Bioversity International




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SouthGreen bioinformatics platform

agap UMR BGPI Biologie et Génétique des Interactions Plante-Parasite LSTM Laboratoire des Symbioses Tropicales et Méditerranéennes

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Bioversity International

Institut de Recherche pour le Développement

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IPME

UMI233 TransVIH-MI

MIVEGEC Maladies Infectieuses et Vecteurs Écologie, Génétique, Évolution et Contrôle

plateau i-trop

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UMR BGPI Biologie et Génétique des Interactions Plante-Parasite

LSTM Laboratoire des Symbioses Tropicales et Méditerranéennes

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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

- TAll trainigs 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 system partitions
- How to use SGE (qusb, 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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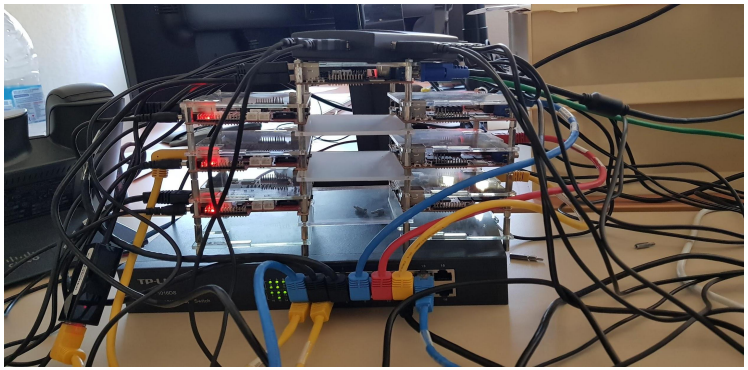

Components of a cluster

- 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

COMPUTING

- Nas servers:

Store the users data and the analyses results

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

Role : Store data

Accessible from the Internet

Connection : filezilla or scp

bioinfo-nas.ird.fr 91.203.34.157

bioinfo-nas2.ird.fr 91.203.34.160

Architecture: rôle des éléments

bioinfo-master.ird.fr
91.203.34.148

Rôle : Lancer et prioriser les jobs sur les nœuds de calcul

Accessible depuis Internet

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

22 noeuds avec bioinfo-inter.ird.fr
91.203.34.150

Rôle : Utilisés par le maître pour exécuter des jobs

Pas accessibles depuis Internet

node0 à node22

Noeud interactif : bioinfo-inter.ird.fr

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

bioinfo-nas3.ird.fr
91.203.34.180

Rôle : Stocker les données utilisateurs

Accessibles depuis Internet

Connexion : filezilla ou scp

bioinfo-nas.ird.fr
91.203.34.157

bioinfo-nas2.ird.fr
91.203.34.160

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 sur le cluster itrop

/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 sur le cluster itrop

/home : Your personal folder
Quota 100Go
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Quota 500Go à 1To
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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

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

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

Partitions sur le cluster itrop

/home : Votre répertoire personnel
Quota 100Go
Hébergée sur : bioinfo-nas.ird.fr
Partagée sur toutes les machines

/team : Données projet partagées
entre plusieurs utilisateurs
d'une même équipe
Quota 200Go
Hébergée sur : bioinfo-nas.ird.fr
Partagée sur toutes les machines

/data2 : Données projet partagées
entre plusieurs utilisateurs
Quota 500Go to 1To
Hébergée sur : bioinfo-nas.ird.fr
Partagée sur toutes les machines

/data : Données projet partagées
entre plusieurs utilisateurs
Quota 500Go à 1To
Hébergée sur : bioinfo-nas2.ird.fr
Partagée sur toutes les machines

/data3 :Données projet partagées
entre plusieurs utilisateurs
Quota 500Go à 1To
Hébergée sur : bioinfo-nas3.ird.fr
Partagée sur toutes les machines

/scratch : Répertoire temporaire de travail
1To à 5To
Hébergée sur : **chaque noeud**
Pas partagée mais uniquement en local
Données conservées **3 semaines**

SUN GRID ENGINE (SGE)

The scheduler sge

- SGE (SUN Grid Engine) est un gestionnaire de ressources de calcul sous linux, capable de gérer de deux à des milliers de serveurs et des centaines de clusters de plusieurs nœuds à la fois.
- 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

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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 :gig need of memory
Nodes: node4 et node7
RAM: 144Go
Cores: 12 cores

Les files d'attentes sge

Bioinfo.q : queue par défaut
Noeuds: node2, node8, node9, node10, node11,node12,node13, ,node14,node15,node16,node17, node19,node20
RAM: de 48Go à 64Go
Coeurs: de 12 à 20 coeurs

dynadiv.q : priorité pour l'équipe dynadiv
Noeuds: node2, node10
RAM: 48Go
Coeurs: 12 coeurs
/scratch de 5To pour node10

dynadiv2.q : priorité pour thomas Couvreur
Noeuds: node20
RAM: 64Go
Coeurs: 20 coeurs

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Noeuds: node17, node18
RAM: 64Go
Coeurs: 12 coeurs

alizon.q : priorité pour l'équipe de samuel Alizon
Noeuds: node8, node9, node12
RAM: 48Go
Coeurs: 12 coeurs

r900.q : queue avec noeud **DELL**
Noeuds: node5, node21
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Coeurs: 16 coeurs

longjob.q : jobs longs ou > à 10 jobs
Noeuds: node0, node1, node11
RAM: 48Go
Coeurs: 12 coeurs

bigmem.q : besoin de mémoire
Noeuds: node3
RAM: 96Go
Coeurs: 12 coeurs

highmem.q : besoin de mémoire
Noeuds: node4 et node7
RAM: 144Go
Coeurs: 12 coeurs

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** With X the node number
• Reserve X core on a node	$~ **qrsh -pe ompi X** 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 • Use several processors	$~ **qsub -N job_name script.sh** $~ **qsub -pe ompi X script.sh** **Avec X le nombre de coeurs à utiliser**
• Have a certain amount of memory	**$~ qsub -l mem_free=XG script.sh** **Avec X le montant de mémoire à réserver**
• 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 • Watch your jobs state	$ **qhost** $~ qstat
• Informations on running jobs	$~ **qstat -j <JOB_ID>** With JOB_ID :the job number
• Informations on completed jobs	$~ **qacct -j <JOB_ID>** With JOB_ID :the job number
• Global informations on queues	$~ **qstat -g c**

Sge commands: deletion

Actions	Commandes
• Deletion of a job	$~ **qdel <JOB_ID>** With JOB_ID : the job id

1

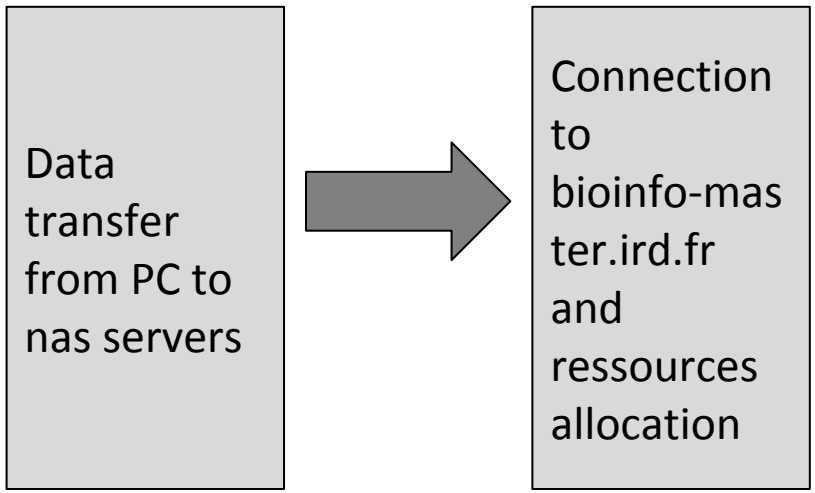
Training: Launch a blast analysis in a interactive way

Analyse steps on the cluster

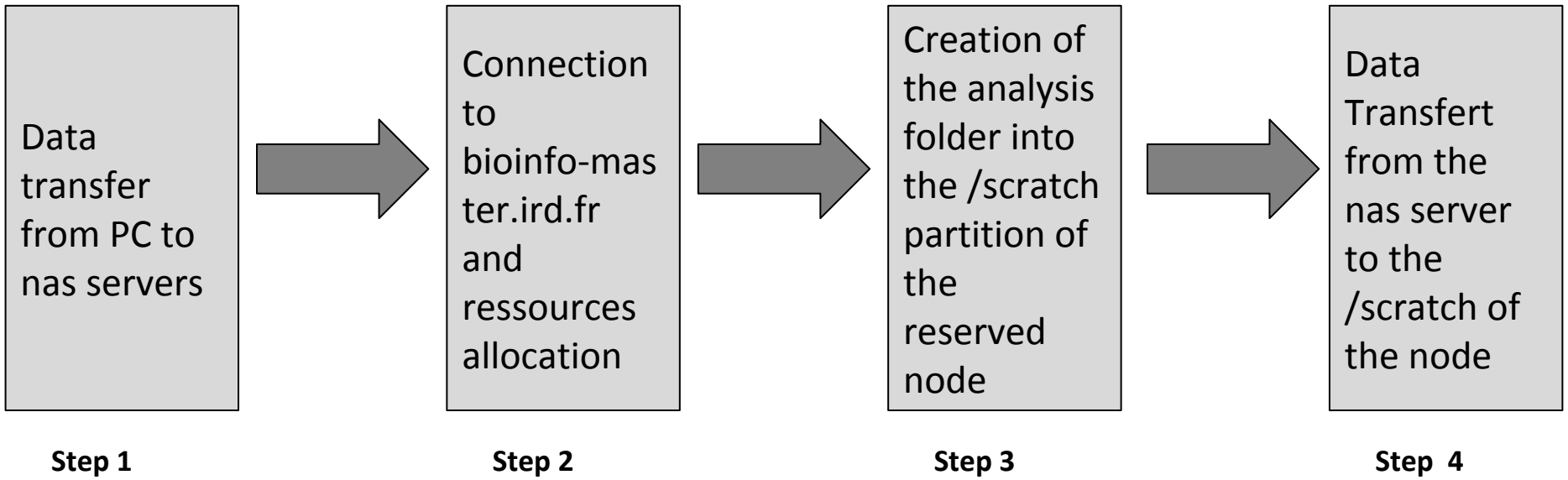
Data transfer from PC to nas servers

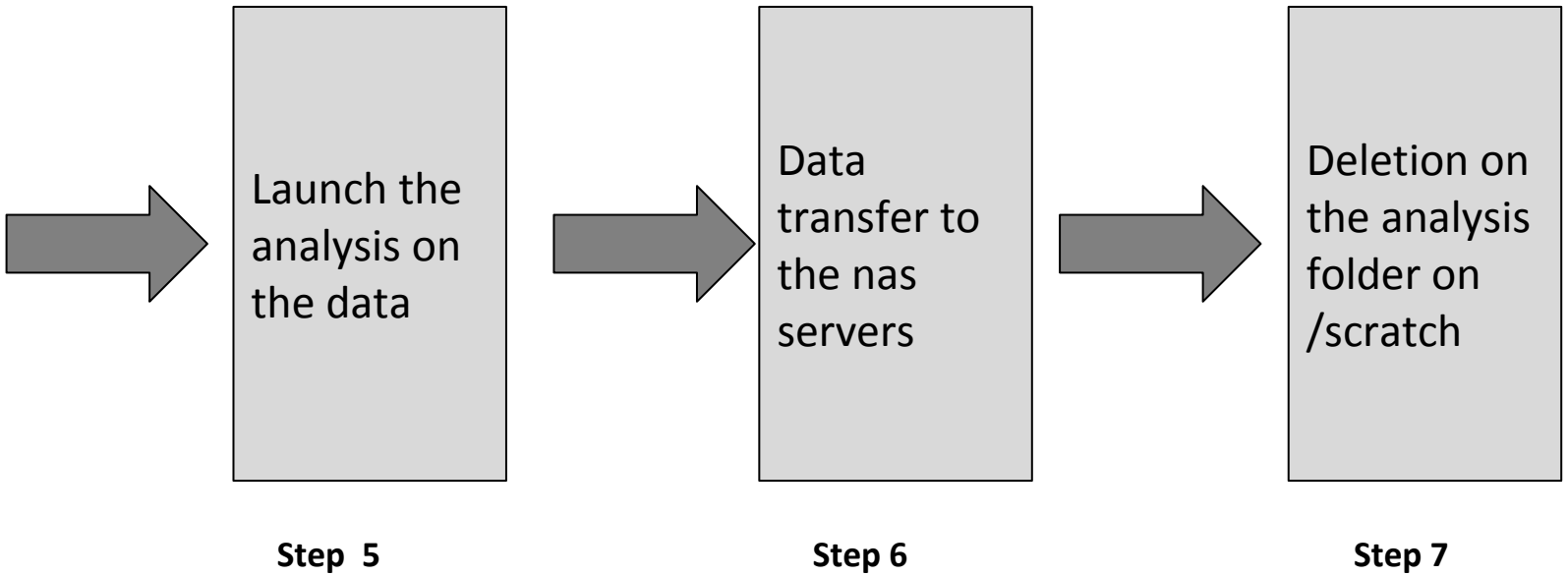
Step 1

Analyse steps on the cluster



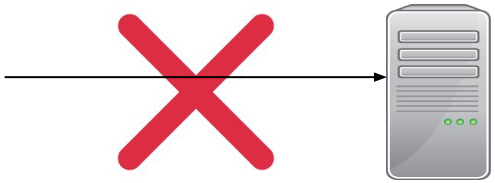
Analysis steps on the cluster





Data transfer on the cluster itrop

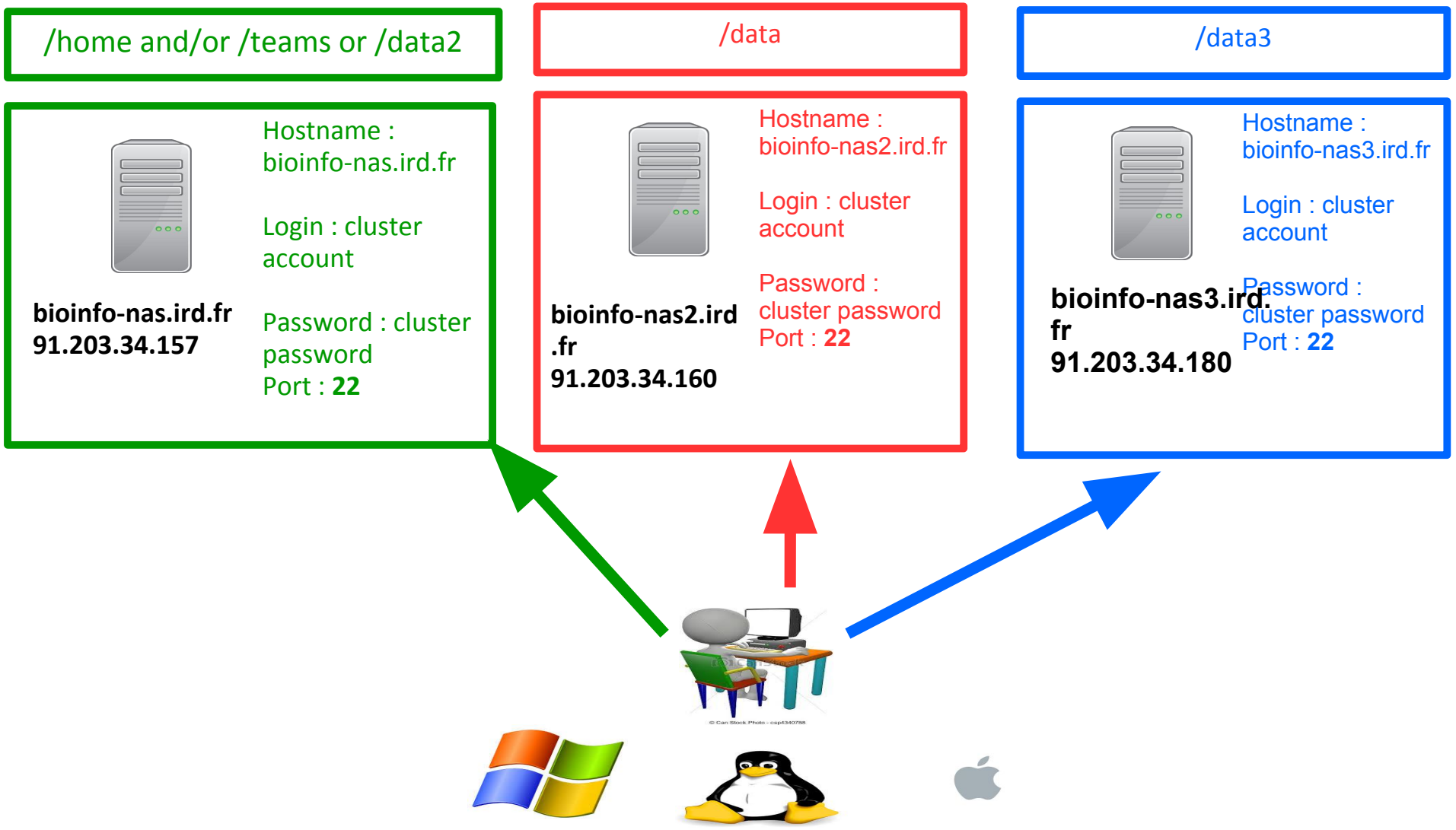
Personal
Computer



direct transfert through filezilla is forbidden

bioinfo-master.ird.fr
91.203.34.148

Data transfer on the cluster itrop



Step 1: Data copy on the cluster

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

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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

Hostname : bioinfo-master.ird.fr

Login : cluster account

Password : cluster password
Port : **22**

Use the qsub command

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

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

/data/projects/tp-cluster/training_2018

Destination ServerA

Source ServerB

Data transfer with scp

Being connected to A

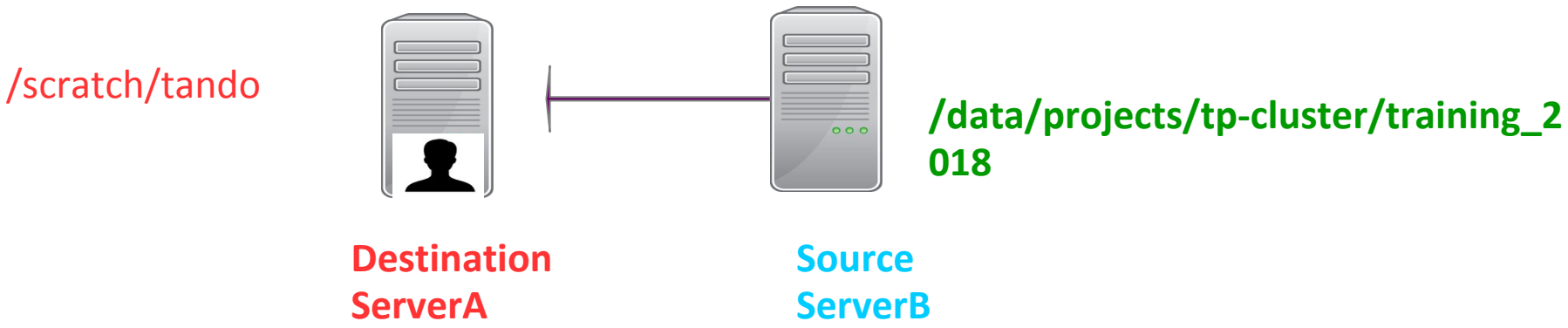
Remote folder to transfer : /data/projects/tp-cluster/training_2018

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

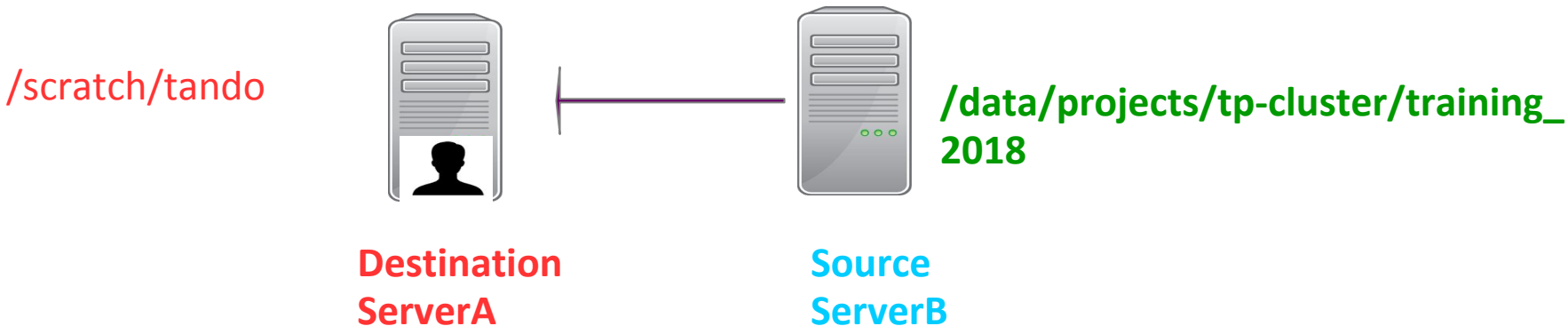
Remote folder to transfer : /data/projects/tp-cluster/training_2018

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



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

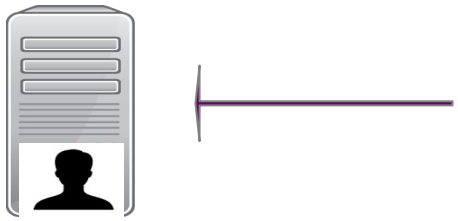
Login : login

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 environement 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

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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*

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     ####################
# Ecrit les erreur dans le fichier de sortie standard
#$ -j y

# Shell que l'on veut utiliser
#$ -S /bin/bash



# Email pour suivre l'execution
#$ -M prenom.nom@ird.fr         ######### Mettre son adresse mail

# Type de message que l'on reçoit par mail
#    -  (b) un message au demarrage
#    -  (e) a la fin
#    -  (a)  en cas d'abandon
#$ -m bea

# Queue que l'on veut utiliser
#$ -q bioinfo.q

# Nom du job
#$ -N Nom_a_choisir
#################################################################
```

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 # choisir nas pour/home, /data2 et /teams ou nas2 pour /data ou nas3 pour /data3
echo "tranfert donnees 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 "Commande executee : $cmd";
$cmd;

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

#### Deletion of the tmp folder
rm -rf $path_to_tmp
echo "Suppression des donnees sur le noeud";
```

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 sript 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 sript has been written under Windows