Getting Started With GLiCID: Beginner Session

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1

Outline: Beginner Session

- Introduction to High Performance Computing (HPC)
 - HPC Use Cases
- Introducing NAUTILUS
 - Architecture of Nautilus
- Working With A Supercomputer
 - Basic Linux Commands
 - SSH Connections and access to Nautilus
- SLURM Workload Manager
 - Basic Slurm Commands
- Modules
- Guix Package Manager
- Data Management
- GLiCID Help

What's HPC?



Data, Data, Everywhere

- Key Statistics 2023
 - **3.5 quintillion bytes of data is created every single day** (Source: Earthweb)
 - 333.2 billion emails are sent per day
 - 100 billion messages are sent through WhatsApp in a day
 - 5 billion Snapchat videos and photos are shared per day
 - 456,000 tweets are made on Twitter each minute of the day
 - 500 million daily story users on Instagram every day
 - People spend \$1 million per minute online



Data, data everywhere, but not a byte to use.



There are only 10 types of people in the world: Those who understand binary and those who don't.





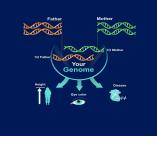
Q. Why would I be interested in High Performance Computing (HPC)?

Frequently, research problems that use computing can outgrow the capabilities of the desktop or laptop. For example,

Use Case 1: AI/ML/Statistics

- A statistics/data science researcher wants to cross-validate a model.
- This involves running the model 1000 times but each run takes an hour.
- Running the model on a laptop will take over a month.
- In this research problem, final results are calculated after all 1000 models have run, but typically only one model is run at a time (in serial) on the laptop.
- Since each of the 1000 runs is independent of all others, and **given enough computers, it's theoretically possible to run them all at once (in parallel) and complete the task in one hour**.

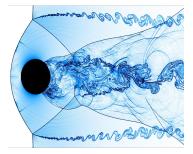




Use Case 2: Genomics

- A genomics researchers use some type of sequencing datasets that are huge.
- It's challenging to open these datasets on a computer analyzing these larger datasets will probably crash it.
- In this research problem, the calculations required might be impossible to parallelize, but a computer with more memory would be required to analyze the much larger future data set.





Use Case 3: Fluid Dynamics/Mechanics

- An engineer using a fluid dynamics package has an option to run in parallel.
- In going from 2D to 3D simulations, the simulation time has more than tripled.
- In this research problem, the calculations in each region of the simulation are largely independent of calculations in other regions of the simulation.
- It's possible to run each region's calculations simultaneously (in parallel), communicate selected results to adjacent regions as needed, and repeat the calculations to converge on a final set of results.
- In moving from a 2D to a 3D model, both the amount of data and the amount of calculations increases greatly, and it's theoretically possible to distribute the calculations across multiple computers communicating over a shared network.

In all these cases, access to more computers with larger memories is needed.

HPC: Other cases

• AI and ML

• HPC supports training deep neural networks, processing large datasets, and accelerating machine learning algorithms

Weather and Climate Modelling

• HPC is used to run complex atmospheric models, simulate weather patterns, and predict climate change phenomena

• Engineering and Design Optimization

• HPC is employed to optimize engineering designs, analyze structural integrity, simulate fluid dynamics, and enhance product performance

• Astrophysics and Cosmology

• HPC facilitates large-scale simulations of the universe, including galaxy formation, stellar evolution, and gravitational wave analysis

HPC: Other cases

• Drug Discovery and Molecular Dynamics

• HPC enables the simulation of drug interactions, protein folding, and molecular dynamics, aiding in the development of new pharmaceuticals

• Financial Modeling and Risk Analysis

- HPC helps in analyzing complex financial models, running Monte Carlo simulations, and assessing investment risks
- And many more...

What is High Performance Computing (HPC)?

- Best-known types of HPC solutions is the **Supercomputer**
- It is made up of thousands of computers that work together
- Fastest Supercomputer is the US-based Frontier, with a processing speed of 1.102 exaflops, or quintillion floating point operations per second (flops)
- HPC solutions can be deployed on-premise, at the edge, or even in the cloud



Top 500	Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
	1	Frontier - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory United States	8,699,904	1,194.00	1,679.82	22,703
	2	Supercomputer Fugaku - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442.01	537.21	29,899
	3	LUMI - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland	2,220,288	309.10	428.70	6,016
	4	Leonardo - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, Atos EuroHPC/CINECA Italy	1,824,768	238.70	304.47	7,404
	5	Summit - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148.60	200.79	10,096

Source: https://www.top500.org/ 11

How does HPC work?

- A standard computing system solves problems primarily using **serial computing**
- It divides the workload into a sequence of tasks, and then executes the tasks one after the other on the same processor
- In contrast, HPC leverages
 - Massively parallel computing
 - Compute clusters (also called HPC clusters)
 - High-performance components

How does HPC work?

• Massively parallel computing

• Parallel computing using tens of thousands to millions of cores

• Compute clusters/HPC clusters

- Consists of multiple high-speed computer servers networked together
- The computers, called nodes, use either high-performance multi-core CPUs or, more likely today, GPUs (graphical processing units)
- Well suited for rigorous computations and graphics-intensive tasks

• High-performance components

 Other computing resources in an HPC cluster - networking, memory, storage and file systems - are high-speed, high-throughput and low-latency components that can keep pace with the nodes and optimize the computing power and performance of the cluster



Introducing GLiCID



14



- Nautilus
- Phileas
- Waves

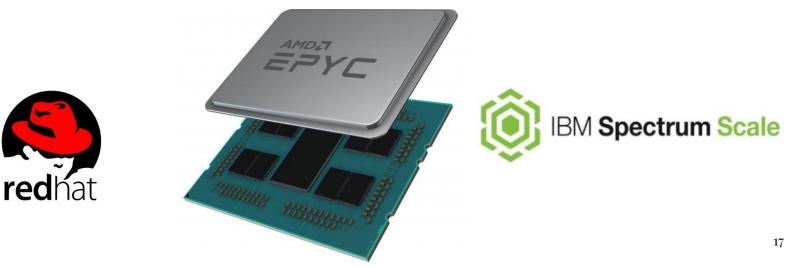
Nautilus Architecture

- Nautilus has 3 main components:
 - Set of nodes communicating with each other
 - Fast interconnect using Infiniband 100 Gb/s technology with high bandwidth and low latency
 - Shared Storage (scratch) 427 TB (IBM/Spectrum Scale- GPFS)



Nautilus Architecture

- Each node consists
 - Red Hat Operating System (RHEL 8.7)
 - 2 AMD EPYC 9474F processors @3.6GHz (4.1GHz Max) with 48 CPU cores
 - TDP (Thermal Design Power)/Power Consumption: 360W
 - 384 GB RAM



Nautilus Architecture

#Computing nodes	Processor and Speed	RAM	#Cores
40 cnode[301-340]	BullSequana X440 (2 AMD EPYC 9474@3.6GHz 48c)	384 GB	3840
8 cnode[701-708]	BullSequana X440 (2 AMD EPYC 9474@3.6GHz 48c)	768 GB	768
4 visu[1-4]	BullSequana X450 (2 AMD EPYC 9474@3.6GHz 48c) with Nvidia A40 (48G) 2 GPUs per node	768 GB	384
4 gnode[1-4]	4 BullSequana X410 (2 AMD EPYC 9474@3.6GHz 48c) with Nvidia A100 (80G) 4 GPUs per node	768 GB	384

Philias/MesoNET

- Bull Sequana X440 X 30 Compute Nodes (+2)
 - Intel Sapphire Rapids (48 cores, 2.1 GHz) X 2
 - 256GB DDR (+2*2TB DDR) + 960GB SSD
- Bull Sequana X450 Display Nodes X 2
 - Intel Sapphire Rapids (48 cores, 2.1 GHz) X 2
 - 512 GB DDR + 960 GB SSD
 - Nvidia A40 GPU 48GB x 2
- DLC Cooling
- Network: IB 100 Gb + 25 Gb eth
- GPFS: 285 TB usable
- 1 login
- 5 years of maintenance
- Available December 2023

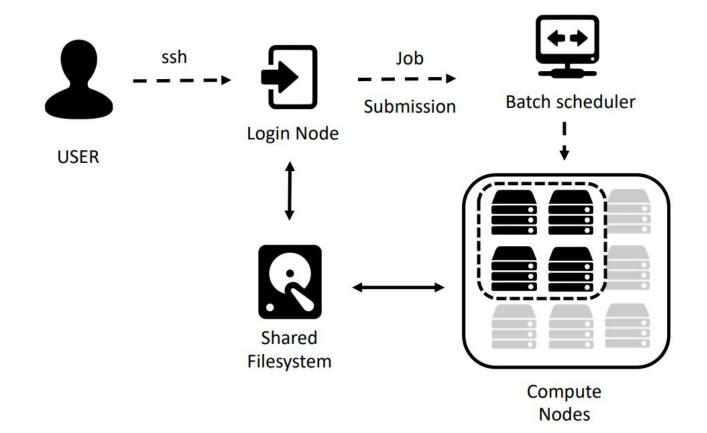
Is NOT like this...







jmir@pc-ici02:~\$ ssh nautilus _____ # This service is restricted to authorized users only. All # activities on this system are logged. # Unauthorized access will be fully investigated and reported # to the appropriate law enforcement agencies. _____ Last login: Mon Sep 25 14:47:01 2023 from 10.50.111.51 1xkkdc 1 + () + ()kWN0dc kW0c VI I kW0c kW0c cOWKl cx0KXWMWXK0xc ccllllloxXWMMMMMMMMMWKo codxk00KXXNNNWWWWMMMMMMMMMMMMW01 coooolc c0WWWWW0 ox0KNWMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWNK0xoc **WMMMWO** kWMMMMNd **ckKKKK**X 1dk0KXNWMMMMMMMMMMMMMMMMMMMMMMMMMWNXK0kd1 clodxkk0000KKKKKKK00000kxdolc Welcome to GLiCID HPC cluster Nautilus === Computing Nodes ======== #RAM/n = #C = cnode[301-340] 40 BullSequana X440 (2 AMD EPYC 9474F@3.6GHz 48c) 384 3840 cnode[701-708] 8 BullSeguana X440 (2 AMD EPYC 9474F03.6GHz 48c) 768 768 visu[1-4] 4 BullSeguana X450 (2 AMD EPYC 9474F@3.6GHz 48c) 768 384 with Nvidia A40 (48G) 2 GPUs per node 4 BullSequana X410 (2 AMD EPYC 9474F@3.6GHz 48c) 768 gnode[1-4] 384 with Nvidia A100 (80G) 4 GPUs per node Fast interconnect using InfiniBand 100 Gb/s technology Shared Storage (scratch) : 427 TB (IBM/Spectrum Scale - GPFS) Remote Visualization Apps through XCS portal @https://xcs.glicid.fr/xcs/ User storage : user directory /home/<username> project directory /LAB-DATA/GLiCID/projects/<projectname> scratch directory /scratch/users/<username> scratch SSD/scratch-shared scratch Liger /scratchliger/<old liger username> (temporary, ro) softwares directory /opt/software Softwares : use modules module avail use GUIX guix install <software> (documentation for details) Useful Links : User DOC https://doc.glicid.fr Support https://help.glicid.fr or support@glicid.fr Chat coming soon Admins tech@glicid.fr Forum coming soon Status page https://ckc.glicid.fr imir@ec-nantes.fr@nautilus-devel-001 ~15





Login node(s)

- Editing and transferring files
- Compile programs
- Prepare simulations



Compute nodes

- Multicore nodes
- Large memories
- High-speed
 interconnections



Batch scheduler

- Resource allocation
- Job queueing
- Accounting and



File system

- Parallel FS
- Efficient I/O
- Node local disks

Getting Started with GLiCID



Prerequisites

- macOS
 - Terminal (pre-installed)
- Windows
 - MobaXterm
 - PowerShell
- Linux
 - You are already well equipped :)

LINUX COMMAND LINE



Linux Command Line - Brief History



- One of the earliest operating systems was called **Unix**
- Designed to run as a multi-user system on **mainframe computers**
- Users connecting to it remotely via individual terminals
- Terminals were pretty basic: just a keyboard and screen
- Send keystrokes to the server and display any data they received on the screen
- No mouse, no fancy graphics, not even any choice of colour
- Everything was sent as text, and received as text
- Programs that ran on the mainframe had to produce text as an output and accept text as an input



Linux Command Line - Brief History



IBM Mainframe, Late 1960's/Early 1970's

Linux Command Line - Brief History



- **Linux** is a sort-of-descendant of Unix
- The core part of Linux is designed to behave similarly to a Unix system
- Most of the old shells and other text-based programs run on it quite happily
- Most of the <u>Top 500</u> supercomputers use Linux

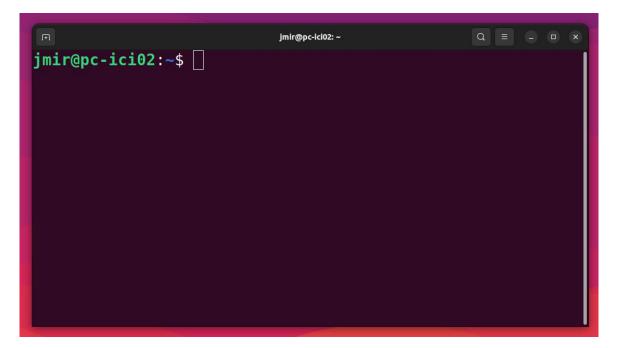
What's A Command Line?



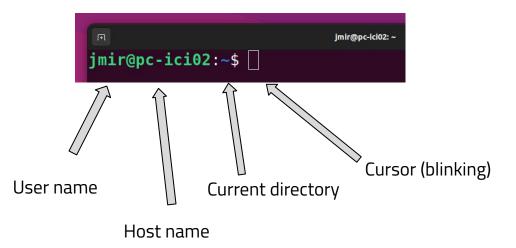
- The Linux command line is a text interface to your computer
- Often referred to as **shell, terminal, console, prompt** or various other names
- It can give the appearance of being complex and confusing to use
- But it is not so scary as it looks
- You just need to memorize a few basic commands



• Launch the Terminal



• Structure of a linux commands

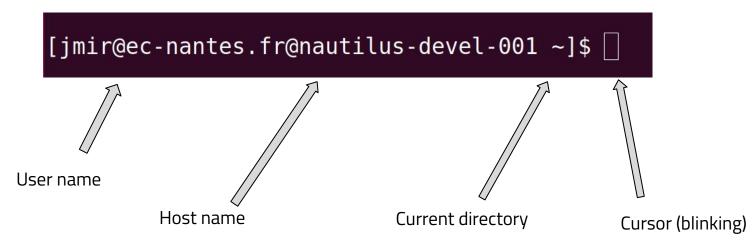


• The system is ready to accept commands





• Structure of a linux commands (in Nautilus)



• The system is ready to accept commands



Command	Syntax	Description
Print Working Directory	pwd	Print present working directory
List	ls	List files and directories at path
Change directory	cd	Change current directory
Make directory	mkdir	Create new directory
Create empty file	touch	Create new file or update timestamp
Move	m∨	Move or rename files and directories
Сору	ср	Copy files or directories from source to destination
Remove	rm	Remove files
Text editor	vim	Vim is a highly configurable text editor



Command	Syntax	Description
Print Working Directory	pwd	Print present working directory

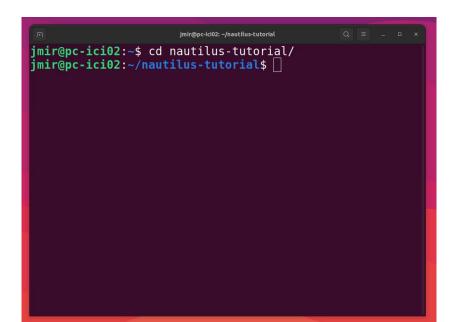
	jmir@pc-ici02: ~	Q = - 0	
jmir@pc-ici02 :~\$ /home/jmir	pwd		
jmir@pc-ici02:~\$	Π		
J			



Command	Syntax	De	scription	
List	ls	Lis	List files and directories at path	
	<pre>imir@pc-ici02:~\$ access-token.txt anaconda3 cv_debug.log Desktop Documents Downloads ghh ghh.pub jmir@pc-ici02:~\$</pre>	git_repo inventory.yaml Music nautilus-tutori Pictures playbook.yaml Public snap	Templates teskey.txt test2.txt al testdir testscript.sh test.txt ust4hpc Videos	

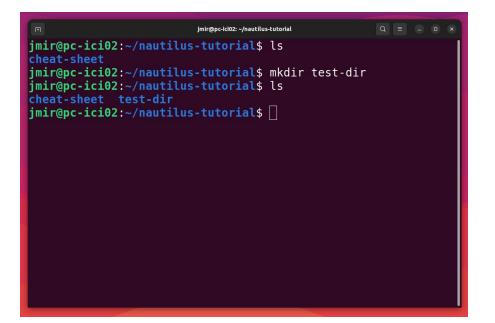


Command	Syntax	Description
Change directory	cd	Change current directory



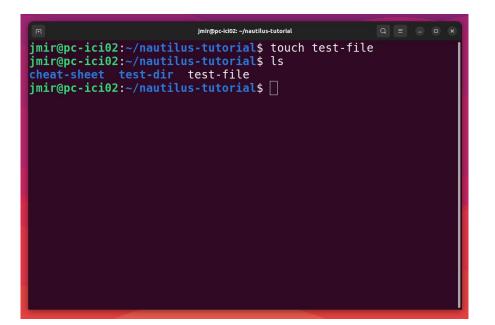


Command	Syntax	Description
Make directory	mkdir	Create new directory





Command	Syntax	Description
Create empty file	touch	Create new file or update timestamp



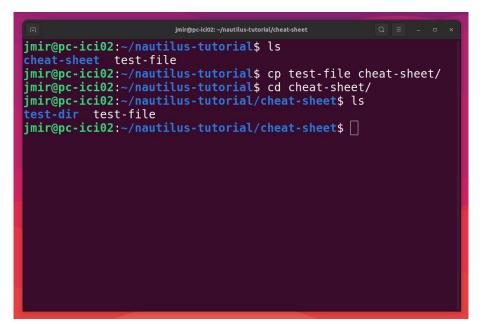


Command	Syntax	Description
Move	mv	Move or rename files and directories

jmir@pc-ici02: -/nautilus-tutorial/cheat-sheet Q ≡ − □ ×
jmir@pc-ici02:~/nautilus-tutorial\$ ls
cheat-sheet test-dir
<pre>jmir@pc-ici02:~/nautilus-tutorial\$ mv test-dir/ cheat-sheet/</pre>
jmir@pc-ici02:~/nautilus-tutorial\$ ls
cheat-sheet
<pre>jmir@pc-ici02:~/nautilus-tutorial\$ cd cheat-sheet/</pre>
jmir@pc-ici02:~/nautilus-tutorial/cheat-sheet\$ ls
test-dir test-file
jmir@pc-ici02:~/nautilus-tutorial/cheat-sheet\$

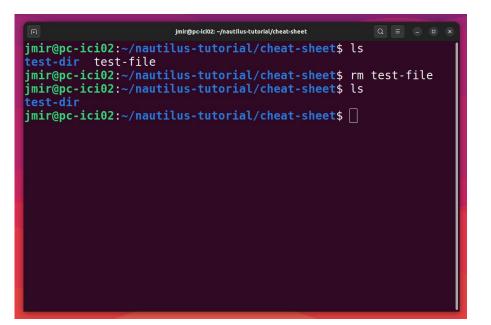


Command	Syntax	Description
сору	ср	Copy files or directories from source to destination





Command	Syntax	Description
Remove	rm	Remove files



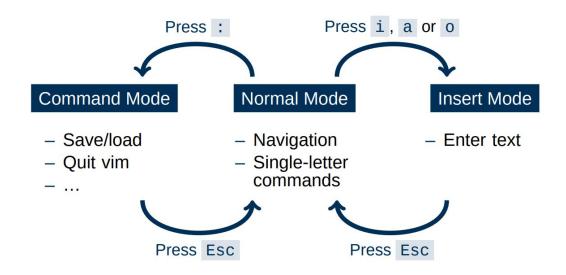


Command	Syntax	Description
Text editor	vim	Vim is a highly configurable text editor

	jmir@pc-ici02: ~/nautilus-tutorial	Q = - • ×
#!/bin/bash		
<mark>nkdir</mark> new-dir && <mark>cd</mark> new	v-dir	
echo "Ciao"		
-		
:wq!		



Command	Syntax	Description
Linux editor	vim	Vim is a highly configurable text editor



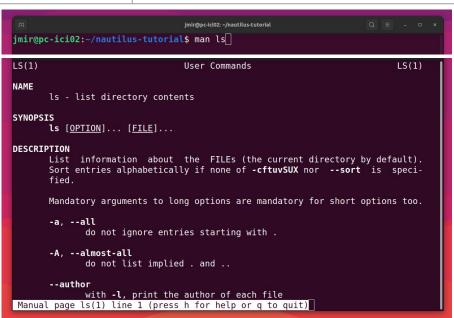


Command	Syntax	Description
Text editor	nano	Comparatively easier (Ctrl+Option)

GNU nano 6.2 !/bin/bash		test_script.sh	
kdir new-dir && cd new-c	ir		
cho "Ciao"			



Command	Syntax	Description
User Manual	man	Displays whole manual of the command



Basic Linux Commands - File Management



Path to folders and files

• Relative Path

 jmir@pc-ici02: ~/nautilus-tutorial/test-dir
 Q = - • ×

 jmir@pc-ici02:~/nautilus-tutorial\$ cd test-dir/
 jmir@pc-ici02:~/nautilus-tutorial/test-dir\$

• Absolute path

jmir@pc-ici02: ~/nautilus-tutorial/test-dir	Q = - • ×
jmir@pc-ici02:~/nautilus-tutorial\$ cd ~/nautilus-tutorial/test-dir/ jmir@pc-ici02:~/nautilus-tutorial/test-dir\$ []	

Basic Linux Commands - Large Files

• Compress

\$ tar -czvf <folder_name.tar.gz> <foldername>

- Decompress
 - \$ tar -xzvf <folder_name.tar.gz>

Basic Linux Commands - File Management

• Local to Remote

\$ scp -r folder_name nautilus:/scratch/nautilus/users/username

Remote to Local

\$ scp -r nautilus:/scratch/nautilus/users/username/folder_name /local_location

Note: Run both commands from the local machine.



Basic Linux Commands - Bash Scripting

- What if we want to run many bash commands?
- ... maybe in a workflow???
- Important part of process automation in Linux
- Plain text file that contains a series of commands
- Any command you run on the command line can be put in a script and vice-versa
- Executed like a program

Basic Linux Commands - Bash Scripting

• Simple bash script

#!/bin/bash mkdir test-dir && cd test-dir echo "Ciao"

- Save as test_script.sh
- To execute ./test_script.sh

File Permissions



chmod u+x <filename>

	jmir@pc-ici02: ~/nautilus-tutorial	Q			
jmir@pc-ici02:~/nautilus-tutoria jmir@pc-ici02:~/nautilus-tutoria jmir@pc-ici02:~/nautilus-tutoria oash: ./test_script.sh: Permissi jmir@pc-ici02:~/nautilus-tutoria jmir@pc-ici02:~/nautilus-tutoria Ciao jmir@pc-ici02:~/nautilus-tutoria cheat-sheet new-dir python py jmir@pc-ici02:~/nautilus-tutoria	<pre>1\$ vi test_script.sh 1\$./test_script.sh on denied 1\$ chmod u+x test_script.sh 1\$./test_script.sh 1\$ ls torch_geometric test-dir test_script.sh</pre>	Lpt	.sh		

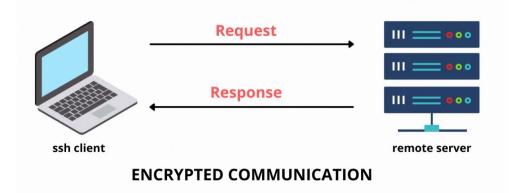
SSH CONNECTIONS



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What is SSH Key?

- SSH is a secure shell (terminal) connection to another computer
- You connect from your computer to the LOGIN NODE
- Security is given by public/private keys
- A connection to the supercomputer needs a
 - о Кеу,
 - Configuration,
 - Key/IP address known to the supercomputer





How to access GLiCID cluster?

- Create an account on <u>https://clam.glicid.fr</u>
- Account validation by an administrator
- User uploads SSH key to CLAM portal (in profile's SSH Access tab)
- SSH connection configuration on local PC

How to configure SSH connection?

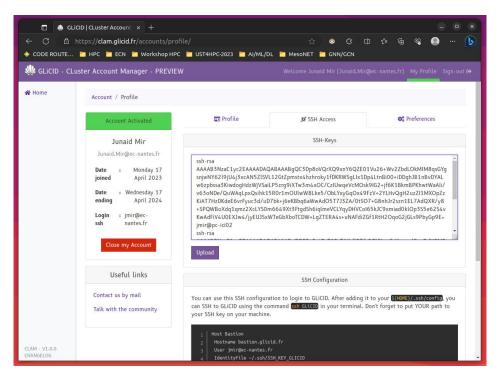
• Generate SSH key and copy the public key (id_ed25519.pub)

jmir@pc-ici02:~\$ ssh-keygen -t ed25519
Generating public/private ed25519 key pair.
Enter file in which to save the key (/home/jmir/.ssh/id_ed25519): y

jmir@pc-ici02:~/.ssh\$ cat id_ed25519.pub
ssh-ed25519 AAAAC3NzaC1lZDI1NTE5AAAAID7Tm0MUiYv62VbE/uyk1Gcan9Wfu1IEsg7sBX8
R6Fjw junaid.mir@ec-nanes.fr
jmir@pc-ici02:~/.ssh\$

How to configure SSH connection?

• Upload this SSH key to the CLAM





How to configure SSH connection?

- Copy Contents to the config file and save it
- Replace <my_username> with your username

```
jmir@pc-ici02:~/.ssh$ cat config
Host Bastion
        Hostname bastion.glicid.fr
        User jmir@ec-nantes.fr
        IdentityFile ~/.ssh/id ed25519
        ForwardAgent yes
Host glicid
        Hostname login-001.glicid.fr
        User jmir@ec-nantes.fr
        ProxyJump Bastion
        IdentityFile ~/.ssh/id ed25519
Host nautilus
        Hostname nautilus-devel-001.nautilus.intra.glicid.fr
        User jmir@ec-nantes.fr
        ProxyJump glicid
        IdentityFile ~/.ssh/id ed25519
```

- Login using SSH by typing this command in the terminal
 - ssh glicid and then press <Enter>

jmir@pc-ici02:~/.ssh\$ ssh glicid The authenticity of host 'bastion.glicid.fr (194.167.60.10)' can't be established. ED25519 key fingerprint is SHA256:0Szy+0r30Rkizt8TXgKeLgD4gRn8Xg+0YmEE4EsfgrU. This key is not known by any other names Are you sure you want to continue connecting (yes/no/[fingerprint])? yes Warning: Permanently added 'bastion.glicid.fr' (ED25519) to the list of known hosts. The authenticity of host 'login-001.glicid.fr (<no hostip for proxy command>)' can't be established. ED25519 key fingerprint is SHA256:0Szy+0r30Rkizt8TXaKeLaD4aRn8Xa+0YmEE4EsfarU. This host key is known by the following other names/addresses: ~/.ssh/known hosts:1: [hashed name] Are you sure you want to continue connecting (yes/no/[fingerprint])? yes Warning: Permanently added 'login-001.glicid.fr' (ED25519) to the list of known hosts. Last login: Wed Nov 29 14:07:00 2023 from 194.167.60.12 imir@ec-nantes.fr@guix-devel-001 ~\$ ls env.yml KEYS ml-container test-containers TP ContainerWorkshop wget-log wget-log.1 jmir@ec-nantes.fr@guix-devel-001 ~\$





- Login directly to nautilus
 - ssh nautilus and then press <Enter>

	jmir@ec-nantes.fr@nautilus-devel-001:~		
parameterized to authorized users only. All of the service is restricted to authorized users only. All of the service is restricted to authorized users only. All of the service is restricted to authorized users only. All of the service is restricted to authorized users only. All of the service is restricted to authorized users only. All of the service is restricted to authorized users only. All of the service is restricted to authorized users only. All of the service is restricted to authorized users only. All of the service is restricted to authorized users only. All of the service is restricted to authorized users only. All of the service is restricted to authorized users only. All of the service is restricted to authorized users on the service is restricted users on the service is restricted users on the service is restricted users on the service is restr			
Velcome to GLICD MPC cluster Novillos 			
Fast interconnect using InfiniBand 100 Gb/s technology Shared Storage (scratch) : 427 TB (IBM/Spectrum Scale - GPFS) Remote Visualization Apps through XCS portal @https://xcs.glicid.fr/xcs/			
User storage : - user directory/home/vusername> - project directory/AB-DATA/GLICE/projects/aprojectmame> - scratch directory/scratchluger/vold_Liger_username> - scratch Liger/scratchluger/vold_Liger_username> (temporary, ro) - scratch Liger			
Softwares : - use modules			
Useful Links : • User DC https://doc.glicid.fr Dait			

- Switch from glicid to nautilus
 - ssh nautilus-devel-001 and then press <Enter>
 - It will not work but ask for a password



- Switch from glicid to nautilus
 - To switch to nautilus, set-up authorized_keys
 - cd ~/.ssh after logging in to glicid
 - Either generate a new key or copy the private key id_ed2259

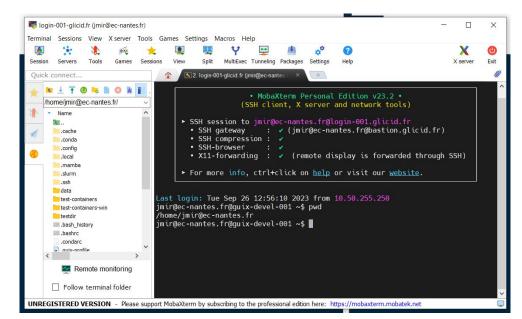
```
jmir@ec-nantes.fr@guix-devel-001 ~/.ssh$ ssh-keygen -t ed25519
Generating public/private ed25519 key pair.
Enter file in which to save the key (/home/jmir@ec-nantes.fr/.ssh/id ed25519):
Enter passphrase (empty for no passphrase):
Enter same passphrase again:
Your identification has been saved in /home/jmir@ec-nantes.fr/.ssh/id ed25519
Your public key has been saved in /home/jmir@ec-nantes.fr/.ssh/id ed25519.pub
The key fingerprint is:
SHA256:7bx0Ee+80Lh9ykhp3/5DGxRPzPXa5DkJqQodBSU6/L0 jmir@ec-nantes.fr@guix-devel-001.waves.intra.glicid.f
The key's randomart image is:
+--[ED25519 256]--+
          000
               00
        + .. 0 .=
         +.00. .*+
        .Sooo. 0+0
         .o.B. o.
          .XE+ . 0
          + 0 0.0
          .= *+0.0
+----[SHA256]----+
imir@ec-nantes.fr@guix-devel-001 ~/.ssh$ ls
id ed25519 id ed25519.pub known hosts known hosts.old
jmir@ec-nantes.fr@quix-devel-001 ~/.ssh$ cat id ed25519.pub > authorized keys
jmir@ec-nantes.fr@quix-devel-001 ~/.ssh$ ls
authorized keys id ed25519 id ed25519.pub known hosts known hosts.old
jmir@ec-nantes.fr@guix-devel-001 ~/.ssh$ ssh nautilus-devel-001
```



jmir@pc-ici02:~\$ ssh nautilus # This service is restricted to authorized users only. All # activities on this system are logged. # Unauthorized access will be fully investigated and reported # to the appropriate law enforcement agencies. _____ Last login: Mon Sep 25 14:47:01 2023 from 10.50.111.51 lxkkdc kWN0dc kW0c kW0c kW0c cOWK1 cx0KXWMWXK0xc ccllllloxXWMMMMMMMMWWKo coocolc codxk00KXXNNNWWWWMMMMMMMMMMMMWW0 ox0KNWMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWNK0xoc c0WWWWW0 MMWX0dc **KWMMMWO** kWMMMMNd ckKKKKKx ldkOKXNWMMMMMMMMMMMMMMMMMMMMMMMMMMMMXK0kdl clodxkk0000KKKKKKK00000kxdolc Welcome to GLiCID HPC cluster Nautilus === Computing Nodes ======= #RAM/n = #C = cnode[301-340] 40 BullSequana X440 (2 AMD EPYC 9474F@3.6GHz 48c) 384 3840 cnode[701-708] 8 BullSequana X440 (2 AMD EPYC 9474F@3.6GHz 48c) 768 768 visu[1-4] 4 BullSeguana X450 (2 AMD EPYC 9474F@3.6GHz 48c) 768 384 with Nvidia A40 (48G) 2 GPUs per node gnode[1-4] 4 BullSeguana X410 (2 AMD EPYC 9474F@3.6GHz 48c) 768 384 with Nvidia A100 (80G) 4 GPUs per node Fast interconnect using InfiniBand 100 Gb/s technology Shared Storage (scratch) : 427 TB (IBM/Spectrum Scale - GPFS) Remote Visualization Apps through XCS portal @https://xcs.glicid.fr/xcs/ User storage : user directory /home/<username> project directory /LAB-DATA/GLiCID/projects/<projectname> scratch directory /scratch/users/<username> scratch SSD/scratch-shared scratch Liger /scratchliger/<old liger username> (temporary, ro) softwares directory /opt/software Softwares : use modules module avail Useful Links : User DOC https://doc.glicid.fr Support https://help.glicid.fr or support@glicid.fr Chat coming soon Admins tech@glicid.fr Forum coming soon Status page https://ckc.glicid.fr [jmir@ec-nantes.fr@nautilus-devel-001 ~]\$



- On Windows
 - Use MobaXTerm
 - Install MobaXterm (Free version) <u>https://mobaxterm.mobatek.net/download.html</u>





- Open Windows PowerShell
 - Run ssh-keygen (Preferably use id_ed25519)
 - Save it in C:\Users\username\.ssh\id_rsa (normally it will be automatic)
 - Don't enter any passwords just press enter (easier)
 - You'll find two files
 - id_rsa.pub and id_rsa.pkk
 - Create an account on https://glicid.clam.fr and upload the public key(id_rsa.pub) (remove spaces if any)(be careful, don't delete anything by mistake)

- Open MobaXterm
- On SSH, configure
 - Remote-host: login-001.glicid.fr
 - Username: jmir@ec-nantes.fr (DON'T USE MINE)
 - Port: 22 (automatic)
 - Click Advanced SSH settings
 - Use private key (upload your private key)(id_rsa.pkk)
 - Go to Network Settings -> SSH gateway (jump host)
 - Gateway host: bastion.glicid.fr
 - Username: jmir@ec-nantes.fr (DON'T USE MINE)
 - Port:22
 - Use SSH key -> upload private key (id_rsa.pkk)
 - Click OKAY
 - Click OKAY in Session Settings
 - Double click OR right click and execute a session
 - You'll be logged in.
 - To exit -> Either write exit in the terminal and press enter or click on the exit option.
- Be careful: Everything is case-sensitive and don't use MobaXterm for key generation



• Open PowerShell

ssh-keygen

		rsa key pair. we the key (C:\	Users∖jmir/.ssh/id	rsa):
Enter pass	phrase (empty f	or no passphras		
	passphrase aga		\Users\imir/.ssh/i	d
			rs\jmir/.ssh/id rs	
The key fi	ngerprint is:			
			/S3/4WdsDE jmir@pc	-gem09
The key's +[RSA 3	randomart image	is:		
	0/2j+ 0+0.			
	0			
	0.+.			
	0 + . 0+E0 .			
	0+E0 . 0+0.+BB0			
	.0.0*0.B			
	.000+			
 +[SHA2	.0++B			
PS C:\User				

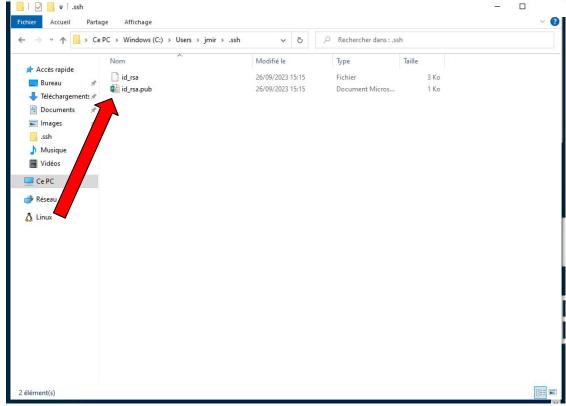


- 0

X

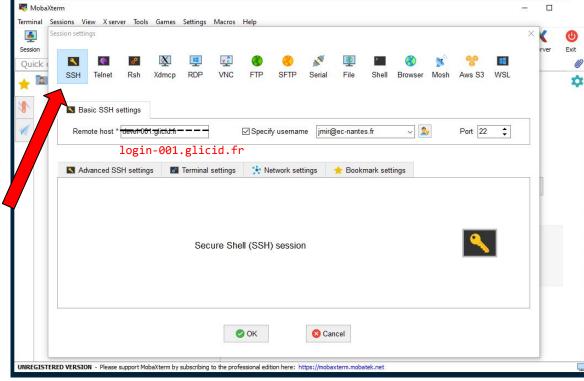


- Keys generated
 - Private key
 - Public key





- Open a session
- Configure SSH



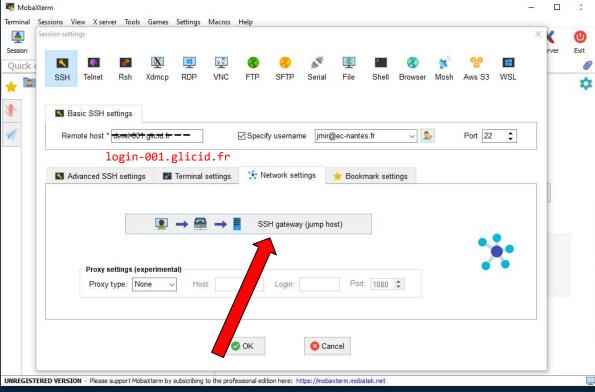


- Advanced SSH
 - Upload id_rsa

Session	n settings														\times	rver	Ex
un i	SSH Telnet		<u>¥</u> imcp	RDP	VNC	FTP	SFTP	Serial	Sile	Shell	Image: Stress of the second se	Mosh	S3 Aws	WSL		-	
	Basic SSH set	tings															
	Remote host *	level 001.gl	ici d fr			Specif	fy usernan	ne jmir@))ec-nante	s.fr	~	}	Port 22	\$			
	lc	ogin-0	01.g	glici	d.fr												
	Advanced SSH	l settings	. 1	Terminal :	settings	🔆 Ne	etwork set	tings	🛨 Booki	mark set	tings						
		Forwarding			settings ompressio		Remote er	nvironment	t: Interac	tive shel]	
	⊠ X11-F Execute	Forwarding command:		⊡ Co	ompressio		Remote er	nvironment	t: Interac	ctive shell	l → I ends						
	⊠ X11-F Execute	Forwarding			ompressio		Remote er	nvironment	t: Interac	ctive shell	l → I ends		•				
	⊠ X11-F Execute SSH-bro	Forwarding command:	SFTP	⊡ Co ? protoco	ompressio	n I	Remote er	nvironment Do not e Follow S	t: Interac	ctive shell command (experim	l ~ l ends ental)		•				
	⊠ X11-F Execute SSH-bro	Forwarding command: pwser type:	SFTP C:\Us	∑ Co ⁹ protoco ers\jmir\.	ompressio	n I	Remote er	nvironment Do not e Follow S	t: Interac exit after c SSH path	ctive shell command (experim	l ~ l ends ental)		•				
	⊠ X11-F Execute SSH-bro	orwarding command: owser type: private key	SFTP C:\Us	∑ Co ⁹ protoco ers\jmir\.	ompressio	a I	Remote er	Do not e Do not e Follow \$	t: Interac exit after c SSH path	ctive shell command (experim	l ~ l ends ental)		ſ				
	⊠ X11-F Execute SSH-bro	orwarding command: owser type: private key	SFTP C:\Us	∑ Co ⁹ protoco ers\jmir\.	ompressio I ssh\id_rs in start: [a I	Remote er	Do not e Do not e Follow \$	t: Interac exit after c SSH path xpert SSH	ctive shell command (experim	l ~ l ends ental)		¢				

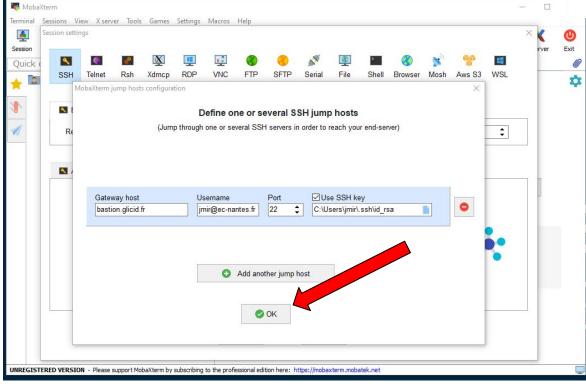


• SSH Gateway



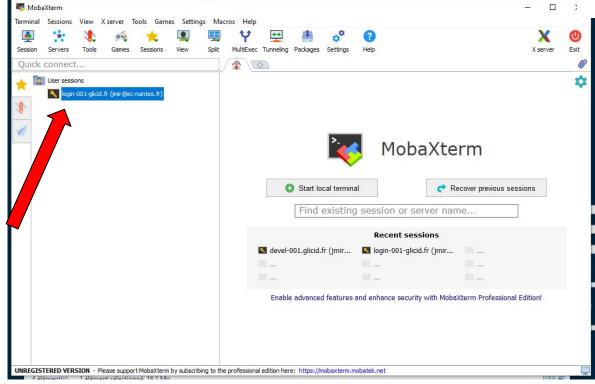


- SSH Gateway
 - Upload id_rsa



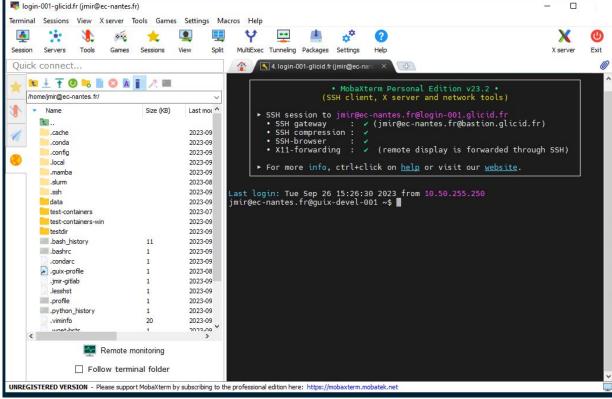


• Execute Session





• Here you go...



WINDOWS: File Management

- File Management
 - Just drag and drop
 - Or using upload option
 - Inside the terminal, it's Unix
 - So if you didn't pay interest in the command line session :(

Get Your Hands Dirty

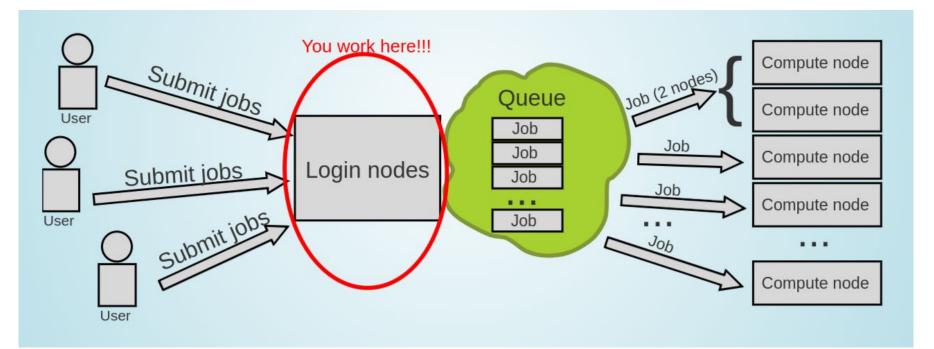




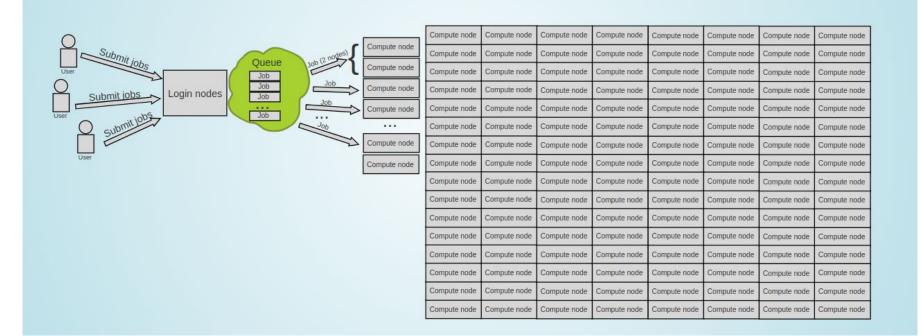
Bringing Order To Chaos



<mark>You submit jobs</mark>



But you don't use the whole Supercomputer



There are many more users

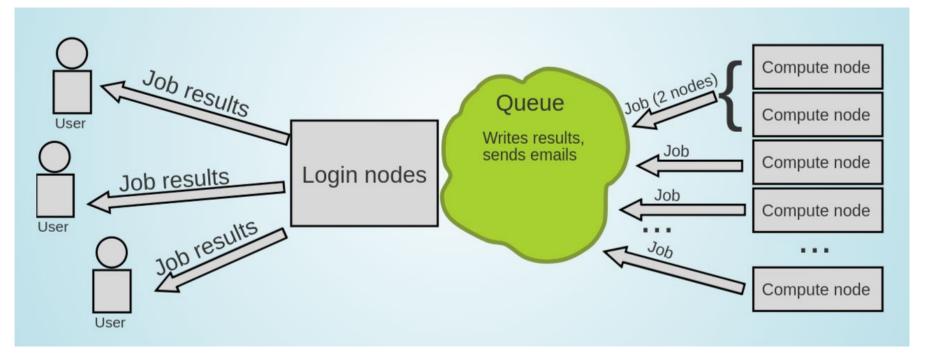
	Compute node C												-			
Queue your Comment	Compute node C							-			-					
	Compute node C				NAMES OF TAXABLE					Contraction of the second						
Submit jobs Login nodes Job Job	Compute node C							Compute node							Compute node	Compute nod
Login nodes	Compute node C							Compute node							Compute node	Compute nod
Submitter node	Compute node C					Compute node			Compute node		Concert Sector Concert		Compute node		Compute node	
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	Compute node C															
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	Compute node C	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node			Compute node		Compute node	
	Compute node C															
	Compute node C	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute no
	Compute node C	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute no
	Compute node C	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute no
	Compute node C	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute not
	Compute node C	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute no
	Compute node C	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute not
	Compute node C	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute not
	Compute node C	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute no
	Compute node C	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute not
	Compute node C	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute not
	Compute node C	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute not
	Compute node C	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute node	Compute not

Enter the queue, and wait

- Your job(s) enter the queue, and wait for its turn
- When there are enough resources for that job, it runs







This it how it works

- User submits jobs
- Job enters the queue
- When it can, it runs
- Sends results back to user

- CAUTION
- Login nodes are for submitting jobs, move files, compile, etc
- NOT FOR TRAINING NEURAL NETS

Who will manage this workload?

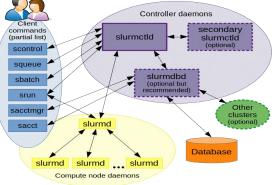
- Need software that will distribute the jobs appropriately and manage the resources
- Keeps track of what nodes are busy/available, and what jobs are queued or running
- Tells the resource manager when to run which job on the available resources



SLURM - Workload Manager



- Simple Linux Utility for Resource Management (SLURM)
- Open source, fault-tolerant, and highly scalable cluster management and job scheduling system for large and small Linux clusters
- It has centralized manager, **slurmctld**, to monitor resources and work
- Each compute node has a **slurmd daemon**, which can be compared to a remote shell: it waits for work, executes that work, returns status, and waits for more work.

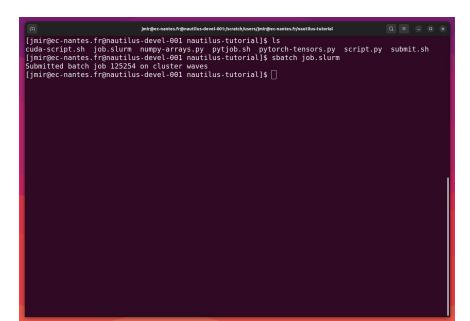




Command	Syntax	Description
sbatch	sbatch <job_name></job_name>	To submit job script for later execution (batch mode)
sinfo	sinfo	Get information about available nodes
squeue	Squeueme	Show information about jobs
scancel	<pre>scancel <job-id></job-id></pre>	To terminate queued or running jobs
salloc	salloc <resource-parameters></resource-parameters>	To get resources and manually run jobs on those allocated resources
sacct	sacct	Show information about current and previous jobs

• To submit a job

sbatch job.slurm







• Get information about available nodes

sinfo

				jmir	@ec-nantes.fr@nautilus-devel-001:~ Q ≡ _ □
		.fr@nautilus	-devel-	001 ~]\$	sinfo
CLUSTER:	nautil	us			
PARTITION	AVAIL	TIMELIMIT	NODES	STATE	NODELIST
standard	up	infinite	1	inval	cnode339
standard	up	infinite	2		cnode[323,329]
standard	up	infinite	10		cnode[302-308,337-338,340]
standard	up	infinite	1	mix	cnode310
standard	up	infinite	2	alloc	cnode[301,309]
standard	up	infinite	22	idle	cnode[312-322,325-328,330-336]
standard	up	infinite	2	down	cnode[311,324]
bigmem	up	infinite	2	drain	cnode[703-704]
bigmem	up	infinite	3	alloc	cnode[701-702,706]
bigmem	up	infinite	3	idle	cnode[705,707-708]
qpu	up	infinite	4	mix	gnode[1-4]
visu	up	infinite	1	alloc	visul
visu	up	infinite	3	idle	visu[2-4]
all*	up	infinite	1	inval	cnode339
all*	up	infinite	2	down*	cnode[323,329]
all*	up	infinite	12	drain	cnode[302-308,337-338,340,703-704]
all*	up	infinite	5	mix	cnode310, gnode [1-4]
all*	up	infinite	6	alloc	cnode[301,309,701-702,706],visu1
all*	up	infinite	28	idle	cnode[312-322,325-328,330-336,705,707-708],visu[2-4]
all*	up	infinite	2	down	cnode[311,324]
CLUSTER:	waves				
PARTITION	AVAIL	TIMELIMIT	NODES	STATE	NODELIST
all*	up	9:00:00	1	unk*	budbud018
all*	up	9:00:00	1	mix	budbud020
all*	up		7		budbud[014-017,019,021-022]
ned	up	4-04:00:00	1		budbud020
ned	up	4-04:00:00	2		budbud[021-022]
devel	up	20:00	1		vmworker-001
		.fr@nautilus	-devel-		

SIUCT workload manager

Basic Slurm Commands

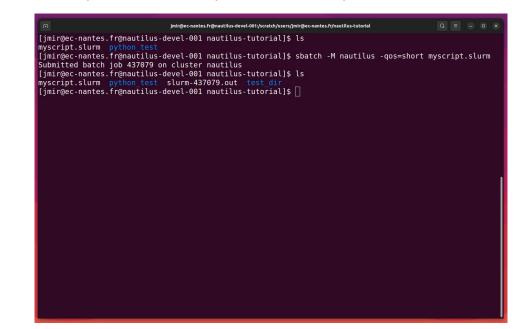
• To check Priority and MaxWall Time

sacctmgr show qos format="name%20,priority,MaxJobsPerUser,MaxWall"

Name	Priority Ma:		saccing snow qus	<pre>format="name%20,priority,MaxJobsPerUser,</pre>	riaxwatt
normal	1	00:05:00			
	50 40	1-00:00:00 3-00:00:00			
	40 30	8-00:00:00			
long unlimited	10	1			
debug	100	00:20:00			
priority	200	8-00:00:00			
mireoc pantos frenau		001 nautilus-tutorial]	+ 		
millingec-nances. Inghat	ititus-uevet-	oor nautrius-tutorratj:	P []		

• Submit your slurm script

sbatch -M nautilus -p standard -q short <script-name>.slurm





Slurm - Batch Script



Sample script to run python code using conda environment

#!/bin/bash	
#SBATCHjob-name=myjob	<pre># create a short name for your job</pre>
#SBATCHnodes=1	# node count
#SBATCHntasks=1	<pre># total number of tasks across all nodes</pre>
#SBATCHcpus-per-task=1	# cpu-cores per task
#SBATCHmem-per-cpu=2G	<pre># memory per cpu-core</pre>
#SBATCHgres=gpu:2	<pre># number of gpus per node</pre>
#SBATCHtime=00:05:00	<pre># total run time limit (HH:MM:SS)</pre>

cd /scratch/user/<username> # go to your working directory / optional

hostname

python myscript.py

Data Management

94

Data management

- HOME (Personal Space/But don't train your neural network here)
- SCRATCH (Train it here)
 - o cd /scratch/nautilus/users/username
 - Move your data to LAB-DATA
- LAB-DATA (Safe Storage)
 - \circ cd /LAB-DATA/

[jmir@ec-nantes.fr@nautilus-devel-001 ~]\$ cd /LAB-DATA/ [jmir@ec-nantes.fr@nautilus-devel-001 LAB-DATA]\$ ls BiRD CEISAM GLiCID LS2N OSUNA [jmir@ec-nantes.fr@nautilus-devel-001 LAB-DATA]\$

Software Modules

96

Software Modules

- Modules
 - Lot of useful software packages
 - Different versions
 - Maintained by experts
 - Optimized for the architecture
 - Users cannot install a module
 - Have to request the administrator

How to use Modules?

• Useful commands

Command	Description
module avail	List modules
<pre>module avail <package_name></package_name></pre>	List all installed versions of python
<pre>module load <package_name></package_name></pre>	Load the default python version
<pre>module load <pakage_name 3.11.5=""></pakage_name></pre>	Load a specific version of python
<pre>module unload <package_name></package_name></pre>	Unload python
module list	List currently loaded modules

How to use Modules?

\$module avail

A	jm	ir@ec-nantes.fr@nautilus-devel-001:~		$Q \equiv - \Box \times$
[jmir@ec-nantes.fr@nautilus-devel-001	~]\$ module avail			
	/usr/share/M	odules/modulefiles/applications		
castem/2021 castem/2023 gaussian/g16	-revA01 hyperworks/2022.2 la	mmps/15Jun2023 turbomole/7.41		
	/usr/share	/Modules/modulefiles/libraries		
aocl-blis/4.0	intel/ccl/2021.9.0	intel/dpl/latest	intel/mkl32/2023.1.0	
boost/1.82.0_gnu	intel/ccl/latest	intel/intel_ipp_ia32/2021.8.0	intel/mkl32/latest	
cuda/12.2.0_535.54.03	intel/dnnl-cpu-gomp/2023.1.0		intel/tbb/2021.9.0	
fftw/3.3.10_intel_serial	intel/dnnl-cpu-gomp/latest	intel/intel_ipp_intel64/2021.8.0	intel/tbb/latest	
fftw/3.3.10_intel_serial_sp fftw/intelmpi/3.3.10 intel intelmpi	intel/dnnl-cpu-iomp/2023.1.0	<pre>intel/intel_ipp_intel64/latest intel/intel_ippcp_ia32/2021.7.0</pre>	intel/tbb32/2021.9.0 intel/tbb32/latest	
fftw/omp/3.3.10 intel omp	intel/dnnl-cpu-tbb/2023.1.0	intel/intel ippcp ia32/latest	libtool/2.4.6 gnu	
gmsh/4.11.1 gnu	intel/dnnl-cpu-tbb/latest	intel/intel ippcp intel64/2021.7.0	netcdf/c-4.9.2 gnu	
hdf5/1.14.1-2_gnu	intel/dnnl/2023.1.0	<pre>intel/intel_ippcp_intel64/latest</pre>	netcdf/f-4.6.1_gnu	
hdf5/1.14.1-2_intel	intel/dnnl/latest	intel/mkl/2023.1.0	rdma/46.0_gnu	
hdf5/intelmpi/1.14.1-2_intel_intelmpi	intel/dpl/2022.1.0	intel/mkl/latest	ucx/1.14.1_gnu	
	/usr/share	/Modules/modulefiles/compilers		
amd/4.0.0 intel/compiler-rt/2023.1			/icc/latest	
<pre>cmake/3.26.4 intel/compiler-rt/latest</pre>	intel/compiler/2023.1.0	intel/compiler32/latest intel	/icc32/2023.1.0	
gcc/13.1.0 intel/compiler-rt32/2023	.1.0 intel/compiler/latest	intel/icc/2023.1.0 intel	/icc32/latest	
	/usr/sha	re/Modules/modulefiles/tools		
				intel/oclfpga/latest
intel/advisor/2023.1.0 intel/dal/2023		/2021.9.0 intel/init opencl/2023.1.		intel/vtune/2023.1.0
intel/advisor/latest intel/dal/late	st intel/dev-utilities	/latest intel/init_opencl/latest	intel/itac/latest	intel/vtune/latest
intel/clck/2021.7.3 intel/debugger	/2023.1.0 intel/dpct/2023.1.0	intel/inspector/2023.1.0	intel/oclfpga/2023.1.0	
	/usr/share	Modules/modulefiles/parallel		
[jmir@ec-nantes.fr@nautilus-devel-001				
<pre>guix/latest intel/clck/lat intel/advisor/2023.1.0 intel/dal/2023 intel/advisor/latest intel/dal/late intel/clck/2021.7.3 intel/debugger intel/mpi/2021.9.0 intel/mpi/latest</pre>	est intel/debugger/late 1.0 intel/dev-utilities st intel/dev-utilities /2023.1.0 intel/dpct/2023.1.0 	st intel/dpct/latest /2021.9.0 intel/init_opencl/2023.1. /latest intel/init_opencl/latest intel/inspector/2023.1.0 :/Modules/modulefiles/parallel	<pre>intel/inspector/latest 0 intel/itac/2021.9.0 intel/itac/latest intel/oclfpga/2023.1.0</pre>	intel/vtune/2023.1.0

Guix Package Manager



What is Guix?



- Package building system/Package manager
- Works on GNU/Linux
- Allows each user to manage his/her own packages
 - without root privilege
 - without interfering with other users
- Easy creation of isolated environments with designated packages
 - useful for per-project dependency management

Guix

Guix Package Manager

• Useful commands

Command	Description
<pre>guix search <package_name></package_name></pre>	Look for a package to install
<pre>guix install <package_name></package_name></pre>	To install a package
<pre>guix remove <package_name></package_name></pre>	To remove a package
guix package -l	List of installed packages

How to use Guix?

\$guix package -1

	jmir@ec-nantes.fr@nautilus-devel-001:~	Q		
[jmir@ec-nantes Generation 1 graphviz	.fr@nautilus-devel-001 ~]\$ guix package -l août 01 2023 15:53:10 7.0.1 out /gnu/store/8ljq5ipy0gs6w69rjigz11vf01zqzaxh-graphviz-7.0.1			
Generation 2 + python	sept. 07 2023 16:33:51 3.10.7 out /gnu/store/3hnmbi6yyn06w4xz7wpsw5nzb12l6xjv-python-3.10.7			
Generation 3 + conda	sept. 20 2023 09:35:38 22.9.0 out /gnu/store/gxrlqm3ggnz3jwz79kwl1125i3lhicb9-conda-22.9.0			
Generation 4 + python-numpy	<pre>sept. 20 2023 09:37:35 1.23.2 out /gnu/store/kz02cd8dcgmryb2fk3ylniky2z333yi2-python-numpy-1.23.2</pre>			
Generation 5	sept. 20 2023 10:10:55			
G eneration 6 + python-panda	sept. 20.2023 11:52:44 s 1.4.4 out /gnu/store/pg68s6204m0sf7g085qa937wwc6nf65m-python-pandas-1.4.4			
Generation 7 + python-pytor	<pre>sept. 20 2023 12:58:54 ch 1.13.1 out /gnu/store/icwxw62i5xpfdczv4sih0f58qvw9ah89-python-pytorch-1.13.1</pre>			
Generation 8 + python-numba	<pre>sept. 20 2023 15:25:47 0.56.4 out /gnu/store/llns1jkzdwsdvpclgkg37kqr7qp0vg4i-python-numba-0.56.4</pre>			
Generation 9 + python-torch	sept. 20 2023 16:20:15 vision 0.15.2 out /gnu/store/gjmf484aq6kw6gfd02474nl1fwi2wvix-python-torchvision-0.15.2			
Generation 10 + python-pytor	sept. 20 2023 16:32:05 ch-lightning 2.0.2 out /gnu/store/v2hvz552j2ywrhx6vs8cjyh51ldhx2hd-python-pytorch-lightning-2.0.2			
Generation 11 + conda - conda	<pre>sept. 22 2023 09:48:01 (current) 22.9.0 out /gnu/store/vf3j4n995jk9zh8yzbvm0mmwajdq71fx-conda-22.9.0 22.9.0 out /gnu/store/gxr1qm3ggnz3jwz79kw11125i3lhicb9-conda-22.9.0</pre>			
[jmir@ec-nantes	.fr@nautilus-devel-001 ~]\$ 🗌			

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