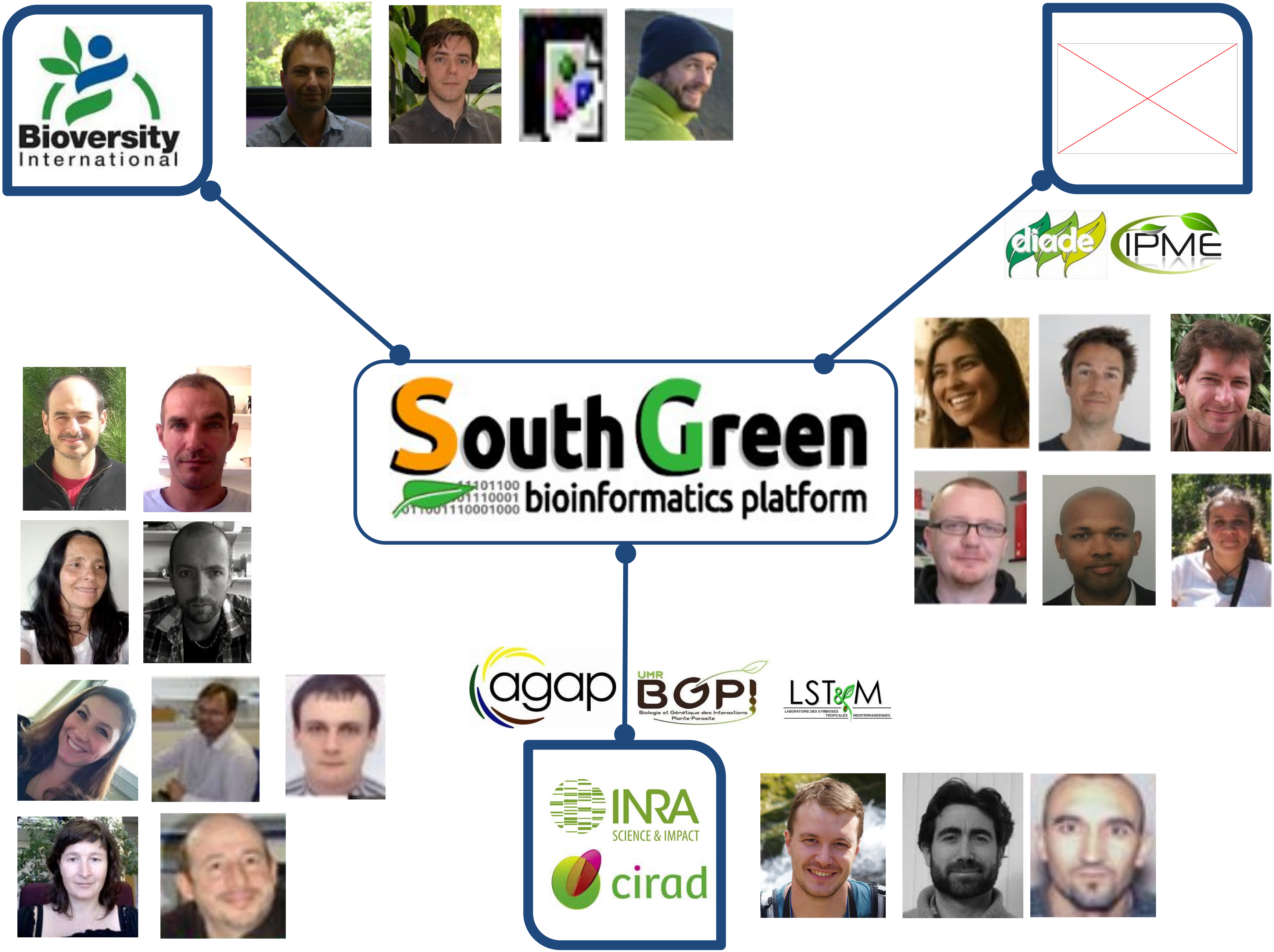
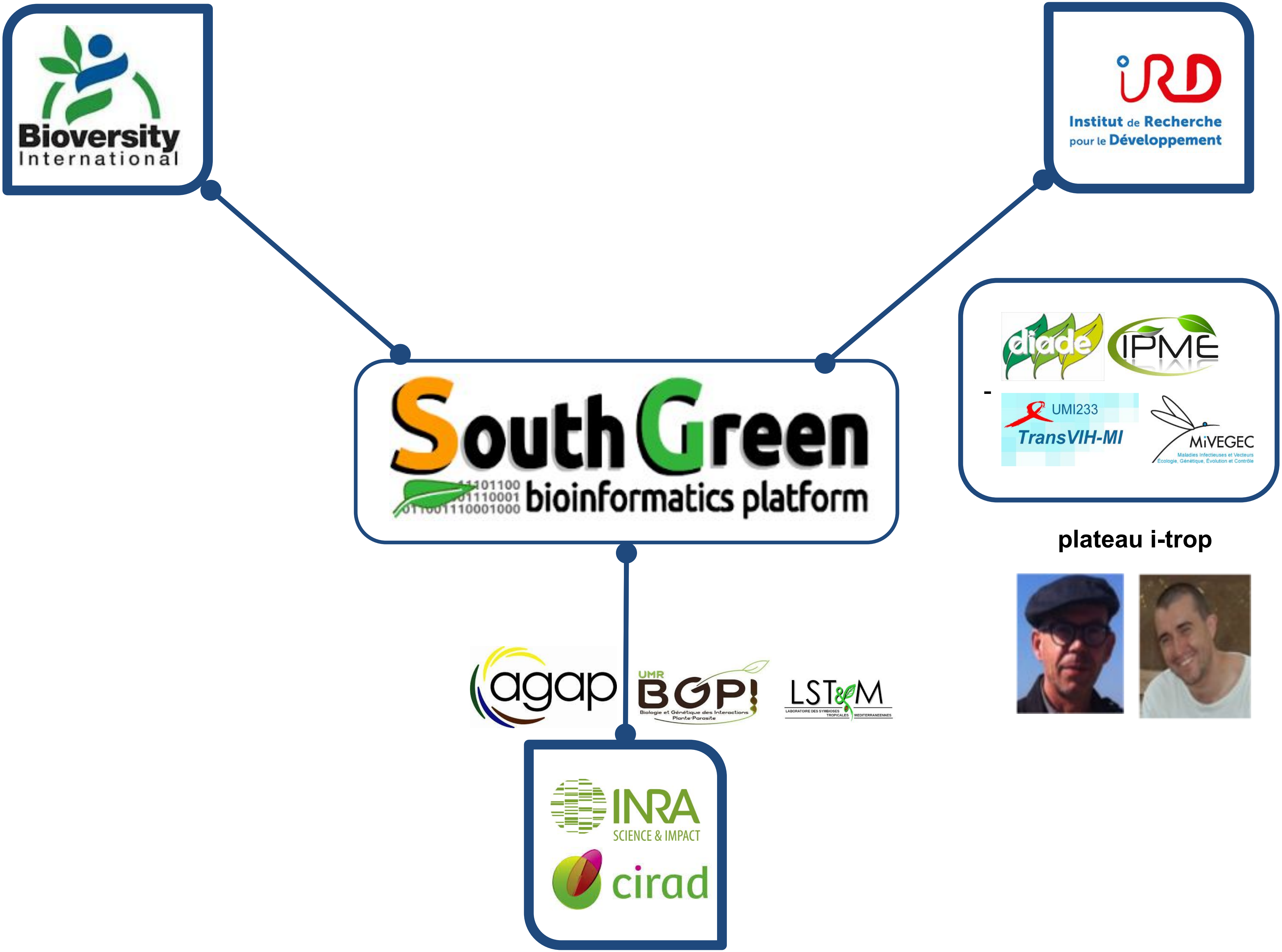

Bioversity International
South Green
bioinformatics platform
diade
IPME
agap
UMR BGPI
Biologie et Génétique des Interactions Plante-Parasite
LST&M
LABORATOIRE DES SYMBIOSES TROPICALES MEDITERRANEENNES
INRA
SCIENCE & IMPACT
cirad


Bioversity International
IRD
Institut de Recherche pour le Développement
SouthGreen
bioinformatics platform
diade
IPME
UMI233
TransVIH-MI
MiVEGEC
Maladies Infectieuses et Vecteurs
Écologie, Génétique, Évolution et Contrôle
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SCIENCE & IMPACT
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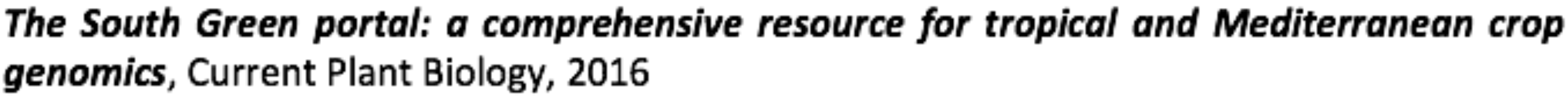
**plateau i-trop**

www.southgreen.fr

https://github.com/SouthGreenPlatform



*The South Green portal: a comprehensive resource for tropical and Mediterranean crop genomics*, Current Plant Biology, 2016

# Trainings 2018

South Green bioinformatics platform

- All trainings here :
  https://southgreenplatform.github.io/trainings/
- Presentation & trainings : HPC IRD
- Work environment : softwares to install

# HPC cluster Introduction

www.southgreen.fr

https://southgreenplatform.github.io/trainings

# Objective

## Objective

**Knowing how to use the itrop HPC Cluster**

## Applications

- Knowing the architecture of the cluster
- Knowing the role of the different systems partitions
- How to use SGE ( qsub, qrsh, qhost, qacct, qstat, qqdel)
- Use the modules environment
- Do some basic scripting

# ARCHITECTURE

# What is a cluster?

- A cluster is a logical unit composed of several servers
- Acts like a unique powerful server
- Allow to obtain a high computing performance
- A bigger storage
- A better reliability
- A high availability of the ressources

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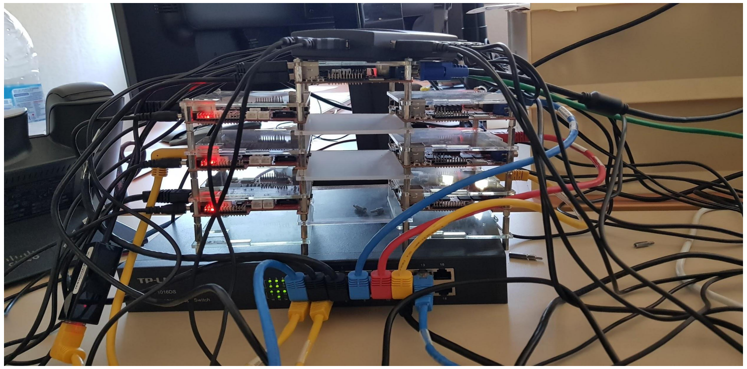

# Components of a  cluster

- Master node : Scheduler.
  Handle the  ressources and priorities of the jobs
- Computing nodes :
  Ressources (CPU or RAM memory ) used by the master

COMPUTING

# Components of a  cluster

- Master node : Scheduler.

Handle the  ressources and priorities of the jobs

- Computing nodes :

Ressources (CPU or RAM memory ) used by the master

- Nas servers:

Store the users data and the analyses results

COMPUTING

STORAGE

# Architecture: role of the components

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

Role : launch and schedule the jobs on the computing nodes

Accessible from the Internet

Connection : ssh login@bioinfo-master.ird.fr

# Architecture: role of the components

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

Role : launch and schedule the jobs on the computing nodes

Accessible from the Internet

Connection : ssh login@bioinfo-master.ird.fr

**25 noeuds with bioinfo-inter.ird.fr**
**91.203.34.150**

Role : Used by the master to execute jobs

Not accessible from the Internet

node0 à node25

Interactive node : bioinfo-inter.ird.fr

Connection : ssh login@bioinfo-inter.ird.fr

**bioinfo-nas3.ird.fr**
**91.203.34.180**

**bioinfo-nas.ird.fr**
**91.203.34.157**

**bioinfo-nas2.ird.fr**
**91.203.34.160**

Role : Store data

Accessible from the Internet

Connection : filezilla or scp

# Partitions on the  itrop cluster

/home : Your personal folder
Quota 100Go
Hosted on : bioinfo-nas.ird.fr
Shared on all servers

/teams : project data shared between users from the same team
Quota 200Go
Hosted on  : bioinfo-nas.ird.fr
Shared on all servers

/data2 : project data shared between several users
Quota 500Go à 1To
Hosted on: bioinfo-nas.ird.fr
Shared on all servers

# Partitions on the itrop cluster

/home : Your personal folder
Quota 100Go
Hosted on : bioinfo-nas.ird.fr
Shared on all servers

/data : project data shared between several users
Quota 500Go à 1To
Hosted on : bioinfo-nas2.ird.fr
Shared on all servers

/teams : project data shared between users from the same team
Quota 200Go
Hosted on : bioinfo-nas.ird.fr
Shared on all servers

/data3 :Données projet partagées entre plusieurs utilisateurs
Quota 500Go à 1To
Hosted on : bioinfo-nas3.ird.fr
Shared on all servers

/data2 : project data shared between several users
Quota 500Go à 1To
Hosted on: bioinfo-nas.ird.fr
Shared on all servers

# Partitions on the itrop cluster

/home : Your personal folder
Quota 100Gb
Hosted on : bioinfo-nas.ird.fr
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Hosted on : bioinfo-nas.ird.fr
Shared on all servers

/data2 : project data shared between several users
Quota 500Gb to 1Tb
Hosted on: bioinfo-nas.ird.fr
Shared on all servers

/data : project data shared between several users
Quota 500Gb to 1Tb
Hosted on : bioinfo-nas2.ird.fr
Shared on all servers

/data3 :project data shared between several users
Quota 500Gb to 1Tb
Hosted on : bioinfo-nas3.ird.fr
Shared on all servers

/scratch : temporary working folder
1Tb to 5Tb
Hosted on : each node
Not shared local only
Data kept **3 weeks only**

# SUN GRID ENGINE (SGE)

# The scheduler sge

- SGE (SUN Grid Engine) is a linux job scheduler, able to handle from 2 to thousands of servers at the same time.
- An opensource tool
- 3 main functions :

  - Allocates ressources (CPU,RAM) to users to allow them to launch their analyses
  - Provides a frame to launch,execute et monitore the jobs on the whole allocated nodes
  - Deals with jobs in queue wait

# Sge queue on the cluster

Bioinfo.q : default queue
Nodes: node2, node8, node9, node10, node11,node12,node13, ,node14,node15,node16,node17, node19,node20
RAM: from 48Go to 64Go
Cores: from 12 to 20 cores

dynadiv.q : priority for the dynadiv team
Nodes: node2, node10
RAM: 48Go
Cores: 12 cores
**/scratch of 5To for node10**

dynadiv2.q : priority for thomas Couvreur
Nodes: node20
RAM: 64Go
Cores: 20 cores

smrtportal.q : priority for the smrtportal software
Nodes: node17, node18
RAM: 64Go
Cores: 12 cores

alizon.q : priority for the samuel Alizon team
Nodes: node8, node9, node12
RAM: 48Go
Cores: 12 cores

# Sge queue on the cluster

Bioinfo.q : default queue
Nodes: node2, node8, node9, node10, node11,node12,node13, ,node14,node15,node16,node17, node19,node20
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Nodes: node17, node18
RAM: 64Go
Cores: 12 cores

alizon.q : priority for the samuel Alizon team
Nodes: node8, node9, node12
RAM: 48Go
Cores: 12 cores

r900.q : queue with **DELL nodes**
Nodes: node5, node21
RAM: 32Go
Cores: 16 cores

longjob.q : long jobs or > to10 jobs
Nodes: node0, node1, node11
RAM: 48Go
Cores: 12 cores

bigmem.q : memory need
Nodes: node3
RAM: 96Go
Cores: 12 cores

highmem.q :big need of memory
Nodes: node4 et node7
RAM: 144Go
Cores: 12 cores

# Sge commands: ressources allocation

| Actions | Commands |
|---|---|
| Reserve a core on a node in an interactive way | $ **qrsh** |
| Reserve a core on a particular node | $ **qrsh -l hostname=nodeX**<br>With X the node number |
| Reserve X cores on a node | $~ **qrsh -pe ompi X**<br>With X : number of processors from 0 to 12 |

# Sge commands: qsub options

| Actions | Commands |
|---|---|
| Launch a script in batch mode | $qsub + script.sh |
| Propagate the load environment to the node | $qsub -V script.sh |
| Name your job | $~ qsub -N job_name script.sh |
| Use several processors | $~ qsub -pe ompi X script.sh<br>With X the nomber of cores to use |
| Have a certain amount of memory | $~ qsub -l mem_free=XG script.sh<br>With X the amount of memory to reserve |
| Have a particular node | $~ qsub -l hostname=nodeX script.sh |
| Directly launch a command with qsub | $~ qsub -b y command |

# Sge commands : Informations

| Actions | Commands |
|---|---|
| Informations on nodes | $ **qhost** |
| Watch your jobs state | $~ qstat |
| Informations on running jobs | $~ **qstat -j <JOB_ID>**<br>With JOB_ID :the job number |
| Informations on completed jobs | $~ **qacct -j <JOB_ID>**<br>With JOB_ID :the job number |
| Global informations on queues | $~ **qstat -g c** |

# Sge commands: deletion

Actions

- Deletion of a job

Commandes

```
$~ qdel <JOB_ID>
```

With JOB_ID : the job id

1

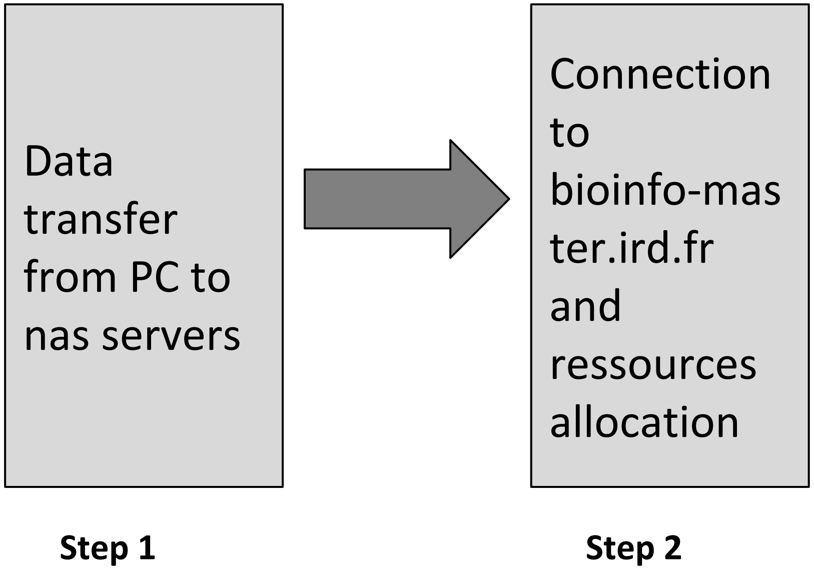
# Training: Launch a blast analysis in a interactive way

# Analyse steps on the cluster

Data transfer from PC to nas servers

**Step 1**

# Analyse steps on the cluster



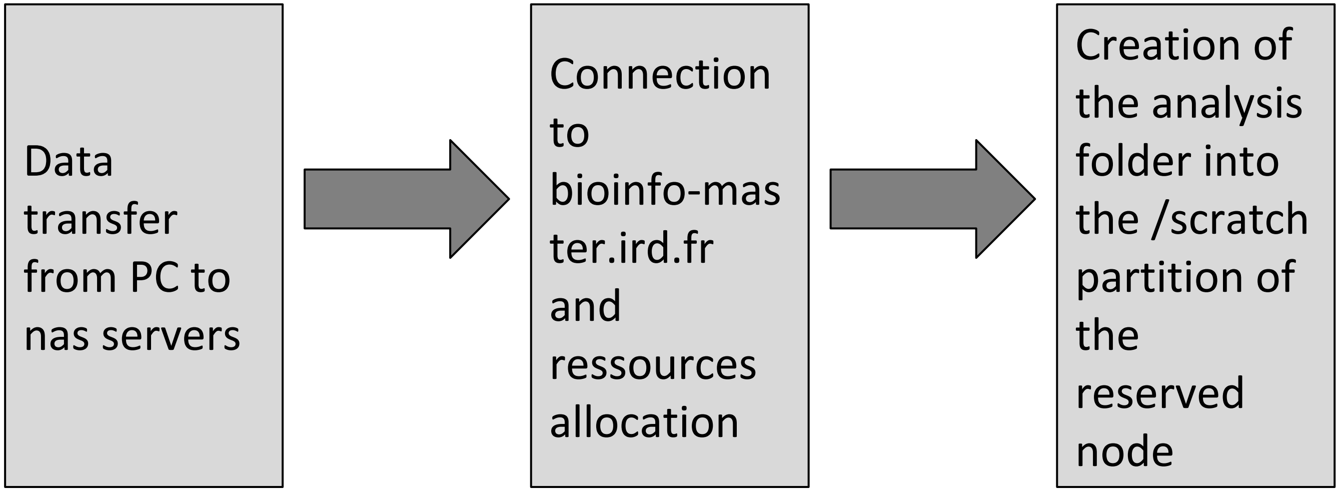
Data transfer from PC to nas servers

Step 1

Connection to bioinfo-master.ird.fr and ressources allocation

Step 2

# Analysis steps on the cluster



Data transfer from PC to nas servers

Connection to bioinfo-master.ird.fr and ressources allocation

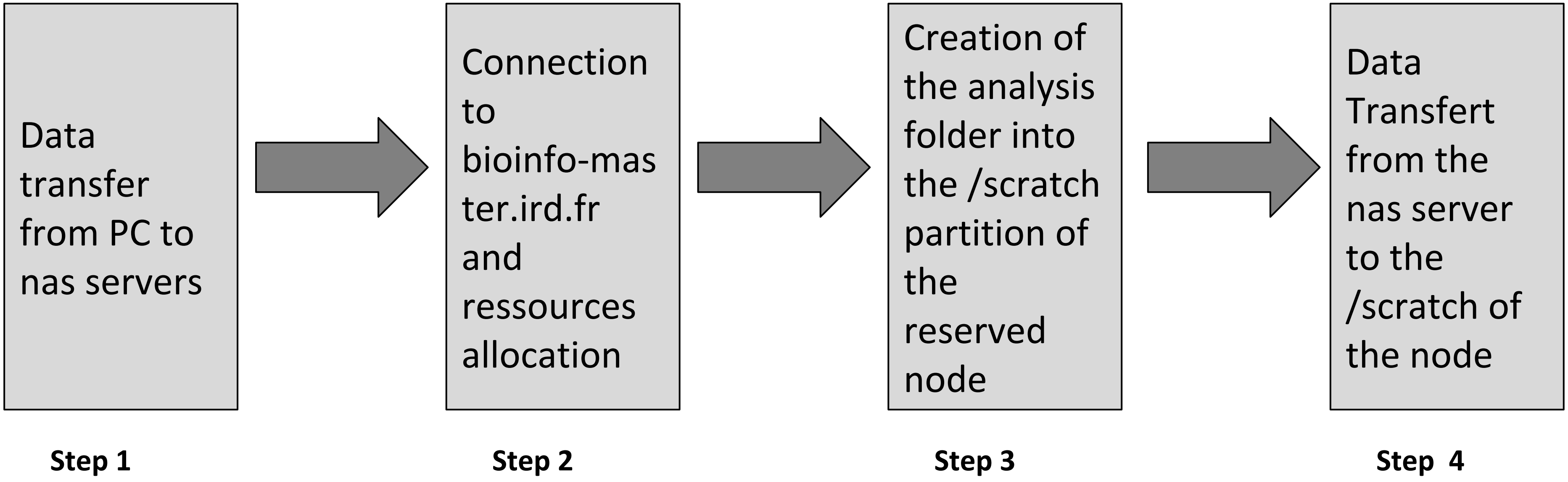
Creation of the analysis folder into the /scratch partition of the reserved node

**Step 1**

**Step 2**

**Step 3**

# Analysis steps on the cluster



Data transfer from PC to nas servers

Step 1

Connection to bioinfo-master.ird.fr and ressources allocation

Step 2

Creation of the analysis folder into the /scratch partition of the reserved node

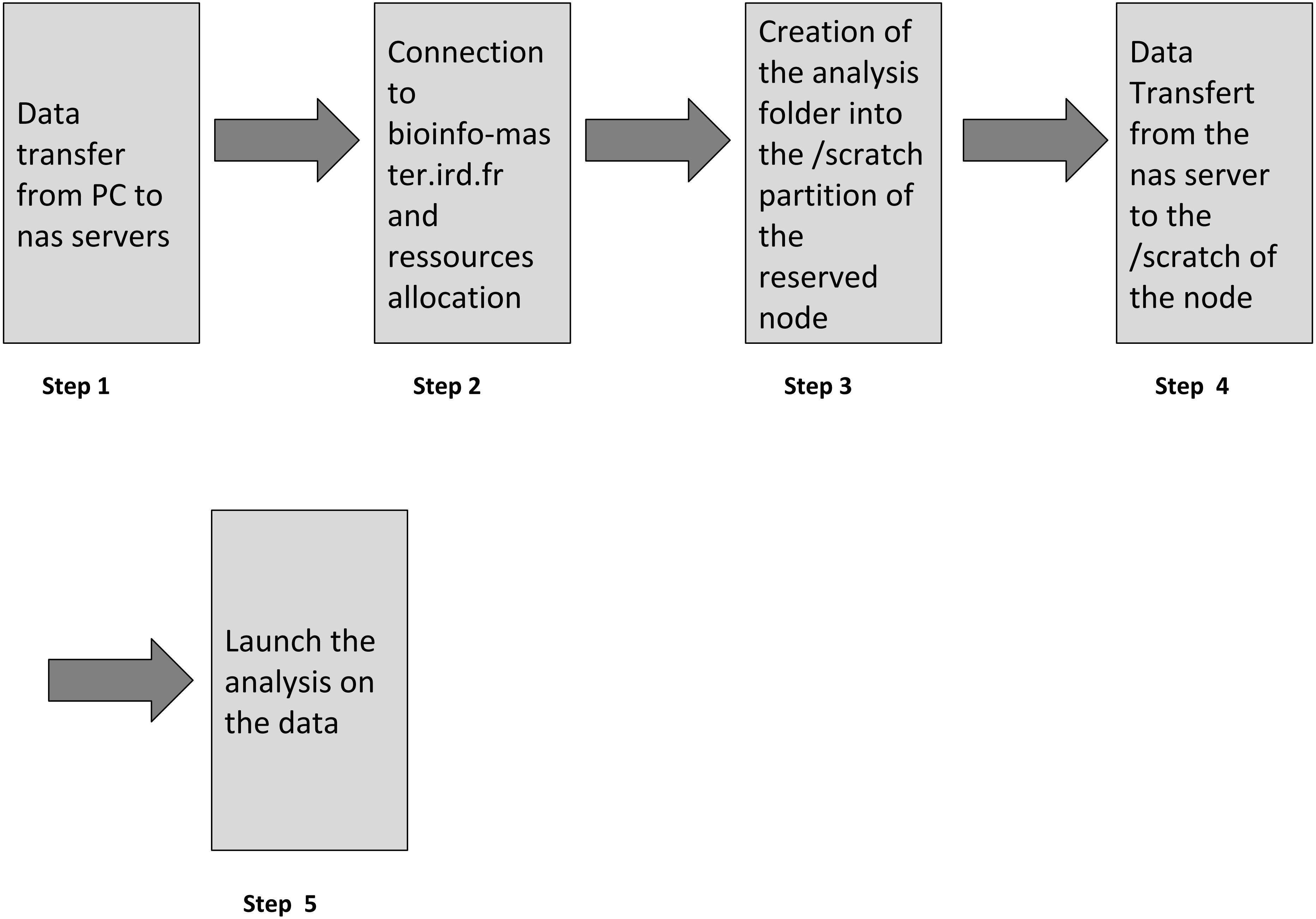
Step 3

Data Transfert from the nas server to the /scratch of the node

Step 4

Step 7

# Analysis steps on the cluster



Data transfer from PC to nas servers

Step 1

Connection to bioinfo-master.ird.fr and ressources allocation

Step 2

Creation of the analysis folder into the /scratch partition of the reserved node

Step 3

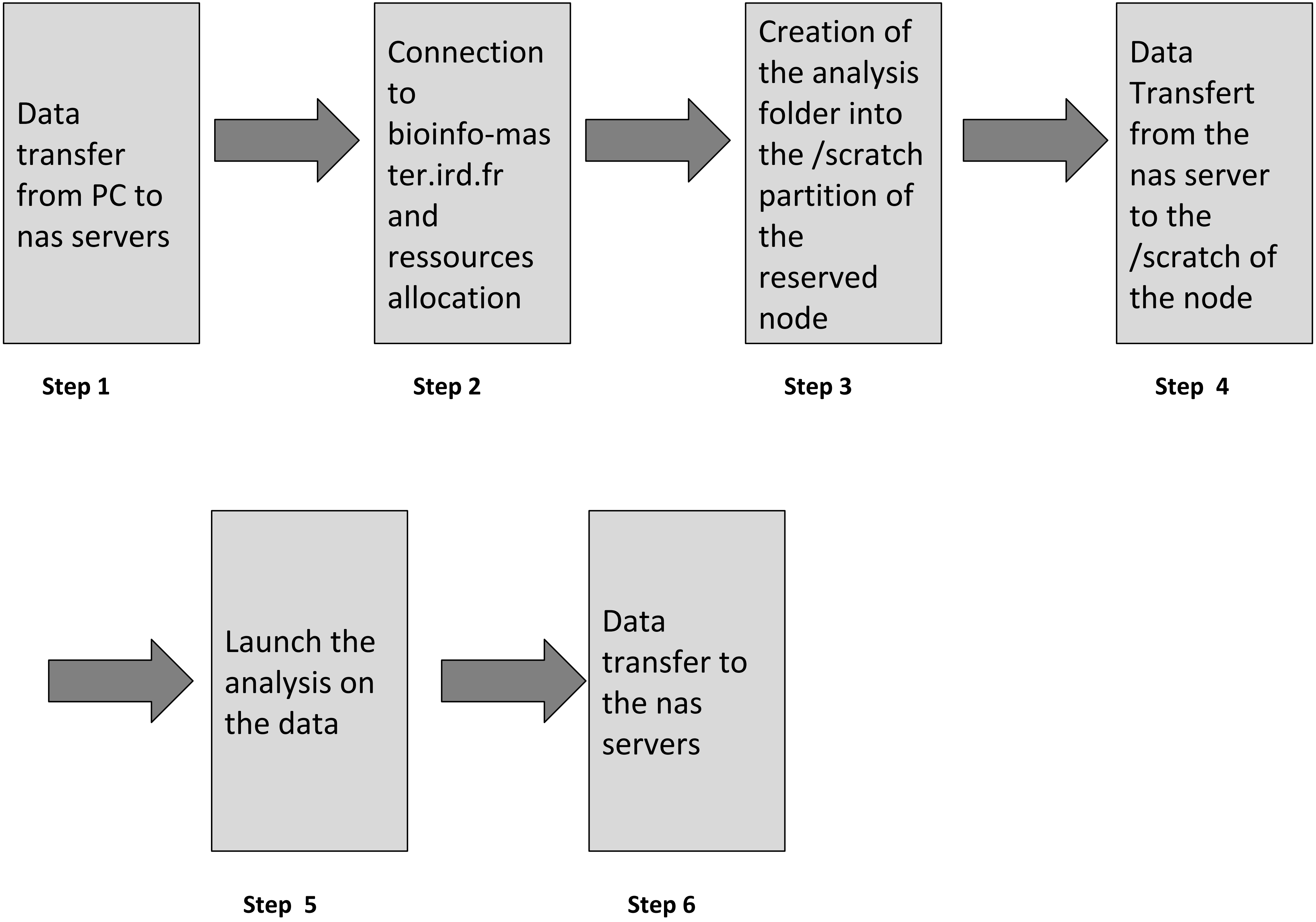
Data Transfert from the nas server to the /scratch of the node

Step 4

Launch the analysis on the data

Step 5

# Analysis steps on the cluster



Data transfer from PC to nas servers

**Step 1**

Connection to bioinfo-master.ird.fr and ressources allocation

**Step 2**

Creation of the analysis folder into the /scratch partition of the reserved node

**Step 3**

Data Transfert from the nas server to the /scratch of the node

**Step 4**

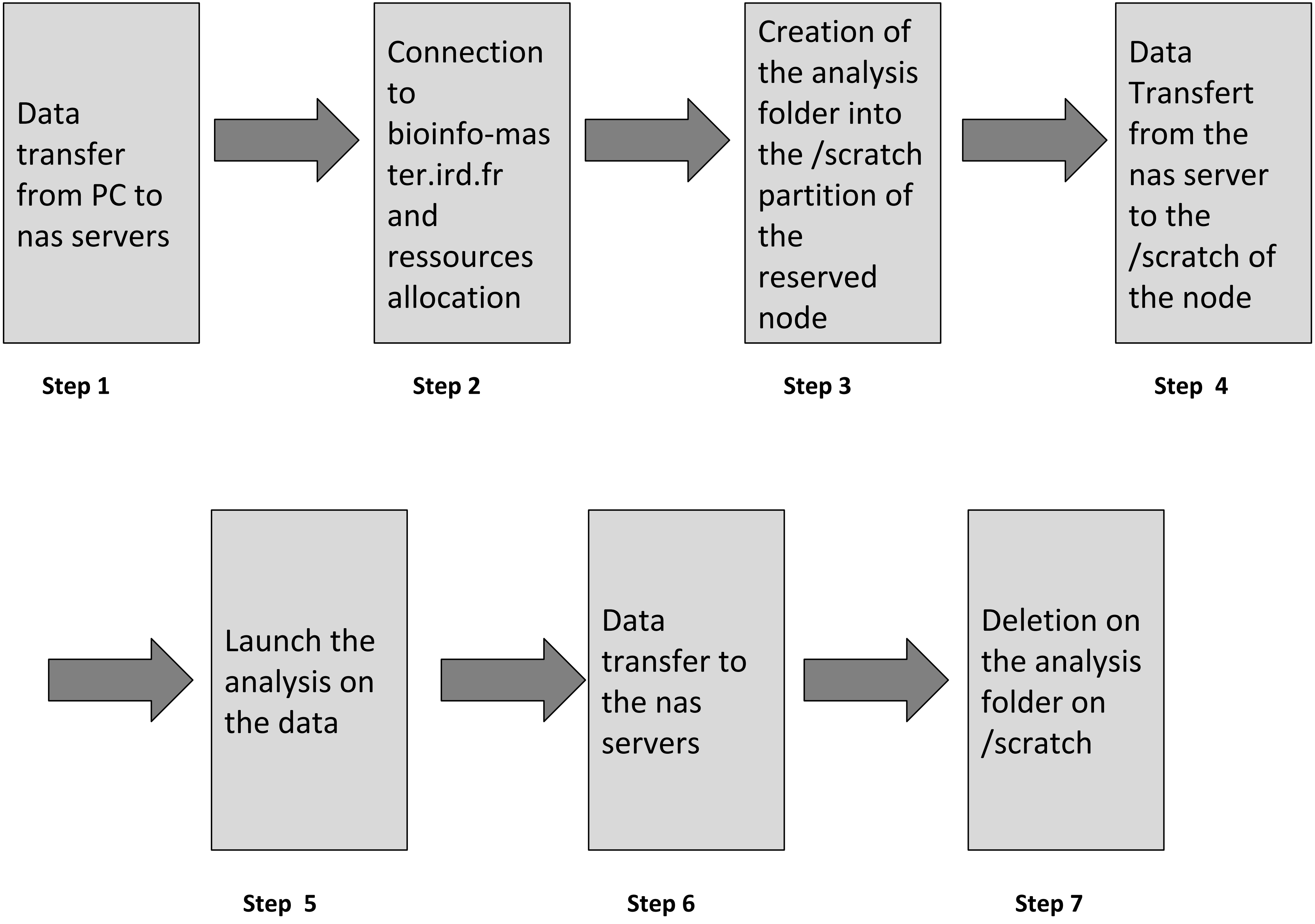
Launch the analysis on the data

**Step 5**

Data transfer to the nas servers

**Step 6**

# Analysis steps on the cluster



Data transfer from PC to nas servers

Step 1

Connection to bioinfo-master.ird.fr and ressources allocation

Step 2

Creation of the analysis folder into the /scratch partition of the reserved node

Step 3

Data Transfert from the nas server to the /scratch of the node

Step 4

Launch the analysis on the data

Step 5

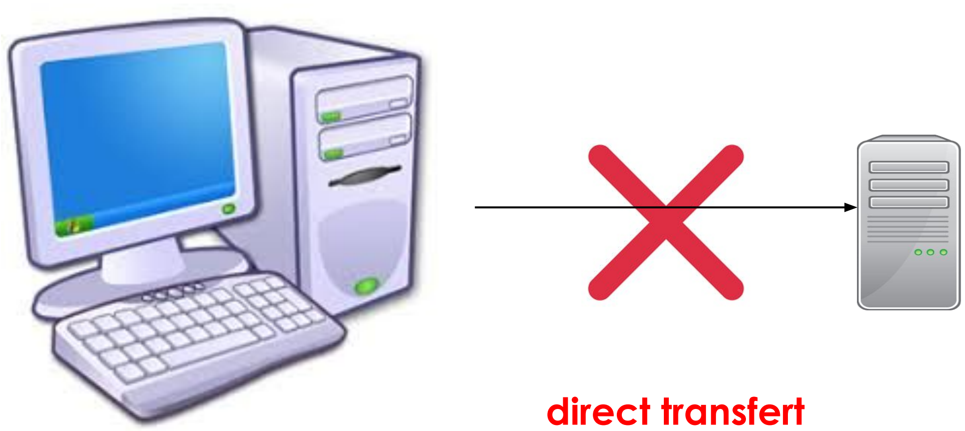
Data transfer to the nas servers

Step 6

Deletion on the analysis folder on /scratch

Step 7

# Data transfer on  the cluster itrop

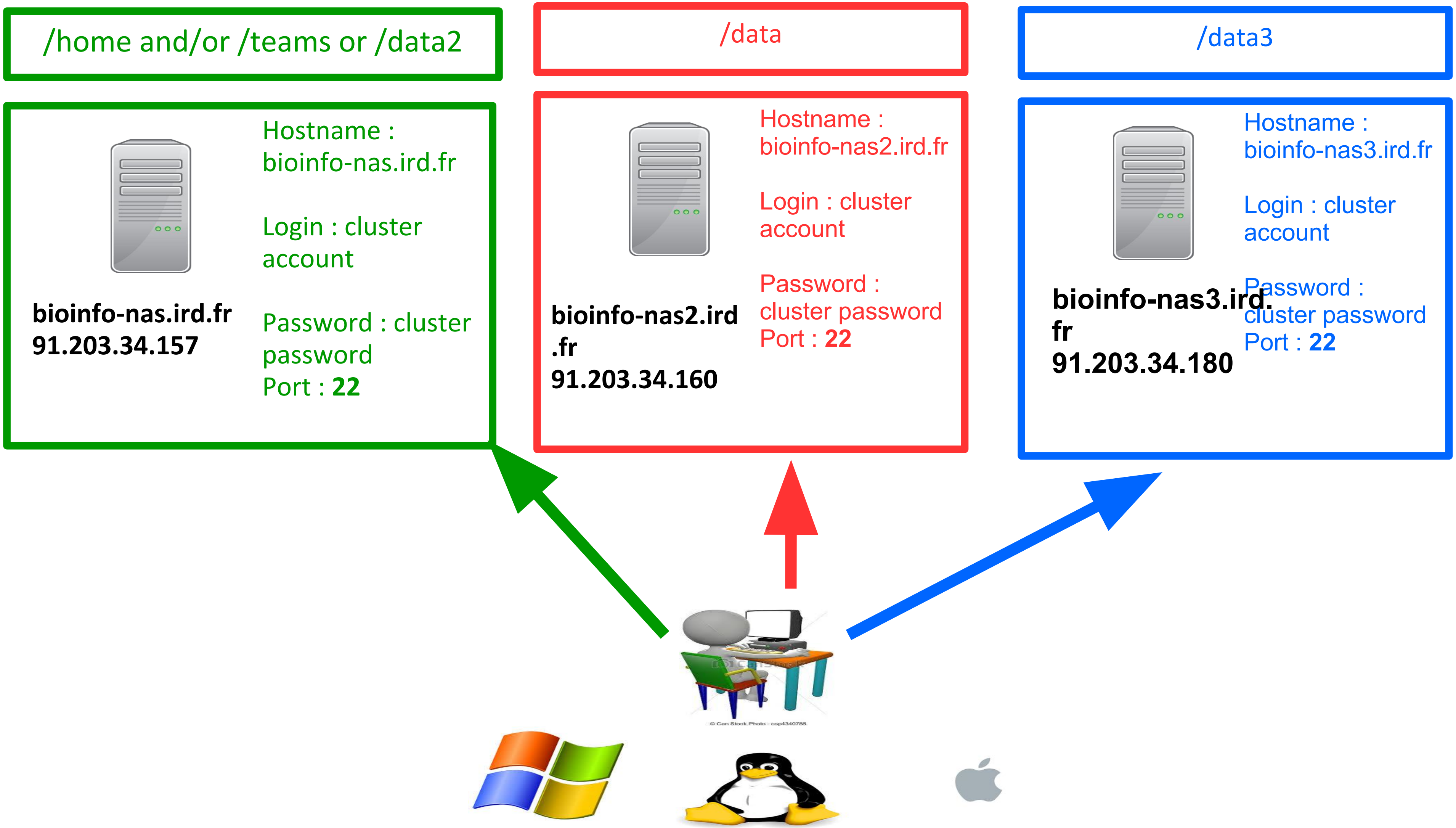


bioinfo-master.ird.fr
91.203.34.148

direct transfert
through filezilla
is forbidden

Personal
Computer

# Data transfer on the cluster itrop



/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**

# Step 1: Data copy  on the cluster

Open filezilla and retrieve the file « HPC_en.pdf »
Hosted in /data/projects/tp-cluster/training_2018

# Step1: Data copy on the cluster

Open filezilla and retrieve the file « HPC_en.pdf »
Hosted in /data/projects/tp-cluster/training_2018

Enter the following parametres:

Hostname : **bioinfo-nas2.ird.fr**
Login : votre login
Password : votre login
Port :**22**
Navigate into the right window through /data/projects/tp-cluster/training_2018
Retrieve the file HPC_en.pdf with a drag-and-drop

# Connection to the itrop cluster

## Launch scripts to several nodes

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

Use the qsub command

Hostname : bioinfo-master.ird.fr

Login : cluster account

Password : cluster password

Port : **22**

## Test your script(s)

**bioinfo-inter.ird.fr**
**91.203.34.150**

Hostname : bioinfo-inter.ird.fr

Login : cluster account

Password : cluster password

Port : **22**

Or use the qrsh command on bioinfo-master.ird.fr

With Putty
Use parameters above

With terminal
Use the ssh command

# Step2:  core reservation on a node

Connect to  bioinfo-master.ird.fr via ssh

Type :
$~ssh login@bioinfo-master.ird.fr onApple or Linux

Under windows : Download Mobaxterm to :
https://mobaxterm.mobatek.net/download-home-edition.html
Then connect to bioinfo-master.ird.fr

# Step2:  core reservation on a node

We can reserve a core of a node to launch an analysis
Through a limited time  using the qrsh  command
Type the qstat command and analyse the result

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We can reserve a core of a node to launch an analysis
Through a limited time using the qrsh command
Type the qstat command and analyse the result

Type :

```
$~qrsh
```

Check on wich node you are with the command

```
$~ uname -a
$~ qstat
```

# Step3 : analyses folder creation

Go into /scratch
Create a folder to host your data

# Step3 : analyses folder creation

Go into /scratch
Create a folder to host your data

Type the commands :

```
$~cd /scratch
$~ mkdir login ( with login the name folder of your choice)
```

# Data transfer with scp

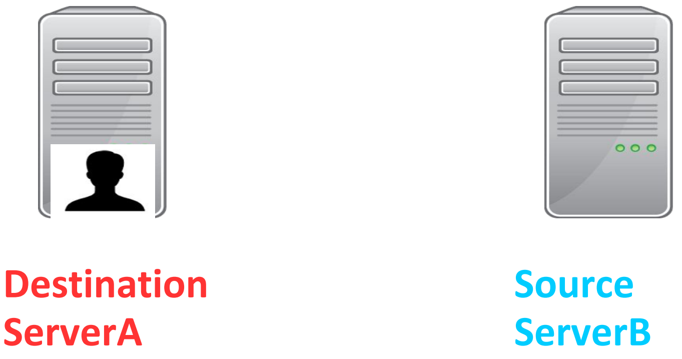
Being connected to A

Remote folder to transfer : /data/projects/tp-cluster/training_2018

Login  : login

Destination folder on the node : /scratch/tando

Copy remote folder from server B to local server A



# Data transfer with scp

Being connected to A

Remote folder to transfer : /data/projects/tp-cluster/training_2018

Login  : login

Destination folder on the node : /scratch/tando

Copy remote folder from server B to local server A

```
scp -r        login@source_server:/remote_path
```

/data/projects/tp-cluster/training_2018

Destination
ServerA

Source
ServerB

# Data transfer with scp

Being connected to A

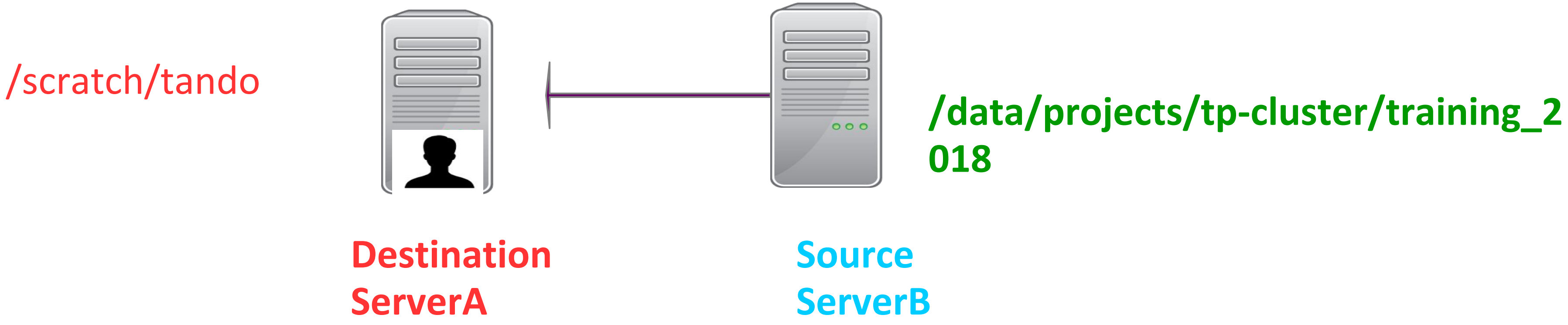
Remote folder to transfer : /data/projects/tp-cluster/training_2018

Login : login

Destination folder on the node : /scratch/tando

Copy remote folder from server B to local server A

```
scp -r      login@source_server:/remote_path      local_folder
```



# Data transfer with scp

Being connected to A

Remote folder to transfer : /data/projects/tp-cluster/training_2018

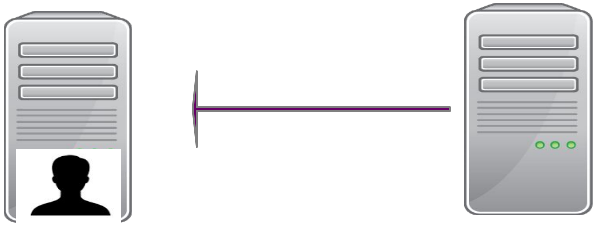
Login  : login

Destination folder on the node : /scratch/tando

Copy remote folder from server B to local server A

```
scp -r      login@source_server:/remote_path      local_folder
```

/scratch/tando



/data/projects/tp-cluster/training_2018

**Destination ServerA**

**Source ServerB**

```
scp -r    login@serverB:/data/projects/tp-cluster/training_2018
```

# Data transfer with scp

Being connected to A

Remote folder to transfer : /data/projects/tp-cluster/training_2018

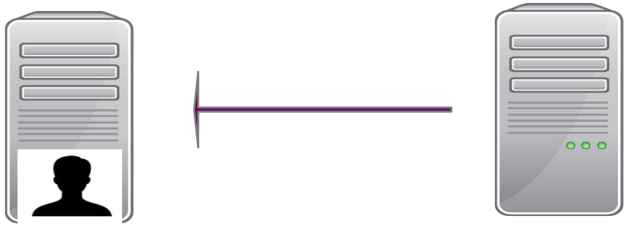
Login : login

Destination folder on the node : /scratch/tando

Copy remote folder from server B to local server A

```
scp -r      login@source_server:/remote_path      local_folder
```

/scratch/tando



/data/projects/tp-cluster/training_2018

Destination
ServerA

Source
ServerB

```
scp -r     login@serverB:/data/projects/tp-cluster/training_2018/scratch/tando
```

# Step 4 : Data copy  to the analyses folder

Copy the folder /data/projects/tp-cluster/training_2018/Blast to /scratch/login

# Step 4 : Data copy  to the analyses folder

Copy the folder /data/projects/tp-cluster/training_2018/Blast to /scratch/login

Type the commands :

```
$~cd /scratch/login
$~ scp -r login@bioinfo-nas2.ird.fr :/data/projects/tp-cluster/training_2018/Blast /scratch/login
```

# Step 5 : Go into the copied folder

Go into the folder /scratch/login/Blast
List the files of the folder

# Step 5 : Go into the copied folder

Go into the folder /scratch/login/Blast
List the files of the folder

Type :

```
$~cd /scratch/login/Blast
$~ ls -ali
```

# 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

- 5 types of commands :

See the available modules : module avail
Obtain infos on a particular module: module whatis + module name
For example module whatis bioinfo/blast/2.4.0+
Load a module : module load + modulename
For example module load bioinfo/blast/2.4.0+
List the loaded module : module list
Unload a module : module unload + modulename
For example module unload bioinfo/blast/2.4.0+
Unload all the modules :
Module purge

# Step 6 : Launch an analysis

Load the blast module version 2.4.0+
Use the blastn  command  to launch a blast analysis
Hat will produce the result file  called blastn.out

# Step 6 : Launch an analysis

Load the blast module version 2.4.0+
Use the blastn command to launch a blast analysis
Hat will produce the result file called blastn.out

Type :

```
$~ module load bioinfo/blast/2.4.0+
$~ blastn -db All-EST-coffea.fasta -query sequence-NMT.fasta -out blastn.out
```

# Step 7: File result analysis

Edit the blastn.out file  with the nano tool

# Step 7: File result analysis

Edit the blastn.out file  with the nano tool

Type :

```
$~ nano blastn.out
```

# Step 8 : Copy the result to your /home

Copy the file blastn.out to your  home folder
Check that the file has been copied

# Step 8 : Copy the result to your /home

Copy the file blastn.out to your  home folder
Check that the file has been copied

Type :

```
$~scp blastn.out login@bioinfo-nas.ird.fr:/home/login
$~ ls -ali /home/login
```

# Step 9 :Deletion of the folder in /scratch

Go into the /scratch folder
Delete your working directory

Type:

```
$~cd /scratch
$~ rm -rf login
```

2

# TP: Launch a bwa in a interactive way

# Training : Launch a bwa analysis

- Follow the steps from the last training and adapt them to this one
- The folder to copy: /data/projects/training_2018/bwa
- Bwa version to use:  0.7.12
- Commands to launch:

```
bwa index referenceIrigin.fasta
bwa mem referenceIrigin.fasta irigin1_1.fastq irigin1_2.fastq >mapping.sam
```

- Retreive the file mapping.sam and place it in your /home/

Cf solution: **practice2**

3

# Training: Launch an analyse via a bash script

# Launch a job in batch mode

- Execute a bash script via sge
- We use the command:

```
$~ qsub script.sh
```

With script.sh : the script name

# Bash scripts syntax

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

```
#!/bin/sh


############      SGE CONFIGURATION      ###################
# wirite errors in standard outputfile
#$ -j y

# Shell we want to use
#$ -S /bin/bash



# Email to follow the job
#$ -M prenom.nom@ird.fr          ######### Mettre son adresse mail

# Type of messges by mail
#    -  (b) beginning message
#    -  (e)end message
#    -  (a) abort message
#$ -m bea

# Queue to use
#$ -q bioinfo.q

# Name of the job
#$ -N name_to_choose
############################################################
```

# Bash scripts syntax

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

```
path_to_dir="/data/projects/rep_a_choisir";
path_to_tmp="/scratch/nom_rep_a_choisir-$JOB_ID"

###### Create the temporary folder on the node and load the blast module
module load bioinfo/blastn/2.4.0+
mkdir $path_to_tmp
scp -rp nas2:$path_to_dir/* $path_to_tmp # choose nas for /home, /data2 and /teams or nas2 for /data or nas3 for /data3
echo "tranfert from master -> noeud";
cd $path_to_tmp

###### Program execution
cmd="blastn -db All-EST-coffea.fasta -query  sequence-NMT.fasta -num_threads $NSLOTS  -out blastn1-$JOB_ID.out";
echo "executed command : $cmd";
$cmd;

##### Data transfer from node to nas
scp -rp $path_to_tmp/ nas:$path_to_dir/
echo "Transfert from node -> master";

#### Deletion of the tmp folder
rm -rf $path_to_tmp
echo "Deletion on the node";
```

# Blastn script creation

- Using the  Training 1  create a script to launch a blastn analysis
- Make the script launchable with

```
$~ chmod 755 script.sh
```

- Launch the script with qsub:

```
$~ qsub script.sh
```

- Check the running script with the command: watch qstat

**solution script blastn**

⚠ Use the dos2unix command when the script has been written under Windows

# Bwa script creation

- Using the  Training 1  create a script to launch a bwa analysys
- Make the script launchable with

```
$~ chmod 755 script.sh
```

- Launch the script with qsub:

```
$~ qsub script.sh
```

- Check the running script with the command: watch qstat

**solution script bwa**

⚠ Use the dos2unix command when the script has been written under Windows