Introduction to the iPOP-UP HPC cluster

Julien Rey   Olivier Kirsh   Magali Hennion

Juin 2023

Table of Contents

Who is this training for

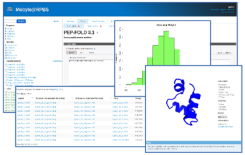
- You work at Université Paris Cité
- You need (or might need) more computational power than you currently have
- You are familiar with Unix systems and Bash

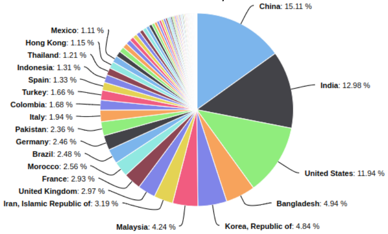
Missions

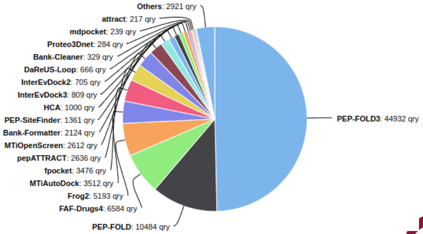
- Development of Structural Bioinformatics methods
- Services deployment on the computing resource
- Expertise and training
- Hardware hosting

Web portal

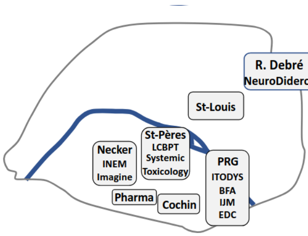
- https://mobyle.rpbs.univ-paris-diderot.fr: free access
- 30+ Structural Bioinformatics services
- 1 million CPU hours /year
- 80,000 jobs /year







The iPOP-UP project

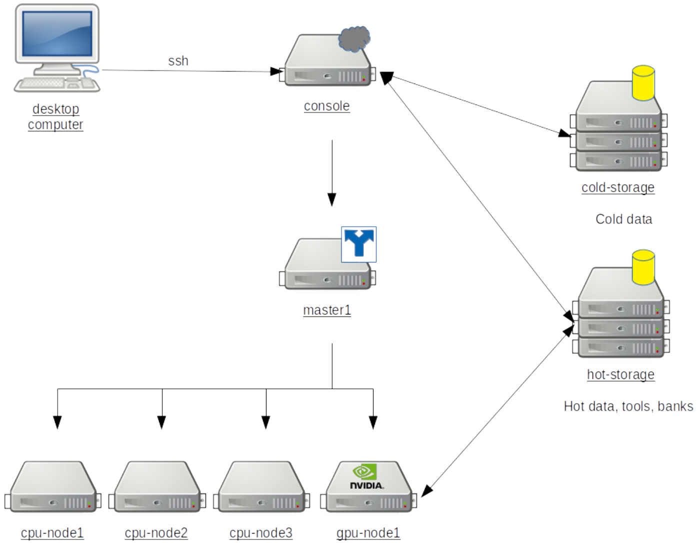


- iPOP-UP: Integrative Platform for Omics Projects at Université de Paris
- Multisite Bioinformatics platform
- Ranging from multiple 'Omics' techniques to structural and chemo- *in silico* Bioinformatics
- Compute nodes

What is a cluster for ?

- High hardware resources needs
- Long running analyses
- A lot of similar analyses
- Shared work between users
- Free your desktop from the task

What is a cluster ?



Computational hardware

Partitions (groups of compute nodes):

- ipop-up: 16 nodes, 2048 CPUs
- rpbs: 20 nodes, 832 CPUs, 9 GPUs (+ 9 nodes, 520 CPUs, 4 GPUs)
- cmpli: 6 nodes, 264 CPUs, 14 GPUs (+ 1 node, 64 CPUs, 2 GPUs)
- epigen: 4 nodes, 128 CPUs
- master-bi: 1 node, 32 CPUs, 3 GPUs

Storage:

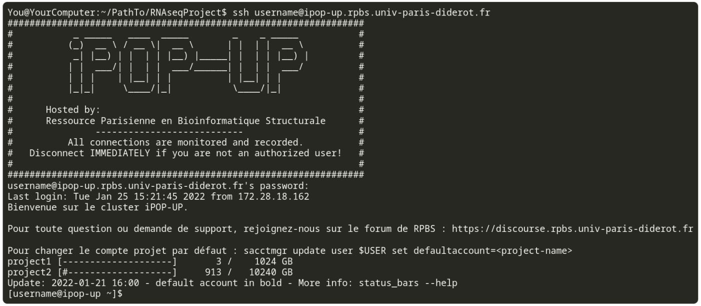
- hot-storage: 125TB, very fast
- cold-storage: 240TB, slow + backup (soon)

In practice

Go to your terminal and connect to the cluster using the following line, don't forget to replace username with your personal username.

```
ssh username@ipop-up.rpbs.univ-paris-diderot.fr
```

Type in your password and enter.



```
You@YourComputer:~/PathTo/RNAseqProject$ ssh username@ipop-up.rpbs.univ-paris-diderot.fr
##################################################################
#           _ _____   ____  _____        _    _ _____            #
#          (_)  __ \ / __ \|  __ \      | |  | |  __ \           #
#           _| |__) | |  | | |__) |_____| |  | | |__) |          #
#          | |  ___/| |  | |  ___/______| |  | |  ___/           #
#          | | |    | |__| | |          | |__| | |               #
#          |_|_|     \____/|_|           \____/|_|               #
#                                                                #
#      Hosted by:                                                #
#      Ressource Parisienne en Bioinformatique Structurale       #
#               ---------------------------                      #
#          All connections are monitored and recorded.           #
#   Disconnect IMMEDIATELY if you are not an authorized user!    #
#                                                                #
##################################################################
username@ipop-up.rpbs.univ-paris-diderot.fr's password:
Last login: Tue Jan 25 15:21:45 2022 from 172.28.18.162
Bienvenue sur le cluster iPOP-UP.

Pour toute question ou demande de support, rejoignez-nous sur le forum de RPBS : https://discourse.rpbs.univ-paris-diderot.fr

Pour changer le compte projet par défaut : sacctmgr update user $USER set defaultaccount=<project-name>
project1 [--------------------]       3 /    1024 GB
project2 [#-------------------]     913 /   10240 GB
Update: 2022-01-21 16:00 - default account in bold - More info: status_bars --help
[username@ipop-up ~]$
```

Note about ssh and security

Your IP will be banned after 5 failed authentication attempts. Each public key count as one authentication attempt. To disable public key authentication:

```
ssh -o PubkeyAuthentication=no
↪  username@ipop-up.rpbs.univ-paris-diderot.fr
```

A good thing to do, change your password:

```
[rey@ipop-up ~]$ passwd
```

Where you can go, write, or execute

User environments

/shared/home/username

Computations (hot data)

/shared/projects/projectname

Processed data (cold data)

/cold-storage/username

Data banks (read-only)

/shared/banks/

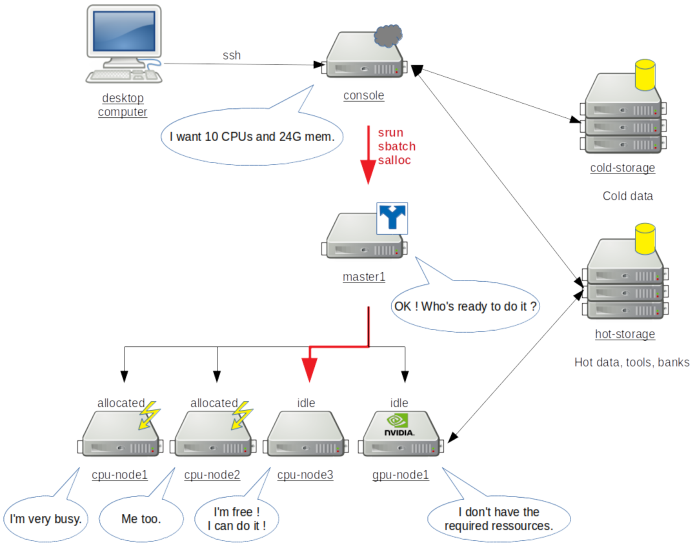
Slurm

Slurm is the job scheduling system.

It is what will take your code and distribute it on the computing nodes, while ensuring they have the CPU(s) and RAM that you asked for.

It requires specific commands to run (srun, sbatch, salloc, etc...)

Slurm


desktop computer
ssh
console
I want 10 CPUs and 24G mem.
srun
sbatch
salloc
cold-storage
Cold data
master1
OK ! Who's ready to do it ?
hot-storage
Hot data, tools, banks
allocated
allocated
idle
idle
cpu-node1
cpu-node2
cpu-node3
gpu-node1
I'm very busy.
Me too.
I'm free !
I can do it !
I don't have the required ressources.

srun

Launch a (simple) interactive job.

```
[rey@ipop-up ~] srun hostname
```

Some parameters can be added to the command line:
–partition/-p: request a specific partition
–account/-A: select the (project) account
–cpus-per-task/-c: request that ncpus be allocated (default: 1 cpu)
–mem-per-cpu: specify the required memory per cpu (default: 2GB)

Example:

```
[rey@ipop-up ~] srun -A training -p ipop-up -c 8 hostname
```

sbatch

Launch more complex jobs.

myscript.sbatch

```
#!/bin/bash
#SBATCH --partition=ipop-up
#SBATCH --account=training
#SBATCH --cpus-per-task=8
#SBATCH --mem-per-cpu=4GB
#SBATCH --output=resultat.log
hostname
```

Example:

```
[rey@ipop-up ~] sbatch myscript.sbatch
```

Associations

Cluster, account, partition and qos must match your user's associations.
To check your associations:

```
[rey@ipop-up ~] sacctmgr show user rey withassoc
User   Def Acct    Cluster    Account  Partition      QOS   Def QOS
------ -------- ----------- ---------- ---------- -------- ---------
 rey       demo  production   training    ipop-up   normal
 rey       demo  production       demo    ipop-up   normal
 rey       demo  production  alphafold      cmpli   normal
 rey       demo  production  alphafold       rpbs   normal
```

squeue

List submitted jobs on the cluster:

```
[rey@ipop-up ~] squeue
          JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
        1008002     cmpli argtoser domingue  R   20:58:09      1 gpu-node14
         993325     cmpli calcam-p   ghoula  R 6-20:23:17      1 gpu-node8
         993574   ipop-up amyloid_   meuret PD       0:00      1 (AssocGrpCPUMinutesLimit)
943019_[165-299]   ipop-up kappa_va  badaoui PD       0:00      1 (JobArrayTaskLimit)
     943019_117   ipop-up kappa_va  badaoui  R 7-17:55:27      1 cpu-node132
```

Some parameters can be added to filter jobs or show more infos:
–**partition/-p**: specify the partition to view
–**user/-u**: request jobs from a list of users
–**format/-o**: specify the information to be displayed

Example:

```
[rey@ipop-up ~] squeue --me -p ipop-up
[rey@ipop-up ~] squeue -o "%10i %.9P %.8j %.12u %.15T %.15M %.15l %.6D %.20R %.6C %.10b %.10Q"
```

scancel

Kill a job:

```
[rey@ipop-up ~] scancel job_id
```

sacct

Display accounting data for your running and completed jobs:

```
[rey@ipop-up ~] sacct --format=JobID,JobName,Start,Elapsed,NCPUS,NodeList,ReqMeM,State --start 2023-06-01 --en
  JobID    JobName                Start    Elapsed    CPUTime  NCPUS        NodeList     ReqMem      State
------- ---------- ------------------- ---------- ---------- ------ ---------------- ---------- ----------
1010778      sleep 2023-06-08T15:37:19   00:00:30   00:00:30      1     cpu-node133     2000Mc  COMPLETED
```

seff

Report a job's efficiency:

```
[rey@ipop-up ~]$ seff 981654
Job ID: 981654
Cluster: production
User/Group: lejal/cmpli
State: COMPLETED (exit code 0)
Cores: 1
CPU Utilized: 04:15:58
CPU Efficiency: 99.72% of 04:16:41 core-walltime
Job Wall-clock time: 04:16:41
Memory Utilized: 243.88 GB
Memory Efficiency: 97.01% of 251.40 GB
```

Some vocabulary

A *job* consists of one or more *steps*, each consisting of one or more *tasks* each using one or more *CPUs*.

- job: A script, typically started with *sbatch*
- step: A step in the job, typically started with *srun*
- task: Requested at the job or step level, with *–array* or *-ntasks*

Job arrays

Job arrays offer a mecanism for launching a lot of tasks at the same time. Each task of the job will have the environment variable $SLURM_ARRAY_TASK_ID set to its array index value.

myscript.sbatch

```
#!/bin/bash
#SBATCH --partition=ipop-up
#SBATCH --account=training
#SBATCH --output=resultat_%a.log
#SBATCH --array=1-3
case "$SLURM_ARRAY_TASK_ID" in
   1) fruit='orange';;
   2) fruit='apple';;
   3) fruit='banana';;
esac
echo $fruit
```

Job arrays

```
[rey@ipop-up ~]$ sbatch myscript.sbatch
```

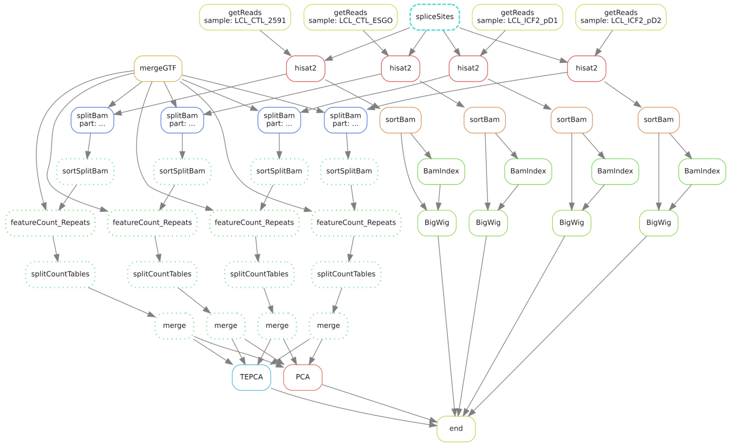
Results:

```
[rey@ipop-up ~]$ ls
resultat_1.log  resultat_2.log  resultat_3.log
[rey@ipop-up ~]$ tail resultat_*
==> resultat_1.log <==
orange

==> resultat_2.log <==
apple

==> resultat_3.log <==
banana
```

Job Array Common Mistakes

- The index of bash lists starts at 0
- Don't forget to have different output files for each task of the array
- Same with your log names (%a or %J in the name will do the trick)
- Do not overload the cluster! Please use %50 (for example) at the end of your indexes to limit the number of tasks (here to 50) running at the same time. The 51st will start as soon as one finishes!
- The RAM defined using `#SBATCH --mem=25G` is for each task

Complex workflows



Use workflow managers such as Snakemake or Nextflow.

Tools

Tools are installed on the cluster in virtual environments:

- each tool has its own dependencies (libraries) and it's not possible to make them all coexist in the same environment
- reproducibility: some users need a specific version of a tool

Conda environments

Containers (Apptainer)

Modules

They can be loaded with the module command.
Look for the different versions of multiqc:

```
[rey@ipop-up ~]$ module avail multiqc
multiqc/1.3  multiqc/1.6  multiqc/1.7  multiqc/1.9
```

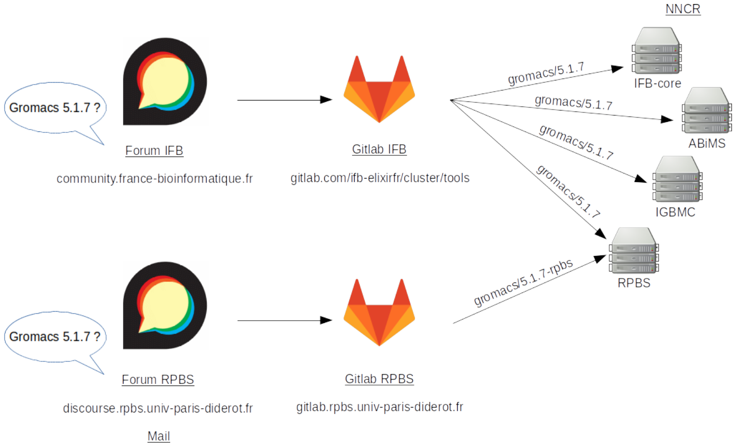
Load an environment:

```
[rey@ipop-up ~]$ module load multiqc/1.9
```

List loaded environments:

```
[rey@ipop-up ~]$ module list
Currently Loaded Modulefiles:
  1) multiqc/1.9    2) blast/2.13.0
```

How tools are installed



ipop-up-installation-request@rpbs.univ-paris-diderot.fr

Useful resources

To find out more, the SLURM manual : `man sbatch` or
https://slurm.schedmd.com/sbatch.html

Ask for help or signal problems on the cluster :
https://discourse.rpbs.univ-paris-diderot.fr/

iPOP-UP cluster documentation:
https://ipop-up.docs.rpbs.univ-paris-diderot.fr/documentation/

Thanks

- Alix Silvert

iPOP-UP's technical and steering committees

Exercices

https://parisepigenetics.github.io/bibs/cluster/training_230612/training/