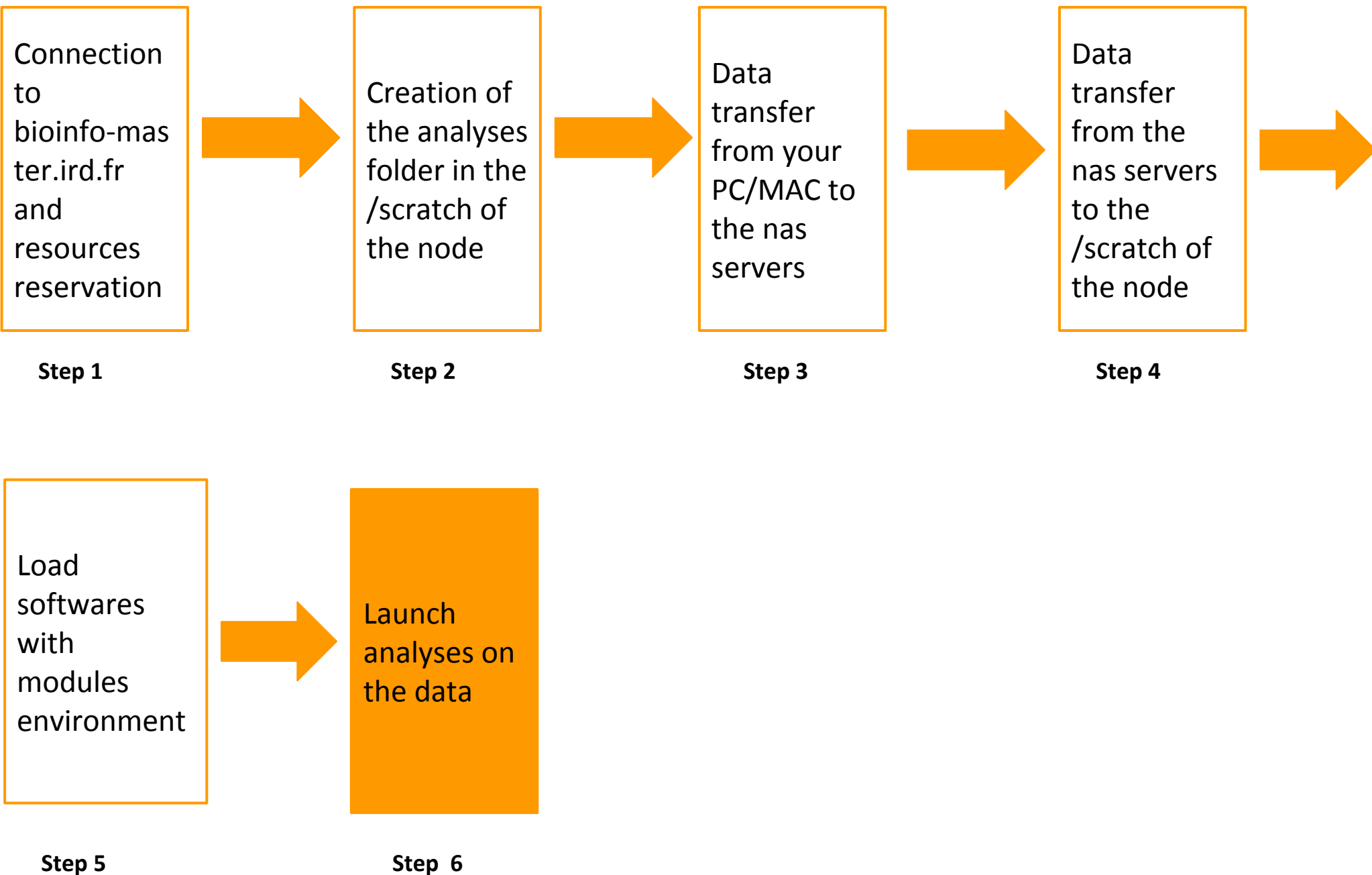
- Load the software version to launch

- Launch the data analysis

$~ *command <options> <arguments>*

With *command*: the command to launch

Practice

6

Go to the Practice6 *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

Analyses steps of the cluster

Step 1 — Connection to bioinfo-master.ird.fr and resources reservation

Step 2 — Creation of the analyses folder in the /scratch of the node

Step 3 — Data transfer from your PC/MAC to the nas servers

Step 4 — Data transfer from the nas servers to the /scratch of the node
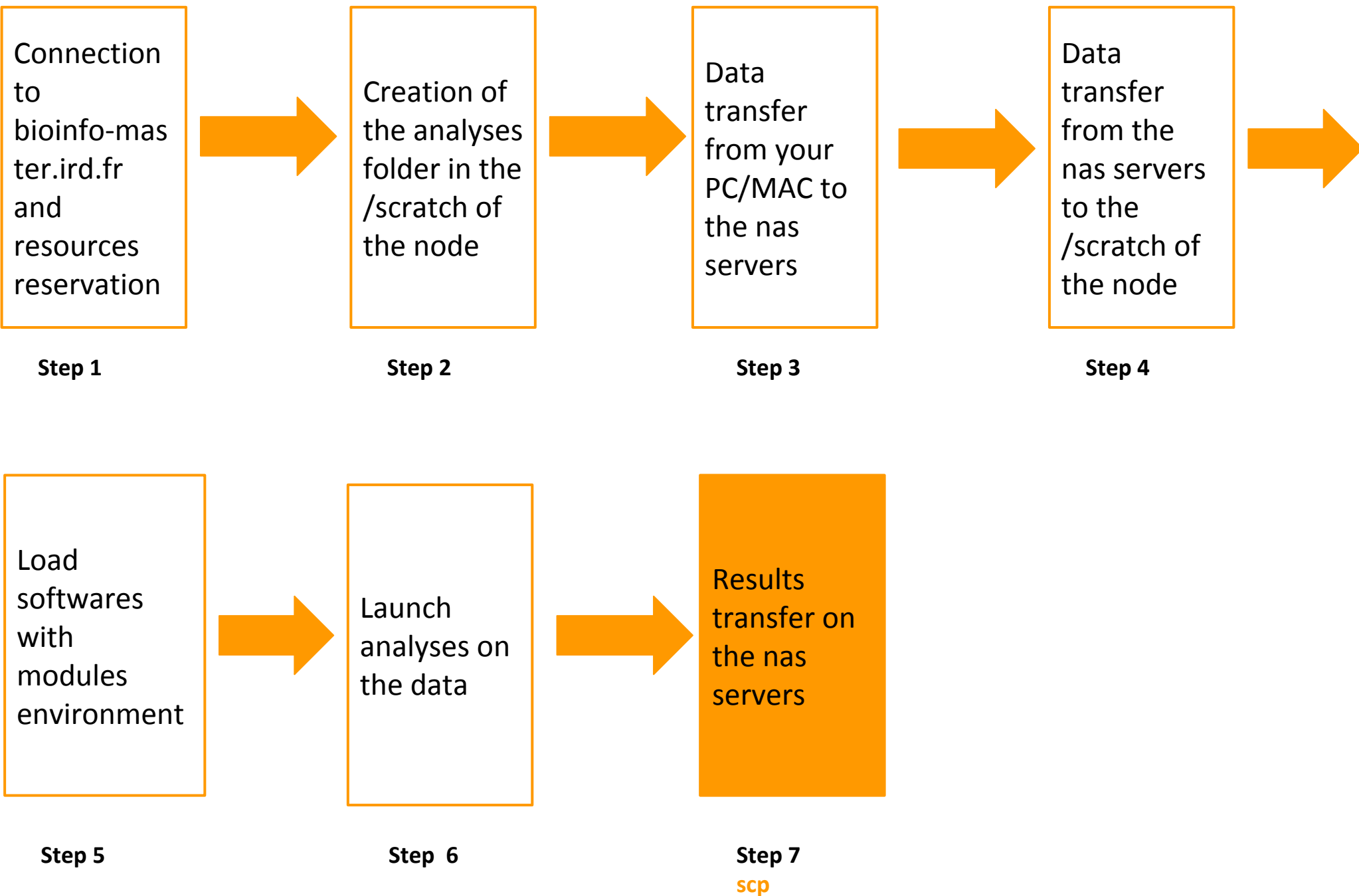
Step 5 — Load softwares with modules environment

Step 6 — Launch analyses on the data

Step 7 — Results transfer on the nas servers

scp

Practice

7

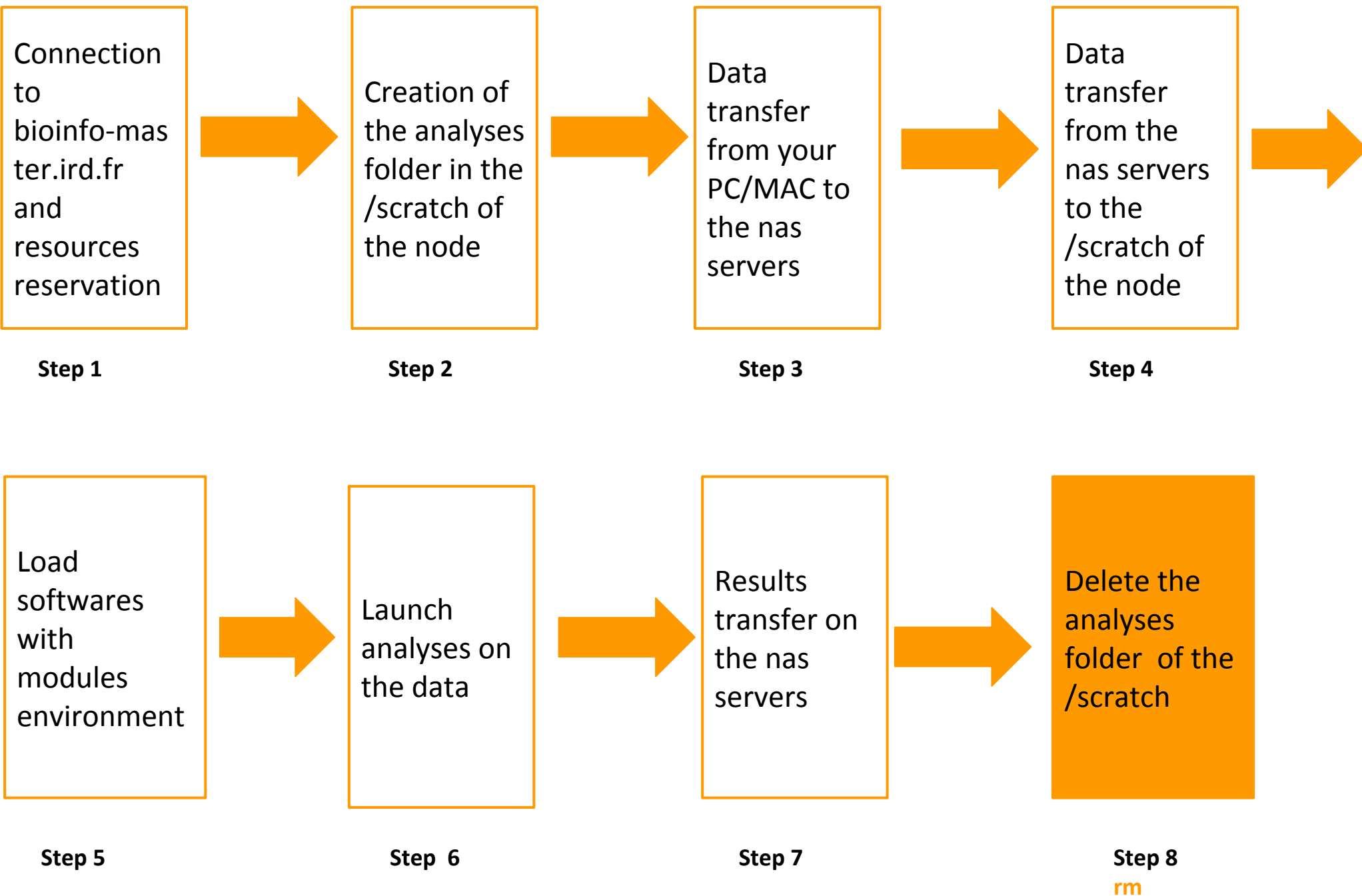*Go to the* Practice7 *of the github*

- Scratch= temporary spaces

- Verify that the copy is OK before

- Use rm command

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

Analyses steps of the cluster

Connection to bioinfo-master.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	Data transfer from the nas servers to the /scratch of the node
Step 1	**Step 2**	**Step 3**	**Step 4**

Load softwares with modules environment	Launch analyses on the data	Results transfer on the nas servers	Delete the analyses folder of the /scratch
Step 5	**Step 6**	**Step 7**	**Step 8**
			rm

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
salloc --time=0X:00	Allocate one or several nodes for a later use	salloc -N 2 --p short --time=05:00
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

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

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
--workdir=[dir_name]	Precise the working directory	sbatch --workdir=/scratch/tando script.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 Slurm
- Use:

$~ **sbatch** *script.sh*

with script.sh : the name of the script

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
--workdir=[dir_name]	Precise the working directory	sbatch --workdir=/scratch/tando script.sh

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

9

Go to the Practice9 of the github

Thank you to fill up the form at this URL:

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

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 !