

New computing infrastructure



Séminar 15/05/2023









A brief introduction

Matthias Zytnicki

Hardware presentation

Didier Laborie

Software utilization

Marie-Stéphane Trotard

Web services

Patrice Dehais



About us

Scientific animation





Matthias Zytnicki (50% FTE)



Claire Hoede (100% FTE)



System administrators

Didier Laborie (100% FTE)



Marie-Stéphane Trotard (80% FTE)

Statistical expertise and data analysis



Patrice Dehais (50% FTE)

Development and data analysis



Christine Gaspin (30% FTE)



Christophe Klopp (30% FTE)



Jérôme Mariette (70% FTE)



Nathalie Vialaneix (25% FTE)

Web Development



Céline Noirot (80% FTE)



Philippe Bordron (100% FTE)



Hanae Chouali (100% FTE)



Julien Touchais (100% FTE)



Team changes

- The management staff has changed (2023/01/01)
 - o operational management: Claire Hoede
 - o scientific management: Matthias Zytnicki
- New arrival:
 - a new IE for Web development: Philippe Bordron
- To be hired
 - o a **biostatistics** IR: permanent position
 - a devops IR: temporarily position (3 years)









User support

Active users: 1062

INRAE: 439

OCCITANIE (not INRAE): 550

o OTHER: 73

• # Software: > **1000**

• % Availability: **99,5**%

• # Tickets: **1773** (2022)

Current projects: 27 (expertise and development)

Annual training sessions: 12









Why limited free usage?

"I can store my data on a hard drive for much less"

What we do not charge academic users for (except. for private companies):

- CPU time
- 1TB work storage + 250GB save storage + 250GB backup

What we charge for:

- Storage extension
- VM (Virtual Machine)
- Most acquisitions are paid by projects (OccalDat, Mudis4LS).
- We pay for the rent (electricity costs are increasing).









Rules of use

User account

- Open to the bioinformatics academic community and private companies
- Gives access to:
 - bioinformatics software
 - genomic and post-genomic databases
 - storage facilities (Home, Save, Work)
 - computing cluster (via a login server)
 - support (FAQ, tickets, training)

Beware

- Password expires 12 months after last password change
- Account is closed after 12 months of inactivity
- Data is purged 3 months after account closure date



Rules of use (continued)

User disk spaces

- Home (10GB): configuration files only
- Save (250GB): 30-day history + replication to remote site
- Work (1TB): 7-day history (only), NO replication

Computing hours

- 100,000 h annual initial quota with possibility of extension
- 3 user groups (contributors, **INRAE / OCCITANIE**, others)

Exceptional requests:

- Rental of additional disk space (projects)
- Rental of virtual machines (website, database...)
- Access to GPU or VIEW resources
- Extension of computing hours
- Access to training accounts



Hardware presentation



New computing cluster

The Bioinfo GenoToul platform has just acquired a new computing infrastructure to replace its obsolete equipment.

Cluster 2007 Cluster 2012 (ceri) Cluster 2017 (genologin)

2007 2008 2009 2010 2011 2012 2013 2014 2015 2016 2017 2018

Cluster 2009 (snp) Cluster 2014 (genotoul)







Bioinfo Timeline of the acquisition

The **timetable** was very **tight** given the shortage of materials, the accommodation at the DROCC and the deadline set by the **REGION** (**FEDER** funding)

- January 2022: drafting of the specifications
- February: setting up of the call for tender procedure
- March: publication of the call for tenders in the BOAMP and the OJEU
- April: receipt of offers from suppliers (4): AXIANS, 2CRSI, ATOS and HPE
- May: selection of the successful bidder: AXIANS integrator with LENOVO equipment
- June: notification of the **public contract**
- October: **delivery** of equipment and start of **installation**
- January 2023: start of INRAE validation period









Migration strategy

2023 (transition period)

- From now, all new user accounts will be created on the new cluster.
- We plan to migrate all users (data, projects, VMs, etc.) by the end of this year
- ~20 projects will be migrated per month (schedule to come)
- We are going to shut down several old cluster nodes every month

	Old cluster (2014, 2017)	New cluster (2023)
#NODES	78	39
#CORES	4424	4928
RAM per core (average)	6GB	16GB
Specific nodes	1 view node	1 view node + 1 GPU node









New computing cluster

VISU

- Authentification SSH
- Bureau à distance
- HTTPS (OOD)

LOGIN (x2)

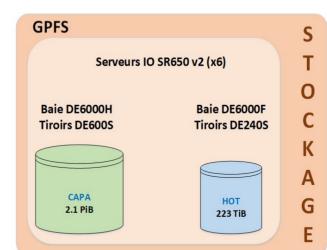
- Authentification SSH
- Transfert de fichiers
- Compilation
- Soumission de jobs

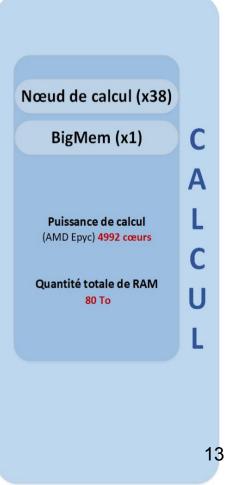
Réseau d'interconnexion Ethernet de production 10G

Réseau d'administration Out-Of-Band 1G: arrêt / démarrage des serveurs, console série, configuration des équipements

Réseau Infiniband HDR: accès aux espaces de stockage (GPFS), calcul (MPI), etc.







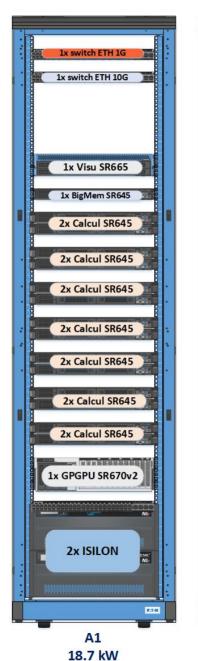


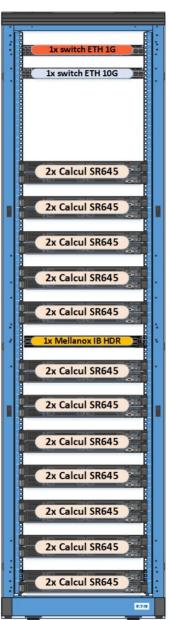
ECA hosting





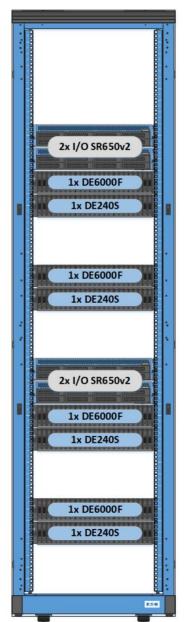
Physical location





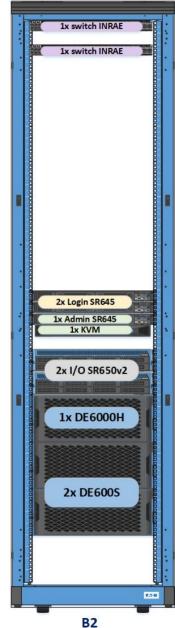
A2

19.9 kW



B1

5,3 kW



5,8 kW



Some vocabulary

Cluster: all compute nodes

Node: a server dedicated to high performance computing (HPC)

Processor: physical computing

units

Core: logical computing unit sharing cache memory

Thread: number of running processes

HT: Hyper Threading (INTEL)

SMT: Simultaneous Multi-Threading (AMD)

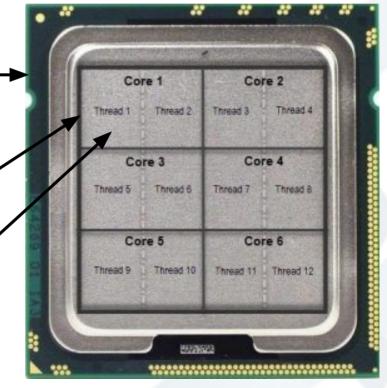


image source:

https://phoenixnap.com/kb/single-vs-dual-processor s-server



Bioinfo Compute nodes (x39)

Server type	LENOVO SR645
Processor	2*AMD 7713 (2*64c)
Frequency	2.0 / 3.7 GHz (turbo)
RAM memory	2048G / 4096G (bigmem01)
Ethernet network (Main communication & storage)	10GbE latency 10 µs Throughput 1,2GB/s
Infiniband network (MPI interconnection & work storage)	HDR-100 latency 1,2 µs Throughput 12,3GB/s



AMD ZEN3 (MILAN) 7NM

The most efficient choice today:

- Smaller process node size (less energy)
- Higher density (more cores, less servers)
- Best performance for bioinformatics computing



VIEW & GPU nodes

	VIEW	GPU
Server	LENOVO SR665	LENOVO SR670 v2
Processor	2*AMD 7513 (2*32c)	2*INTEL Gold 6338 (2*32c)
Frequency	2.6 GHz	2.0 GHz
RAM memory	512G	1024G
Local disks	2*SSD 2T (Raid 1)	4*NVMe 4T (Raid 5)
GPU	RTX 6000 24G	4*A100 80G
Networks	2*10GbE + HDR-100	10GbE + 2*HDR-100



Bioinfo ADMIN and LOGIN nodes

	ADMIN	LOGIN (*2)	
Server	LENOVO SR645	LENOVO SR645	
Processor	2*AMD 7313 (2*16c)	2*AMD 7513 (2*32c)	
Frequency	3.0 GHz	2.6 GHz	
RAM memory	512G	512G	
Local disks	2*SSD 2T (Raid 1)	2*SSD 2T (Raid 1)	
Networks	2*10GbE + HDR-100	10GbE + 2*HDR-100	

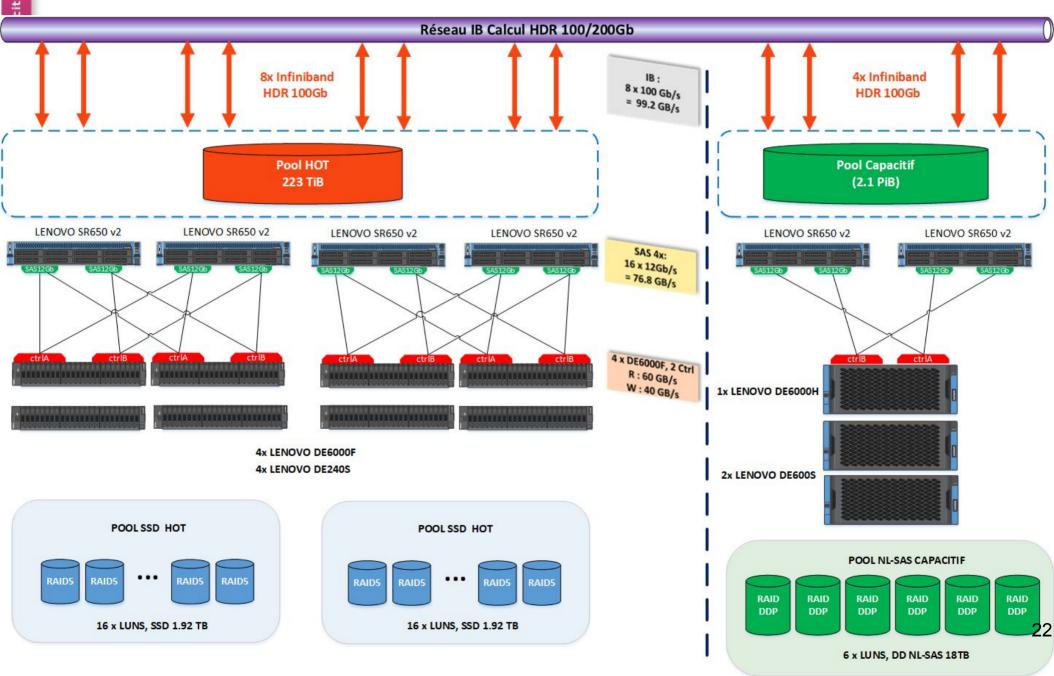


High Performant storage (/work)

- Provided by the "integrator"
- Parallel File System IBM Spectrum Scale
- Integration of servers + disk array
- Hot data: SSD 1,92 TB (192 disks)
- Cold data: NL-SAS 18 TB (160 disks)
- 2,3 PB usable, 40 GB/s bandwidth (R/W)
- NFS export to virtual machines
- Snapshots, quotas (users, groups)



Performant storage /work





Software utilization



Genobioinfo: new environment

New environment

- => changes between the 2 clusters.
- => user access.

Software usage

=> reminder: run a soft.

Help

=> reminder: software help, other help.

Others services

=> monitoring, account information.

Best practices

- => security.
- => shared resources and environmental constraint.
- => infrastructure.









New environment Changes

			Current cluster	New cluster
Login server name (reconfigure MobaXerm, Filezilla, etc.)		genologin.toulouse. inra.fr	genobioinfo.toulo use.inrae.fr	
Location		INRAE Auzeville	ECA Toulouse	
Authent	ification		same accounts	
	Цото	Storage	current	New (from scratch)
	Home	Path	/home/ <login></login>	
		Storage	current	New (from scratch)
Data	Work	Path	/work/ <login></login>	/work/user/ <login></login>
Cove	Storage	Shared (current)		
	Save	Path	/save/ <login></login>	/save/user/ <login></login>
	Banks	Storage	current	ated New



New environment Changes

		Current cluster	New cluster
CPU (you may need to recompile your binaries)		Intel Broadwell	AMD Zen3 Milan (except gpu node)
os		CentOS 7.9	Red Hat 8.6
Software*		<category>/<soft>-<version></version></soft></category>	<category>/<soft>/<version></version></soft></category>
Scheduler		slurm 21.08.8-2	slurm 22.05.6
Accountin (including cp		current	New (from scratch)
Queues	unlimitq	180 days	90 days

^{*} Some categories have changed, some (not bioinfo) softwares don't belong to the same categories in current and new cluster



New environment User access

Access to the platform: via a command line SSH connection or MobaXterm for Windows

New frontal/login servers: genobioinfo1 & genobioinfo2

New hostname for the connection: genobioinfo.toulouse.inrae.fr

Example: \$ ssh <login>@genobioinfo.toulouse.inrae.fr









Software usage Reminder: Run a soft

"Environment Modules package"

"Modules" provides a dynamic modification of a user's environment via modulefiles (add command in your PATH, define specific environment variable, add paths to dependencies, add paths to specific libraries).

(see Appendix 1 & 2 and https://modules.sourceforge.net/)

Run a software

To run a software you need to load the corresponding module.

\$ module load <modulename>

To run a software with others software dependencies, you need to load all required modules.

Best practices

Check modules already loaded: \$ module list

Purge modules already loaded if not needed:

\$ module purge (all modules)

\$ module unload <modulename> (only one module)



New environment Software installation

Genologin to Genobioinfo cluster: new installations

- ~ 100 software already installed on Genobioinfo cluster.
- To ask for new software on Genobioinfo cluster:

on demand by filling form on our website (Ask for/Software installation) https://bioinfo.genotoul.fr/index.php/ask-for/install-soft/

Installation and update

Default installation on **Genobioinfo** (if not specified in the request).

Reminder: updates only upon user request



New environment Search/Find a soft (Web)

Website (Resources/Software): https://bioinfo.genotoul.fr/index.php/resources-2/softwares/

Not installed on Genobioinfo Clusterlink to ask for

All software

Application Description Avaibility/Use Scaffolding genome sequence assemblies using 10X Genomics GemCode/Chromium data. This project is a new kmer-Genologin Cluster: How to use based (alignment free) implementation of ARCS. It provides improved runtime performance over the original ARCS Genobioinfo Cluster (soon available): Ask for Install ARKS implementation by removing the requirement to perform alignments with bwa mem.

Burrows-Wheeler Aligner (BWA) is an efficient program that aligns relatively short nucleotide sequences against a long reference sequence such as the human genome. It implements two algorithms, bwa-short and BWA-SW. The former works for query sequences shorter than 200bp and the latter for longer sequences up to around 100kbp. Both algorithms do gapped alignment. They are usually more accurate and faster on queries with low error rates.

> Installed on Genobioinfo Clusterlink to help

Link to soft website

Genologin Cluster: How to use

Genobioinfo Cluster (soon available): How to use



New environment Search/Find a soft (Command line)

New installation paths (new storage spaces)

Bioinfo: /usr/local/bioinfo/src/ Compilers: /tools/compilers

Libraries: /tools/lib

Languages (Python, R, Java, Singularity..): /tools/statistics,/tools/containers,tools/devel

Other system tools: /tools/others tools

Useful scripts: /tools/bin (sarray, squota_cpu, saccount_info...). In user's default PATH.

Commands

- with useful scripts:

\$ search_module <soft_name>: display available versions for a specific application (case insensitive)

\$ search_R_package <package_name>: find if R package already installed (case insensitive)
\$ search_Python_package <package_name>: find if Python package already installed (case insensitive)

- with module or Is command: see our FAQ

https://bioinfo.genotoul.fr/index.php/faq/software_faq/ -> Is a software is already installed on the cluster?



Help Software help (1/2)

Software documentation

- official software documentation in the installation folder: /usr/local/bioinfo/src/<soft_name>/<soft_version>
- our website Software page: https://bioinfo.genotoul.fr/index.php/resources-2/softwares/

Use on SLURM cluster: "How_to_use_SLURM_<soft_name>" file

- on our website Resources/Software page (Availability/Use column, click on Genobioinfo cluster link).
- in software installation directory /usr/local/bioinfo/src/<soft_name>
- find "How_to_use_SLURM_<soft_name>" file path : \$ module help <modulename>
- a basic « example_on_cluster » directory in the software installation directory: /usr/local/bioinfo/src/<soft_name>/example_on_cluster



Help Software help (2/2)

HOW TO USE ON GENOBIOINFO CLUSTER

```
SOFT: bwa
Site du soft: https://github.com/lh3/bwa
                                                                      Software
LICENSE:
                                                                    informations
GPL-v3
See software documentation for more informations.
Location: /usr/local/bioinfo/src/bwa
Load binaries and environment:
                                                                      Usage and
-> Version v0.7.17
                                                                       versions
module load bioinfo/bwa/0.7.17
Example directory for use on cluster:
                                                                       Example
/usr/local/bioinfo/src/bwa/example on cluster
To submit: sbatch test bwa-0.7.17.sh
```



Help Usage examples

Use STAR-v2.7.5a:

\$ search_module Star bioinfo/STAR/2.7.10b bioinfo/STAR/2.7.5a

\$ module help bioinfo/STAR/2.7.5a

Module Specific Help for /tools/modulefiles/bioinfo/STAR/2.7.5a:

See How_to_use file:
/usr/local/bioinfo/src/STAR/How_to_use_SLURM_STAR

\$ module load bioinfo/STAR/2.7.5a \$ which STAR /usr/local/bioinfo/src/STAR/STAR-2.7.5a/source/STAR \$ STAR --version 2.7.5a

\$ module unload bioinfo/STAR/2.7.5a

\$ STAR --version

-bash: STAR: command not found





Browse all "How_to_use_SLURM_<soft_name>" files (in your web browser)

https://web-genobioinfo.toulouse.inrae.fr/How to Softs/

Useful scripts (already in your default path or /tools/bin)

saccount_info, sq_long or sq_debug (squeue long format), sa_debug (sacct long format), sarray (wrapper for sbatch to create a job array that will execute in parallel SHELL lines from a file), squota_cpu to see your CPU time limit, sq_veille (summary of current jobs, running, pending...), sq_run or sq_pend for running or pending job,last_soft.sh (last softs installed)...

FAQ: https://bioinfo.genotoul.fr/index.php/faq/

Newsletters: https://bioinfo.genotoul.fr/index.php/about-us/newsletters/

Training slides:

Linux (for Genologin cluster):

https://genoweb.toulouse.inra.fr/~formation/unix/doc/Formation_LINUX_GenoToul.pdf

Cluster (for Genologin cluster):

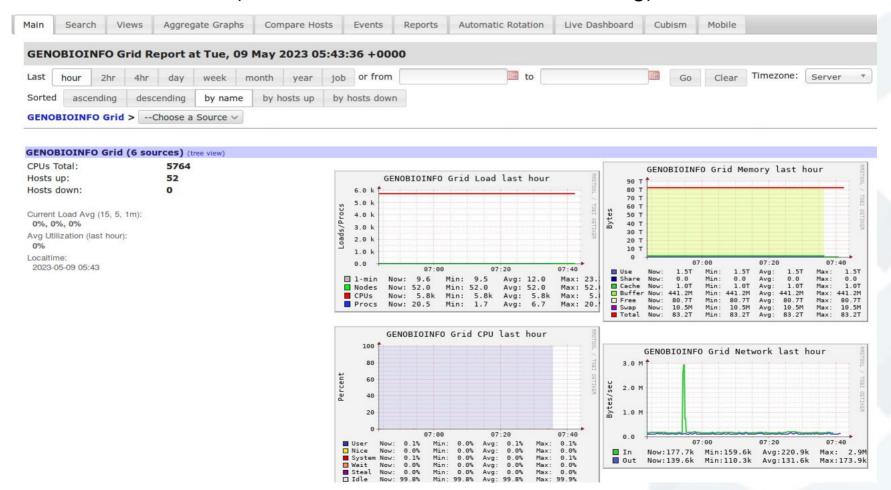
https://genoweb.toulouse.inra.fr/~formation/cluster/doc/Formation_cluster_SLURM.pdf



Others services Monitoring

Ganglia: https://web-genobioinfo.toulouse.inrae.fr/ganglia/

(or our website : Resources/Monitoring)



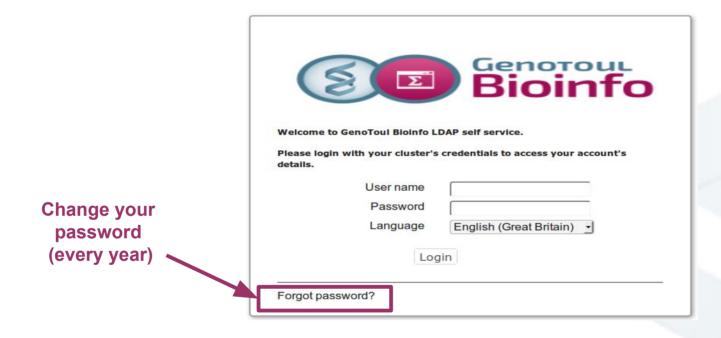
Some help to understand Ganglia view here.



Others services

Account information, password change

Self Service → https://selfservice.bioinfo.genotoul.fr



CLI command: saccount_info <login>

- account expiration date and last password change date your primary Linux group your secondary Linux groups if you have any status of your Linux primary group in Slurm (contributors, inrae, region or others) your groups' members
- some Slurm limitations of your account : cpu and memory limit, CPU Time ...



Best practices Security

One user = one account

You are responsible of the damage caused by your login.

Default permissions directories

- home: drwxr-x--x Read, Write, eXecution for the owner, Read and eXecution for the group members, eXecution for all.
- save and work: drwxr-x--- Read, Write, eXecution for user, Read and Execution for your group members, no permissions for all.

To change permissions: **chmod** command or ACL

https://bioinfo.genotoul.fr/index.php/faq/linux_faq/
-> How to change permissions on file or folder?



Best practices

Shared resources and environmental concerns (1/2)

Cluster is a shared and power-consuming resource, so ... think about others and environmental preservation.

Objectives: Go faster and save time + Free up resources for others + Calculate less, better and therefore consume less energy: different objectives but same means.

Means: ask yourself the right questions.

In which case to use a cluster?

Cluster use ≠ faster process

It is useful to use a computing cluster rather than a personal computer when:

- you need more resources than available on your PC (RAM, CPU, disk space),
- the same job needs to be run several times on different data (possibility to run it in parallel on several nodes),
- the program you want to run would benefit from being "multi-threaded" via MPI or OpenMP.

Resources (CPU, memory, I/O...) are shared on a node with other users and this can create latencies.



Best practices

Shared resources and environmental concerns (2/2)

How to request resources adapted to your needs? (including in workflows as nf_core ...)

The smaller a job is (cpu, memory, time), the faster it will be launched. You don't save time by overbooking or misbooking; you stay in the queue longer and you block the others.

A best practice is to run a **test** on a sample **and adjust** your resources before launching identical jobs massively:

- choose the **right queue**: unlimitq is very limited in resources. Only use unlimitq when a job requires more than 4 days.
- adjust the memory: first do a test and check the memory consumed by the job in COMPLETED state with the seff command: \$ seff <jobid>
- reserve several **cpus** only if the program used can do multithreading. The number of cpu reserved with Slurm must match the number of cpus set in the software parameters.
- adjust the time option -t



Best practices Infrastructure

Help in keeping the infrastructure and the support to run smoothly.

- DO NOT run jobs on frontal servers (tmux, screen, R, snakemake):

Why?

- overloading frontal servers slows down everyone. overloading frontal servers can crash them and block everyone.

Check your processes on frontal servers before exit: \$ pstree -u < login> Kill them and close Screen/Tmux session when they are no longer useful

Any job launched on the servers "genobioinfo" will be immediately killed by the system administrators.

- Configure your antispam to accept these e-mails: support.bioinfo.genotoul@inrae.fr,support.bioinfo.genotoul@inrae.fr,support.bioinfo.genotoul@inrae.fr,bioinfo.genotoul@groupes.renat er.fr,ldap admin@genobull.toulouse.inra.fr (changement de mot de passe)
- Inform us of a departure: the number of accounts is limited so when we can delete some and leave room for others, it's better.
- Respect our charter.
- Be precise in support requests support (and/or use our forms to give the right information)





Bioinfo genotoul website

https://bioinfo.genotoul.fr/

Bioinfo Genotoul Chart

https://bioinfo.genotoul.fr/wp-content/uploads/ChartPFBioinfoGenoToul.pdf

FAQ

https://bioinfo.genotoul.fr/index.php/faq/

Support

Mail: support.bioinfo.genotoul@inrae.fr

Fill form (best for us): https://bioinfo.genotoul.fr/index.php/ask-for/support/



What about:

Web services?



Web services

- New infrastructure implies:
 - New computing facilities access (new Slurm scheduler)
 - New storage locations (home & work)
- Migration is required for web services/servers that use:
 - Current cluster (2017) facilities
 - Current storage for home or save
- Impacted services/servers are (among other):
 - https://genoweb.toulouse.inra.fr (public_html)
 - https://vm-galaxy-prod.toulouse.inrae.fr (Galaxy)
- => New servers will be set up, and users will be guided through the migration steps.
- => Web admin will be contacted and assisted as well.
- Migration will be as smooth as possible, and public URL will stay unchanged.



Thank you for your attention

Any questions?







WORK Data Migration



From the new genobioinfo node (on new cluster): Replace "**username**" by your own login and type:

"rsync -avh /oldwork/username /work/user/username"



Appendix 1 :Software usage

Create your own environment

Create your modulefile

Basic example for the modulefile ~/save/my_own_module :

module load bioinfo/STAR/2.7.5a prepend-path PATH /save/<login>/my_binaries/

Load your module

\$ module load -f ~/save/my_own_module

Verify your environment

\$ which STAR

/usr/local/bioinfo/src/STAR/STAR-2.7.5a/source/STAR

Unload one module

\$ module unload bioinfo/STAR/2.7.5a

Unload all module and specific variable

\$ module purge



Appendix 2: Software usage Environment modules

Basic command to use module:

module: (no arguments) print usage instructions

module avail: list available software module

module load modulename: add a module to your environment

module unload modulename: unload remove a module

module purge : remove all modules

module show modulename: show what changes a module will make to your environment module help modulename: path to the hel ("How_to_use_SLURM_<soft_name>" file for us)

For more documentation, see the Environment Module website: https://modules.sourceforge.net/



Appendix 3: hot or cold data?

How to know if file or directory is on hot or cold work space storage?

\$ mmlsattr -L <file or directory>

Example:

\$ mmlsattr -L scripts_test

file name: scripts_test metadata replication: 1 max 2

immutable: no appendOnly: no

flags:

storage pool name: system

fileset name: user

snapshot name:

creation time: Wed Aug 18 14:09:57 2021

Misc attributes: DIRECTORY

Encrypted: no

system=hot space capacitive=cold space



Storage benches (/work)

Caractéristique			Par baie	Solution proposée
Max Random IOPS Read (4KB)			1 M	4M
Max Random IOPS Write (4KB)			160 000	640 000
Max Sequential Reads (1MB)			15 GB/s	60 GB/s
Max Sequential cache mirroring disc	Writes bled	(1MB)	14 GB/s	56 GB/s
Max Sequential cache mirroring end	Writes bled	(1MB)	10 GB/s	40 GB/s



Storage benches (/work)

Plateform	Per disk array	Our solution (4 disk arrays)
Max random IOPS Read (4 KB)	1M	4M
Max random IOPS Write (4 KB)	160 000	640 000
Max Sequential Reads (1 MB)	15 GB/s	60 GB/s
Max Sequential Write (1 MB) Cache mirroring disabled	14 GB/s	56 GB/s
Max Sequential Write (1 MB) Cache mirroring enable	10 GB/s	40 GB/s

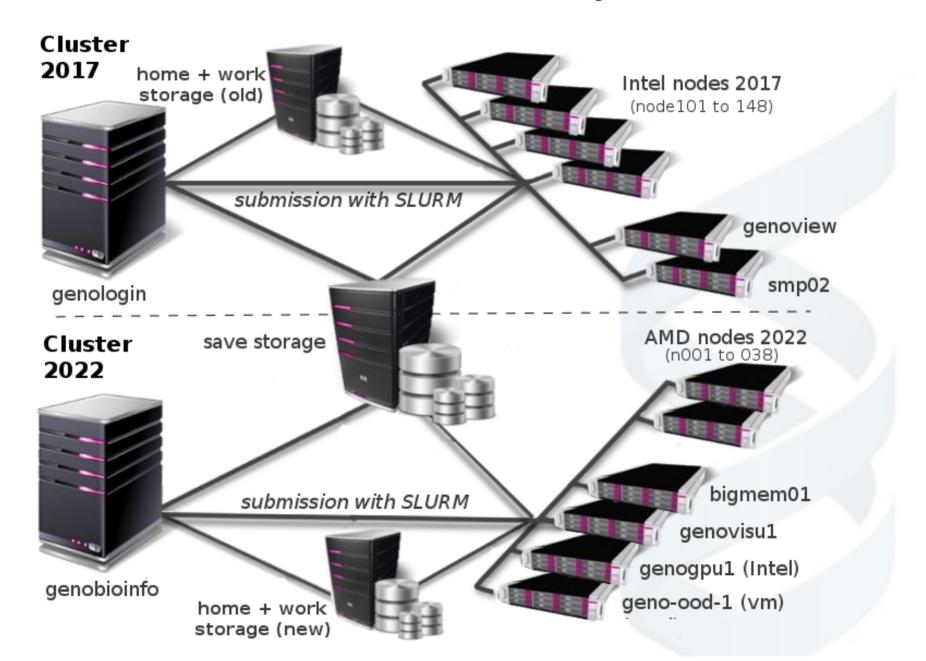


Compute benches

- Bench HPL (39 nodes): 136 TFlops/s
- Bench HPL GPU: 55 TFlops/s
- Bench STREAM memory (1 nodes): de l'ordre de 300GB/S
- Bench **BWA**, **SAMTOOLS** (1 instance on 1 node): 100s
- Bench BWA, SAMTOOLS (128 instances on 1 node): 250s
- Bench STAR (1 instance * 128 threads): 193s
- Bench STAR (16 instances * 16 threads): 1775s



New environment For one year, 2 clusters





Open On Demand portal

=> Work In Progress (currently being deployed)

Launch **interactive sessions** on the virtualization node through the Web browser:

Tools:

- Linux 3D desktop,
- Jupyter Notebook,
- Rstudio

Submit jobs (SLURM) on the compute cluster

Browse the files

Transferts from/to the user desktop



Portal Open On Demand

GENOBIOINFO HPC Portal

Files ▼

Jobs ▼

Shells ▼

Interactive Apps ▼



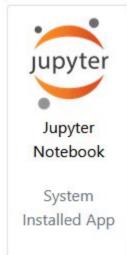


OnDemand provides an integrated, single access point for all of your HPC resources.

Pinned Apps A featured subset of all available apps

Message

Interactive Apps









What about:

https://vm-galaxy-prod.toulouse.inrae.fr



Galaxy

- Current Galaxy server uses your account for:
 - job submission on current cluster (2017)
 - temp processing files in the work storage
- A new Galaxy server will be installed this year:
 - With latest version of Galaxy server
 - Submission on new cluster (still with your account)
 - Use of new storage locations
- Waiting for this new server for every body:
 - Old one will still be available for current and new users
 - Migration support will be provided (dataset and tools)
- Old server will be stopped at the end of the year