Getting Started With GLiCID: Beginner Session

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January 18, 2024

Outline: Whole Session

- Introduction to High Performance Computing (HPC)
- Introducing NAUTILUS
- Working With A Supercomputer
- SSH Connections and Access to GLiCID
- SLURM Workload Manager
- Modules/Software Stack
- Guix Package Manager
- Data Management on GLiCID
- Anaconda Distribution/Micromamba
- Apptainer Containers
- Hands-on Everything

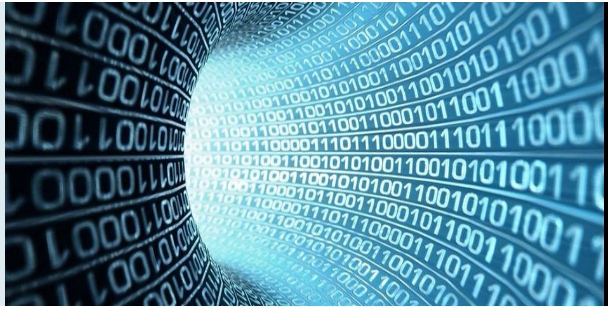
Outline: Beginner Session

- Introduction to High Performance Computing (HPC)
  - What’s 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
  - Batch Scripting
- Modules
- Guix Package Manager
- Data Management

What’s HPC?

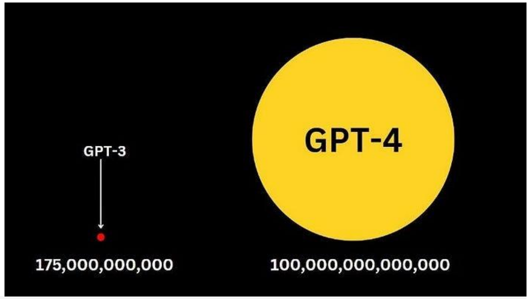
Data, Data, Everywhere

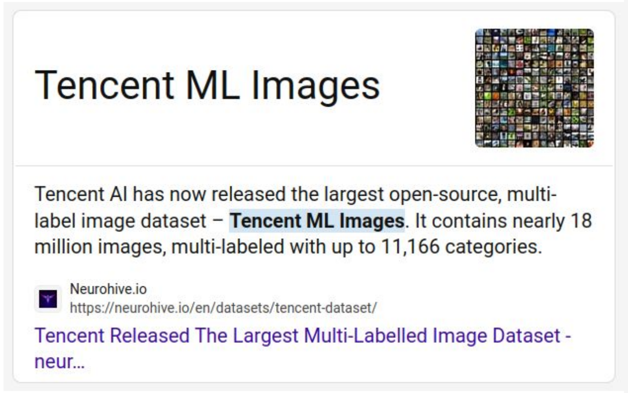
- Key Statistics 2023
  - **3.5 quintillion bytes of data is created every single day** (Source: Earthweb)
  - 333.2 billion emails are sent per day
  - 100 billion messages are sent through WhatsApp in a day
  - 5 billion Snapchat videos and photos are shared per day
  - 456,000 tweets are made on Twitter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



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

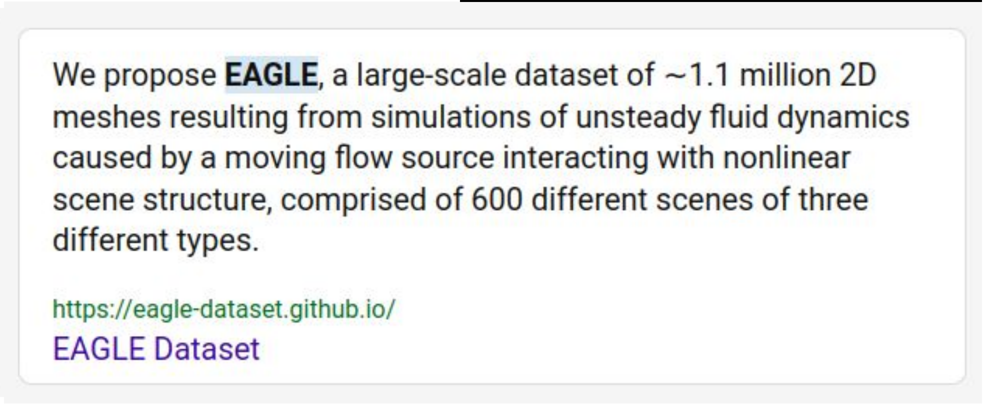
Data, Data, Everywhere



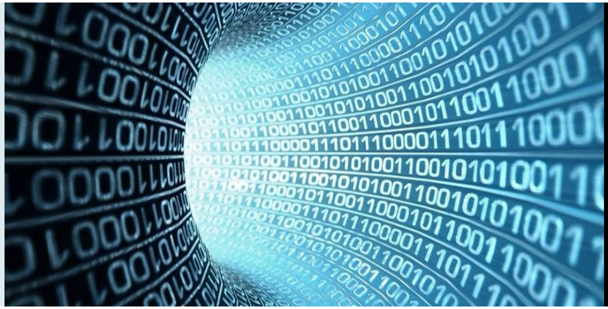

Tencent ML Images

Tencent AI has now released the largest open-source, multi-label image dataset – **Tencent ML Images**. It contains nearly 18 million images, multi-labeled with up to 11,166 categories.

Neurohive.io
https://neurohive.io/en/datasets/tencent-dataset/
Tencent Released The Largest Multi-Labelled Image Dataset - neur...


We propose **EAGLE**, a large-scale dataset of ~1.1 million 2D meshes resulting from simulations of unsteady fluid dynamics caused by a moving flow source interacting with nonlinear scene structure, comprised of 600 different scenes of three different types.

https://eagle-dataset.github.io/
EAGLE Dataset



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

What to do with this data?

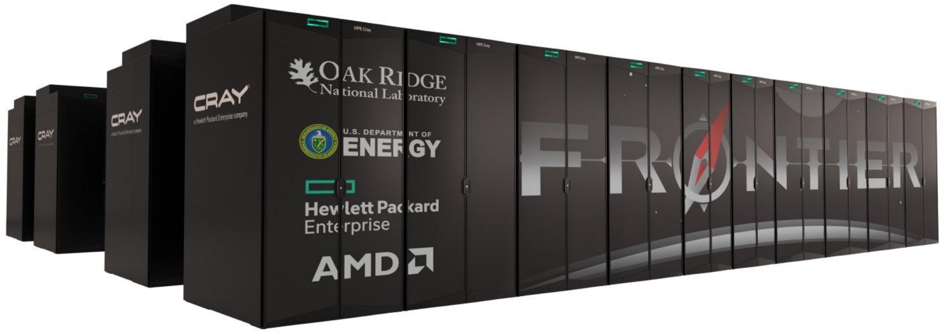
- It is through data that
  - groundbreaking scientific discoveries are made,
  - game-changing innovations are fueled, and
  - quality of life is improved for billions of people around the globe.
- But we need huge computing power/resources to analyze this humongous data
- **HPC** gives us the power to deal with this data

What is High Performance Computing (HPC)?

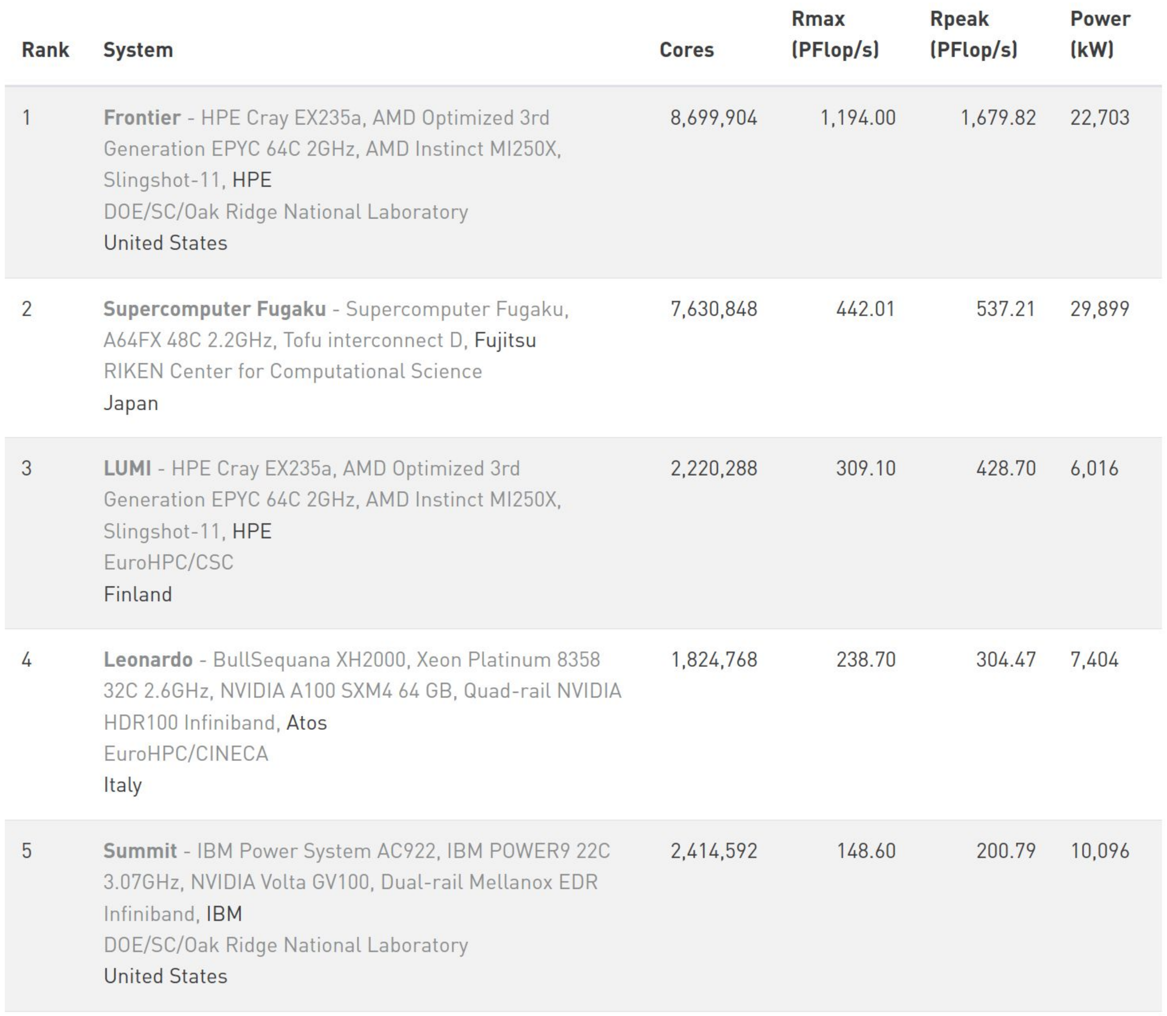
- HPC is the ability to process data and perform complex calculations at high speeds
- Laptop/desktop (3 GHz processor) can perform around 3 billion calculations/sec
- HPC solutions can perform quadrillions of calculations/sec (million times faster)
- **HPC** is the foundation for scientific, industrial, and societal advancements

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


CRAY
OAK RIDGE National Laboratory
U.S. DEPARTMENT OF ENERGY
Hewlett Packard Enterprise
AMD
FRONTIER

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/

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

HPC: Use 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: Use 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…

Introducing Nautilus

Name: Why Nautilus?

- **Nautilus** is the fictional submarine belonging to Captain Nemo featured in Jules Verne's novels Twenty Thousand Leagues Under the Seas (1870) and The Mysterious Island (1874).
- Verne took the name "Nautilus" from one of the earliest successful submarines, built in 1800 by Robert Fulton, who also invented the first commercially successful steamboat.

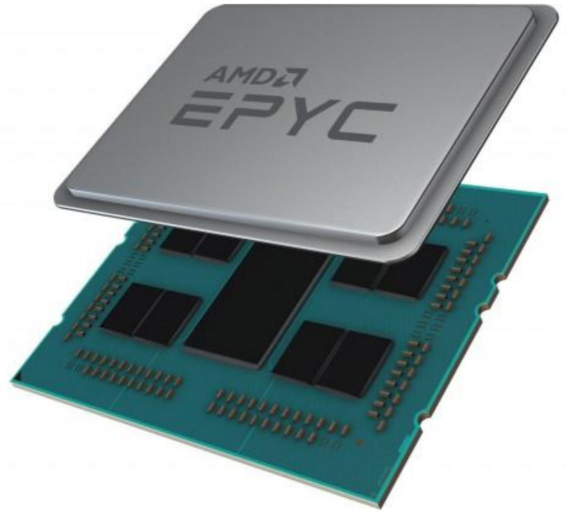
Source: Wikipedia

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

NANTES

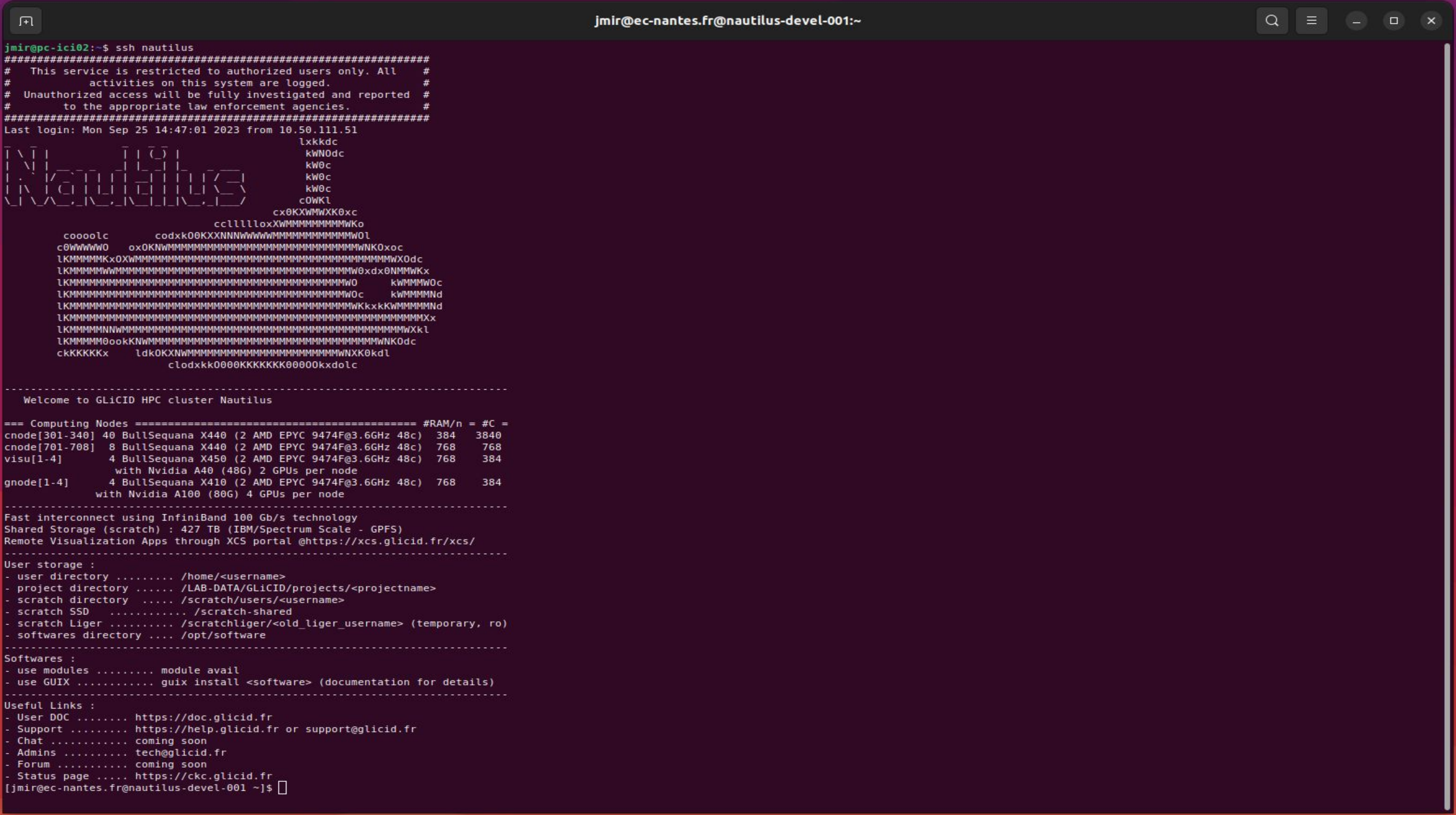
- Bull Sequana X440 X 30 Compute Nodes (+2)
    - Intel Sapphire Rapids (48 cores, 2.1 GHz) X 2
    - 256GB DDR (+2*2TB DDR) + 960GB SSD
- Bull Sequana X450 Display Nodes X 2
    - Intel Sapphire Rapids (48 cores, 2.1 GHz) X 2
    - 512 GB DDR + 960 GB SSD
    - Nvidia A40 GPU 48GB x 2
- DLC Cooling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

Working With A Supercomputer

Working With A Supercomputer

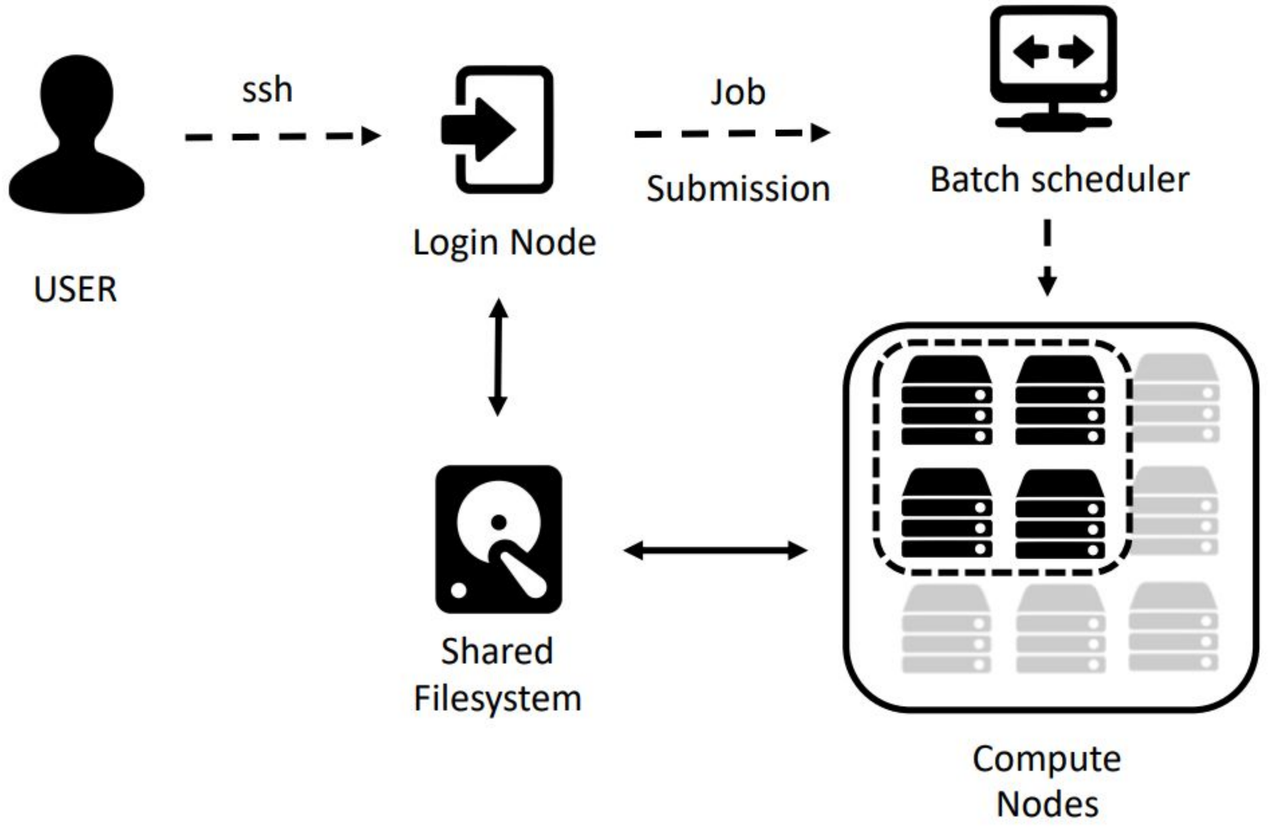
Is NOT like this…

Working With A Supercomputer



```
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
| \ | |                | | (_) |                  kWNOdc
|  \| | __ _ _   _ _| |_ _| |_   _ ___            kW0c
| . ` |/ _` | | | | __| | | | | / __|             kW0c
| |\  | (_| | |_| | |_| | | |_| \__ \             kW0c
\_| \_/\__,_|\__,_|\__|_|_|\__,_|___/            cOWKl
                                         cx0KXWMWXK0xc
                                cclllllloxXWMMMMMMMMWKo
         coooolc       codxkO0KXXNNNWWWWWMMMMMMMMMMMMWOl
        c0WWWWWO   oxOKNWMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWNKOxoc
        lKMMMMMKxOXWMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWXOdc
        lKMMMMMWMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMW0xdx0NMMWKx
        lKMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWO     kWMMMWOc
        lKMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWOc    kWMMMMNd
        lKMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWKkxkKWMMMMMNd
        lKMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMXx
        lKMMMMMNNWMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWXkl
        lKMMMMM0ookKNWMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWNKOdc
        ckKKKKKx    ldkOKXNWMMMMMMMMMMMMMMMMMMMMMMMWNXK0kdl
                         clodxkkO000KKKKKK0000Okxdolc

-----------------------------------------------------------------------------
   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 BullSequana X450 (2 AMD EPYC 9474F@3.6GHz 48c)  768    384
                 with Nvidia A40 (48G) 2 GPUs per node
gnode[1-4]      4 BullSequana 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
- 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
[jmir@ec-nantes.fr@nautilus-devel-001 ~]$ 
```

Working With A Supercomputer



Working With A Supercomputer

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

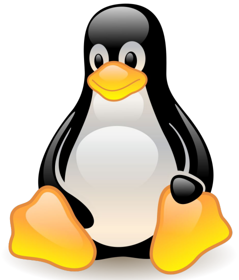
Getting Started with GLiCID

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

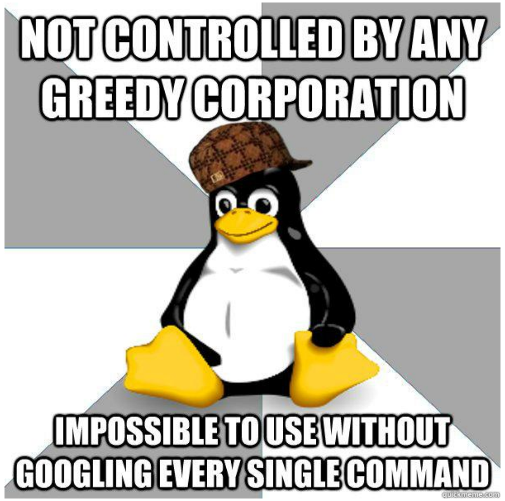
IBM Mainframe, Late 1960's/Early 1970's

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 Top 500 supercomputers use Linux

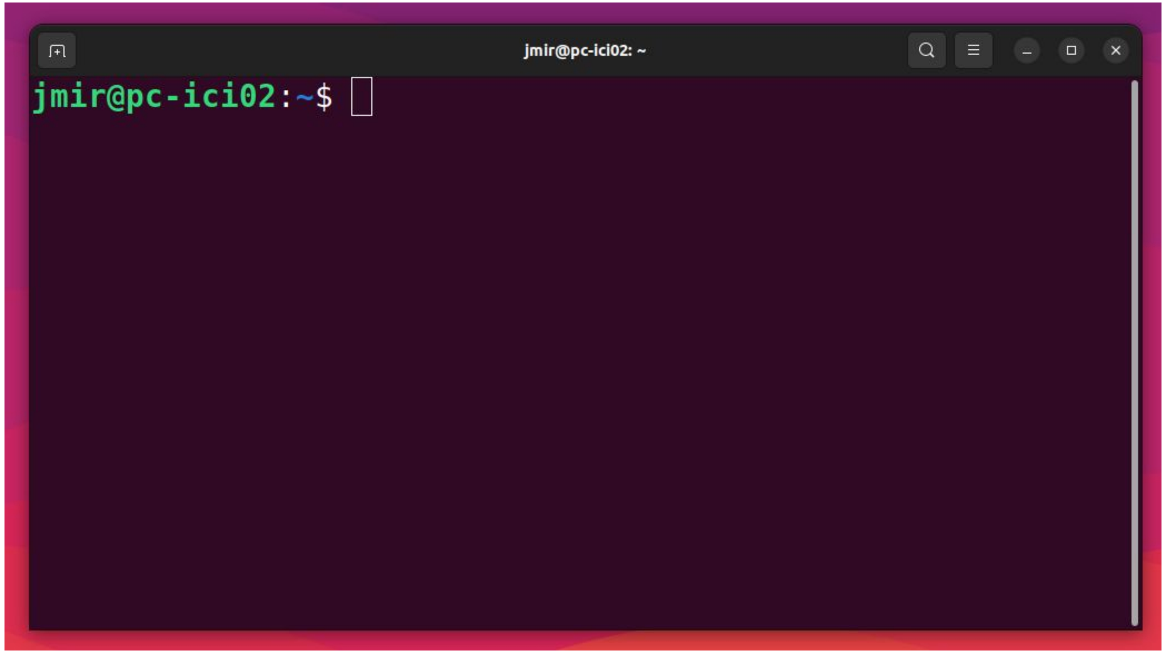
What’s A Command Line?

- 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


NOT CONTROLLED BY ANY GREEDY CORPORATION
IMPOSSIBLE TO USE WITHOUT GOOGLING EVERY SINGLE COMMAND
quickmeme.com

Basic Linux Commands

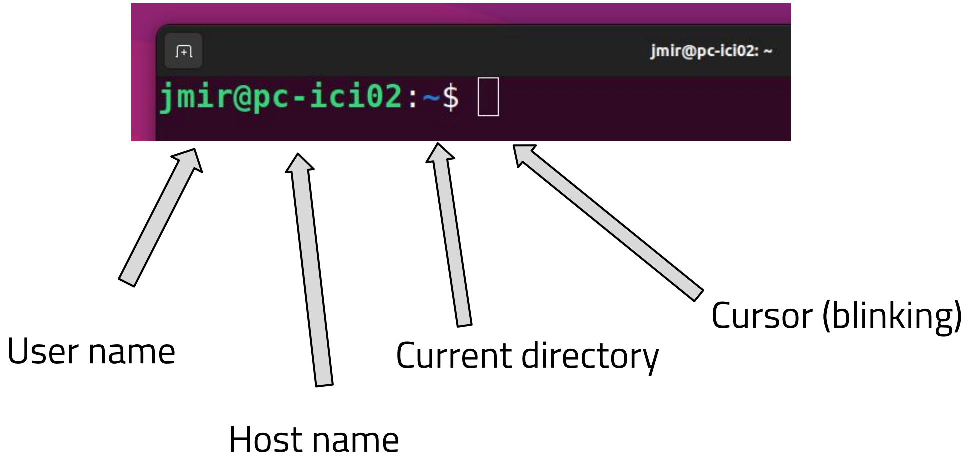
- Launch the Terminal



```
jmir@pc-ici02:~$ 
```

Basic Linux Commands

- Structure of a linux commands

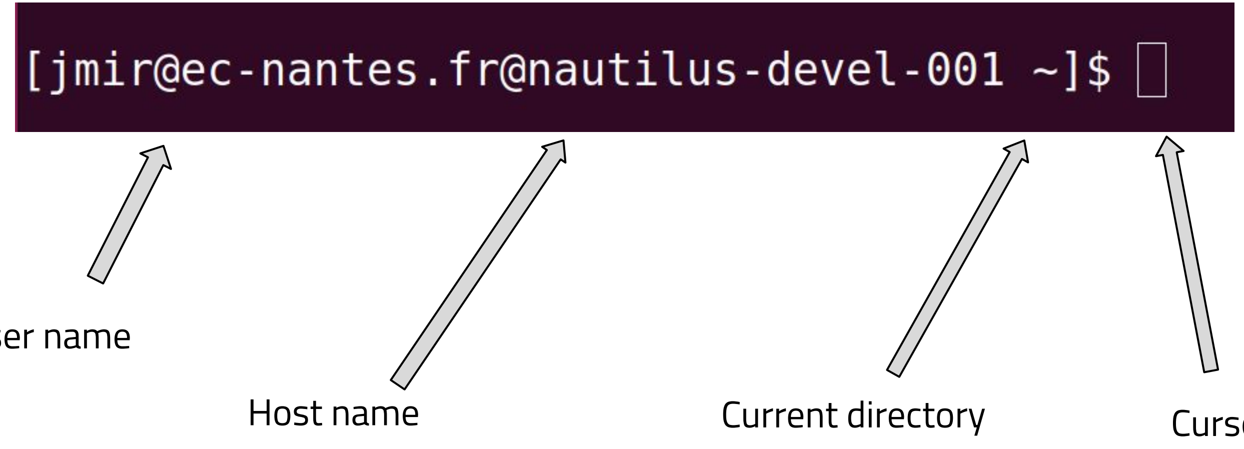


```
jmir@pc-ici02: ~
jmir@pc-ici02:~$ 
```

- The system is ready to accept commands

Basic Linux Commands

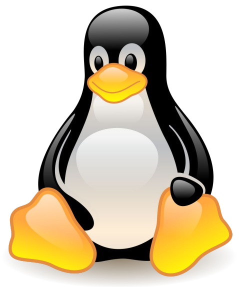
- Structure of a linux commands (in Nautilus)



```
[jmir@ec-nantes.fr@nautilus-devel-001 ~]$ 
```

- The system is ready to accept commands

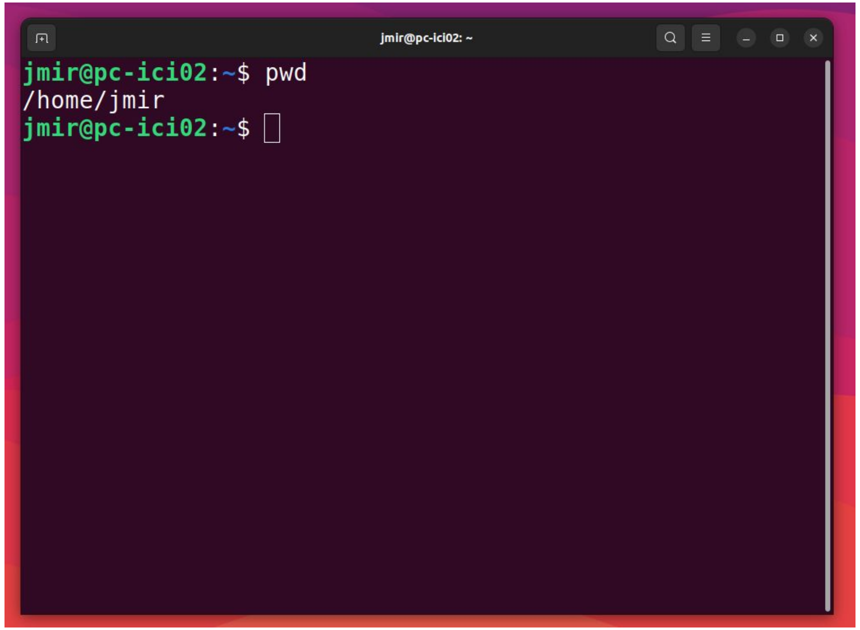
Basic Linux Commands



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	`mv`	Move or rename files and directories
Copy	`cp`	Copy files or directories from source to destination
Remove	`rm`	Remove files
Text editor	`vim`	Vim is a highly configurable text editor

Basic Linux Commands

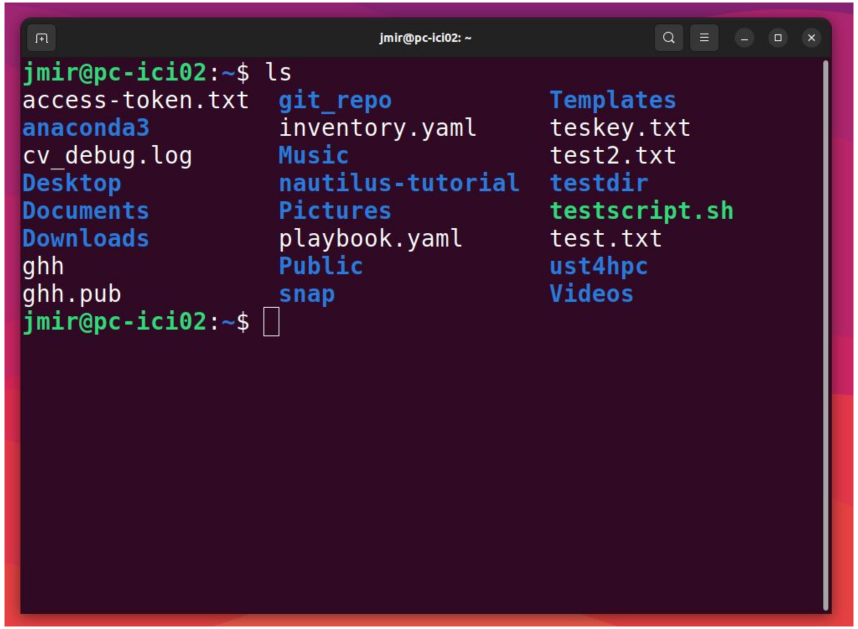
Command	Syntax	Description
Print Working Directory	pwd	Print present working directory



```
jmir@pc-ici02:~$ pwd
/home/jmir
jmir@pc-ici02:~$ 
```

Basic Linux Commands

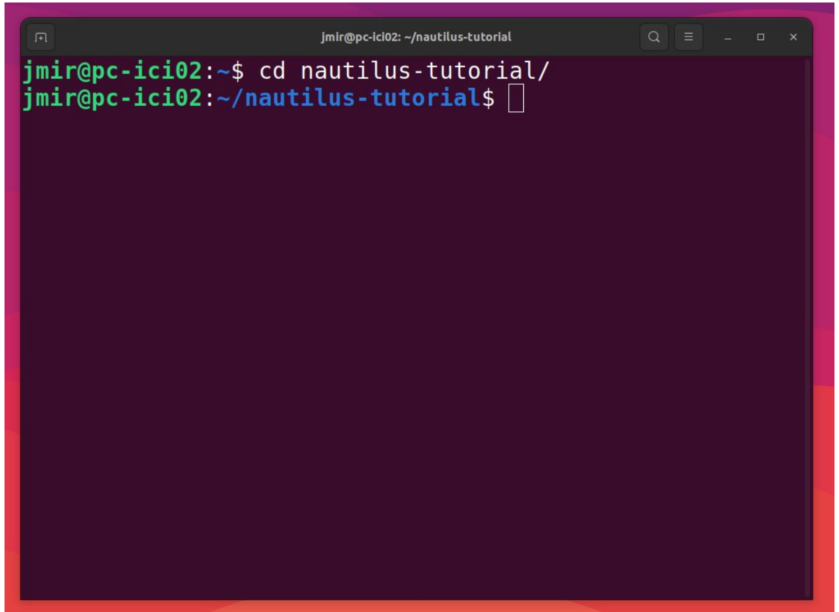
Command	Syntax	Description
List	`ls`	List files and directories at path



```
jmir@pc-ici02:~$ ls
access-token.txt  git_repo            Templates
anaconda3         inventory.yaml      teskey.txt
cv_debug.log      Music               test2.txt
Desktop           nautilus-tutorial   testdir
Documents         Pictures            testscript.sh
Downloads         playbook.yaml       test.txt
ghh               Public              ust4hpc
ghh.pub           snap                Videos
jmir@pc-ici02:~$ 
```

Basic Linux Commands

Command	Syntax	Description
Change directory	cd	Change current directory

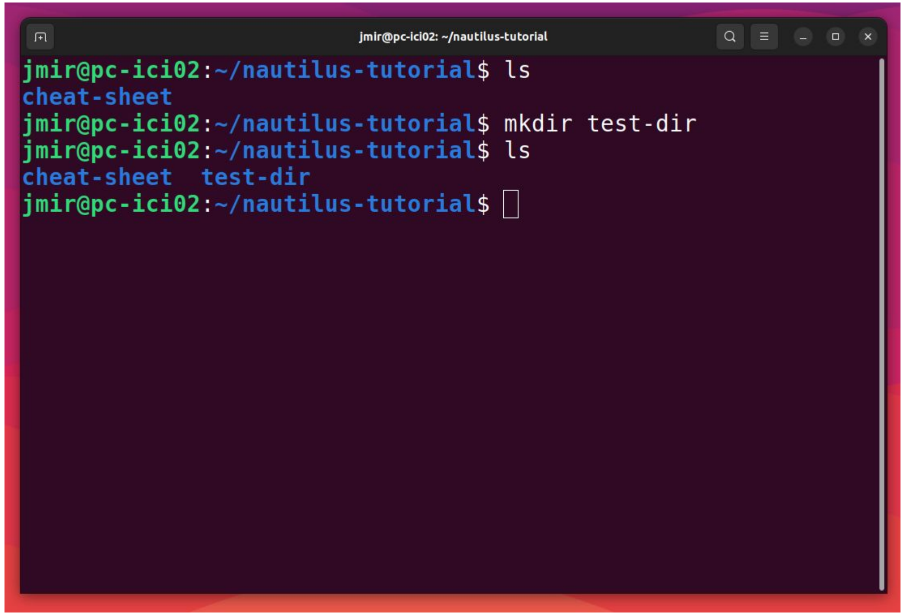


jmir@pc-ici02: ~/nautilus-tutorial

```
jmir@pc-ici02:~$ cd nautilus-tutorial/
jmir@pc-ici02:~/nautilus-tutorial$ 
```

Basic Linux Commands

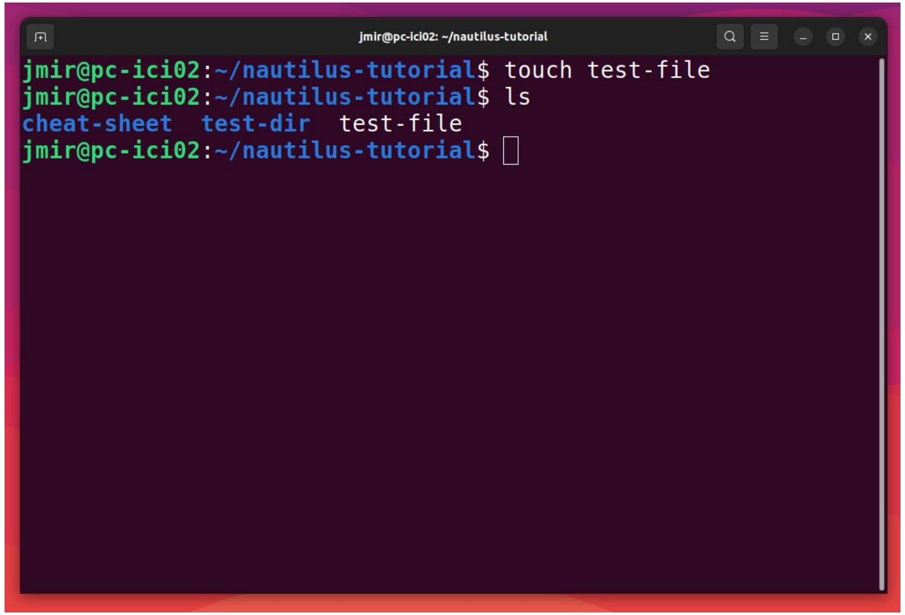
Command	Syntax	Description
Make directory	`mkdir`	Create new directory



```
jmir@pc-ici02:~/nautilus-tutorial$ ls
cheat-sheet
jmir@pc-ici02:~/nautilus-tutorial$ mkdir test-dir
jmir@pc-ici02:~/nautilus-tutorial$ ls
cheat-sheet  test-dir
jmir@pc-ici02:~/nautilus-tutorial$ 
```

Basic Linux Commands

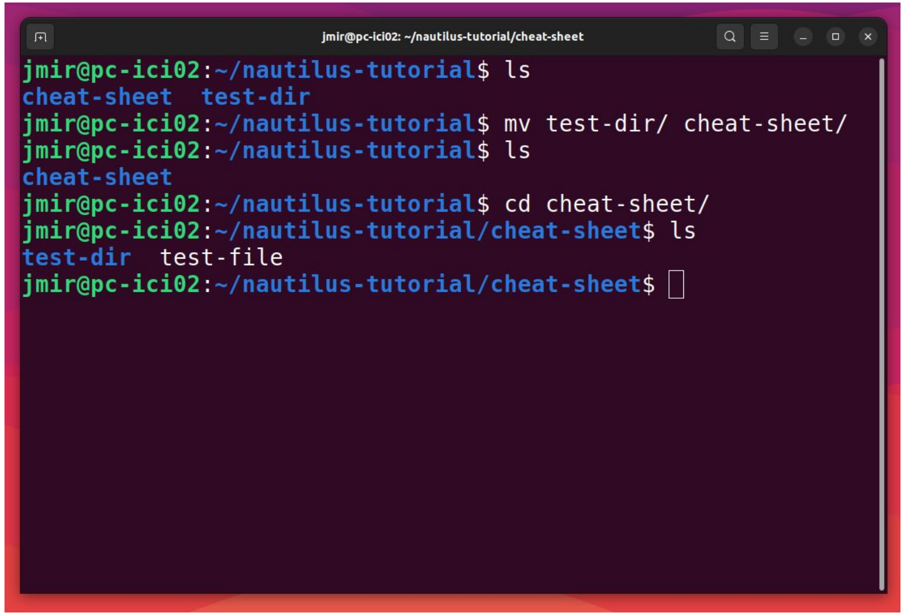
Command	Syntax	Description
Create empty file	`touch`	Create new file or update timestamp



```
jmir@pc-ici02:~/nautilus-tutorial$ touch test-file
jmir@pc-ici02:~/nautilus-tutorial$ ls
cheat-sheet  test-dir  test-file
jmir@pc-ici02:~/nautilus-tutorial$ 
```

Basic Linux Commands

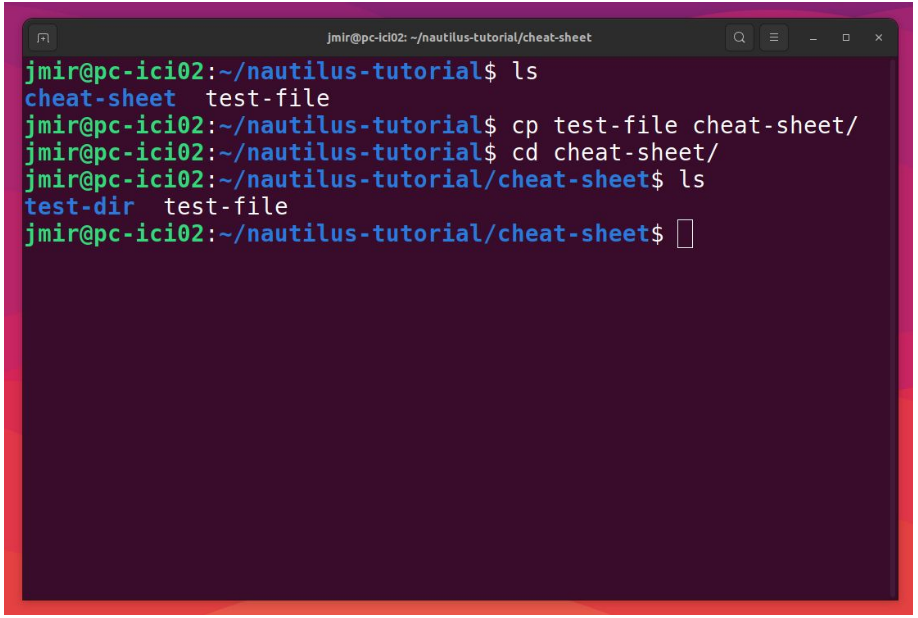
Command	Syntax	Description
Move	`mv`	Move or rename files and directories



```
jmir@pc-ici02:~/nautilus-tutorial$ ls
cheat-sheet  test-dir
jmir@pc-ici02:~/nautilus-tutorial$ mv test-dir/ cheat-sheet/
jmir@pc-ici02:~/nautilus-tutorial$ ls
cheat-sheet
jmir@pc-ici02:~/nautilus-tutorial$ cd cheat-sheet/
jmir@pc-ici02:~/nautilus-tutorial/cheat-sheet$ ls
test-dir  test-file
jmir@pc-ici02:~/nautilus-tutorial/cheat-sheet$ 
```

Basic Linux Commands

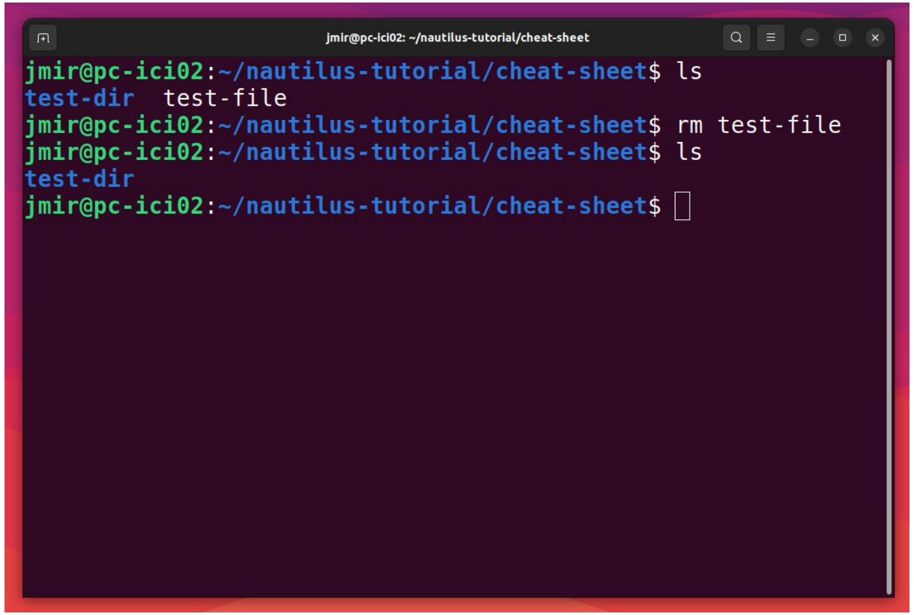
Command	Syntax	Description
copy	cp	Copy files or directories from source to destination



```
jmir@pc-ici02:~/nautilus-tutorial$ ls
cheat-sheet  test-file
jmir@pc-ici02:~/nautilus-tutorial$ cp test-file cheat-sheet/
jmir@pc-ici02:~/nautilus-tutorial$ cd cheat-sheet/
jmir@pc-ici02:~/nautilus-tutorial/cheat-sheet$ ls
test-dir  test-file
jmir@pc-ici02:~/nautilus-tutorial/cheat-sheet$ 
```

Basic Linux Commands

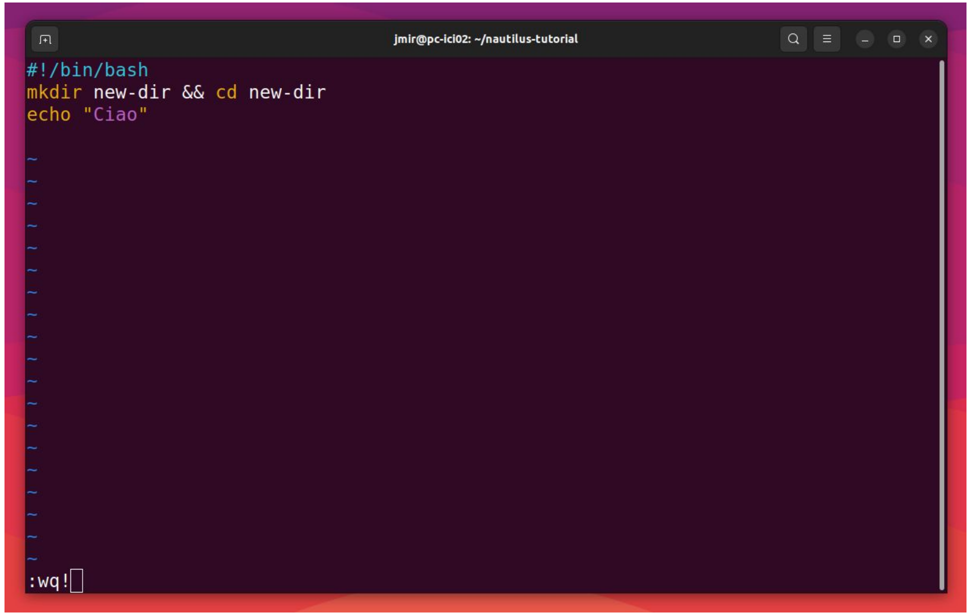
Command	Syntax	Description
Remove	rm	Remove files



```
jmir@pc-ici02:~/nautilus-tutorial/cheat-sheet$ ls
test-dir  test-file
jmir@pc-ici02:~/nautilus-tutorial/cheat-sheet$ rm test-file
jmir@pc-ici02:~/nautilus-tutorial/cheat-sheet$ ls
test-dir
jmir@pc-ici02:~/nautilus-tutorial/cheat-sheet$ 
```

Basic Linux Commands

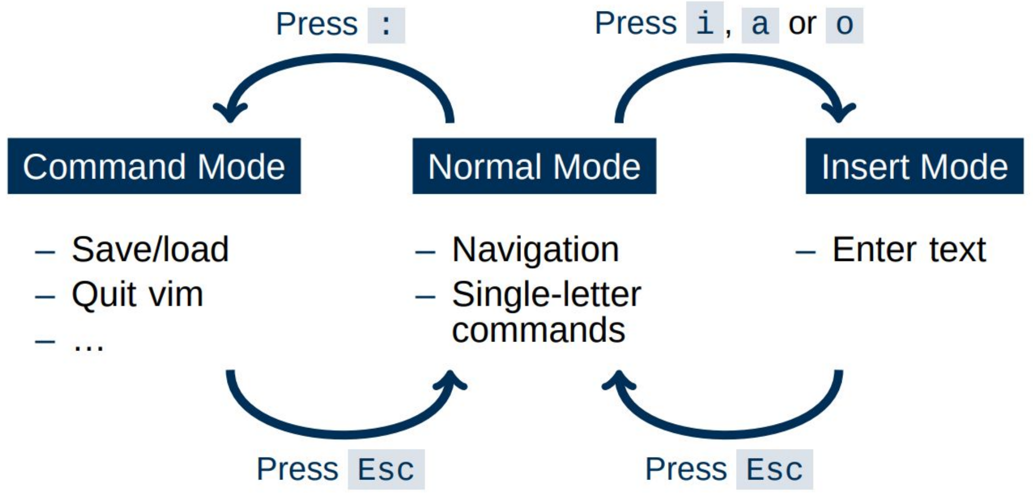
Command	Syntax	Description
Text editor	`vim`	Vim is a highly configurable text editor



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

~
~
~
~
~
~
~
~
~
~
~
~
~
~
~
~
~
~
~
:wq!
```

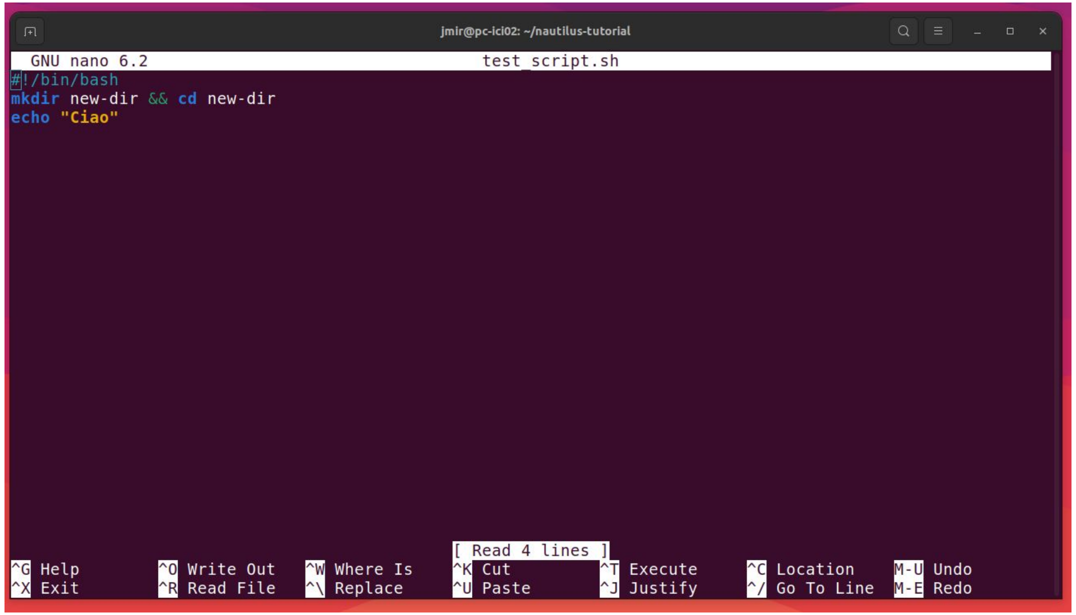
Basic Linux Commands

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



Basic Linux Commands

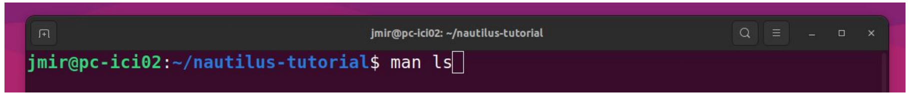
Command	Syntax	Description
Text editor	nano	Comparatively easier (Ctrl+Option)



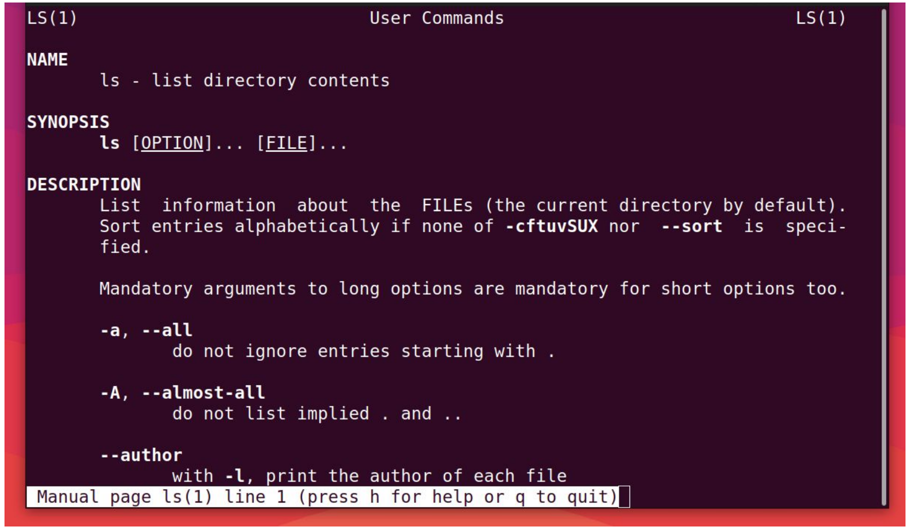
```
  GNU nano 6.2                                 test_script.sh
#!/bin/bash
mkdir new-dir && cd new-dir
echo "Ciao"

                                        [ Read 4 lines ]
^G Help        ^O Write Out   ^W Where Is    ^K Cut         ^T Execute     ^C Location    M-U Undo
^X Exit        ^R Read File   ^\ Replace     ^U Paste       ^J Justify     ^/ Go To Line  M-E Redo
```

Basic Linux Commands

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



```
jmir@pc-ici02:~/nautilus-tutorial$ man ls
```

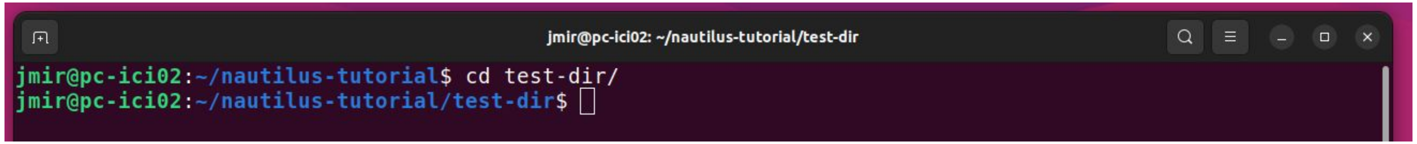


```
LS(1)                            User Commands                           LS(1)

NAME
       ls - list directory contents

SYNOPSIS
       ls [OPTION]... [FILE]...

DESCRIPTION
       List  information  about  the  FILEs (the current directory by default).
       Sort entries alphabetically if none of -cftuvSUX nor  --sort  is  speci‐
       fied.

       Mandatory arguments to long options are mandatory for short options too.

       -a, --all
              do not ignore entries starting with .

       -A, --almost-all
              do not list implied . and ..

       --author
              with -l, print the author of each file
 Manual page ls(1) line 1 (press h for help or q to quit)
```

Basic Linux Commands - File Management

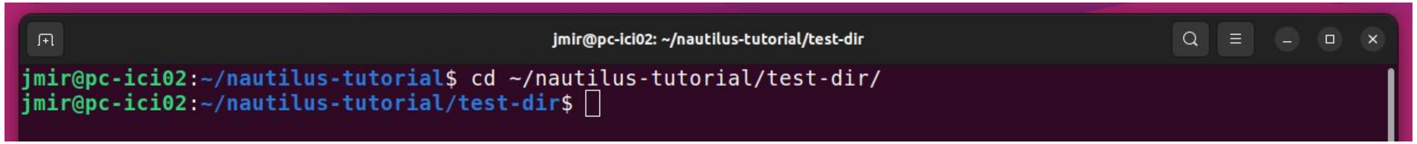
Path to folders and files

- Relative Path



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

- Absolute path

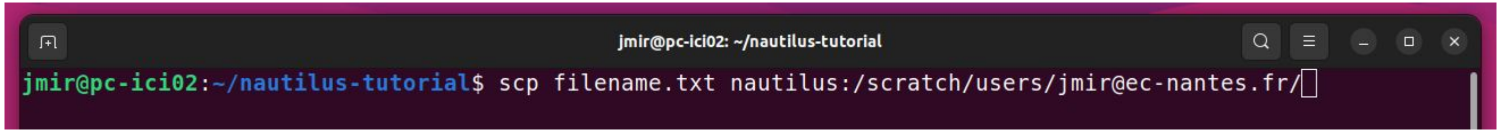


```
jmir@pc-ici02:~/nautilus-tutorial$ cd ~/nautilus-tutorial/test-dir/
jmir@pc-ici02:~/nautilus-tutorial/test-dir$ 
```

Basic Linux Commands - File Management

- Local to Remote

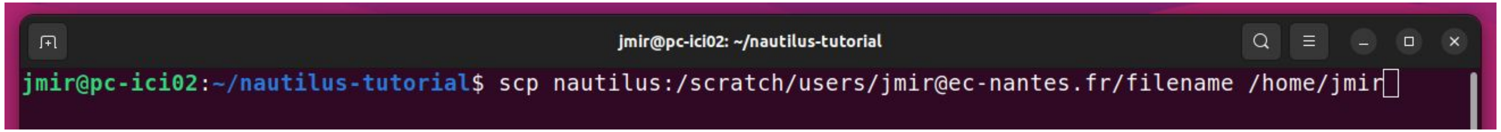
```
scp <file_name> nautilus:/scratch/users/<username>
```



```
jmir@pc-ici02:~/nautilus-tutorial$ scp filename.txt nautilus:/scratch/users/jmir@ec-nantes.fr/
```

- Remote to Local

```
scp nautilus:/scratch/users/<username>/<file_name> /<local_path>
```



```
jmir@pc-ici02:~/nautilus-tutorial$ scp nautilus:/scratch/users/jmir@ec-nantes.fr/filename /home/jmir
```

Not recommended: `scp <file_name> nautilus:/home/<username>`

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/users/username
```

- Remote to Local

```
$ scp -r nautilus:/scratch/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

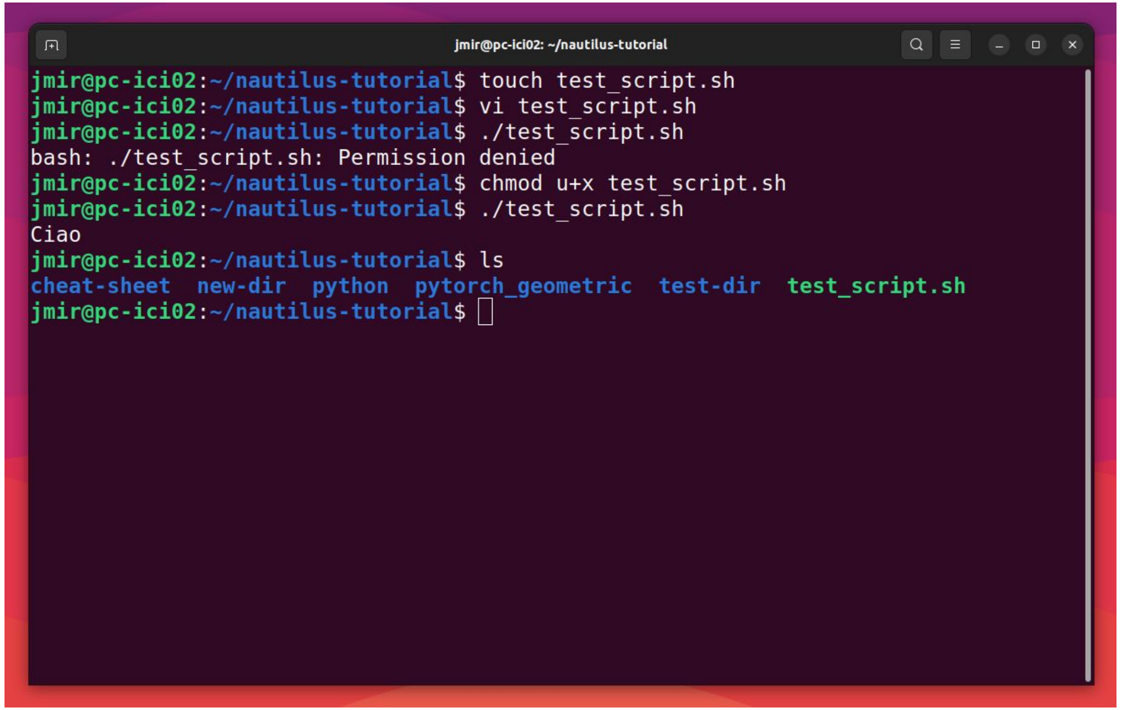
- Simple bash script

```
#!/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>`



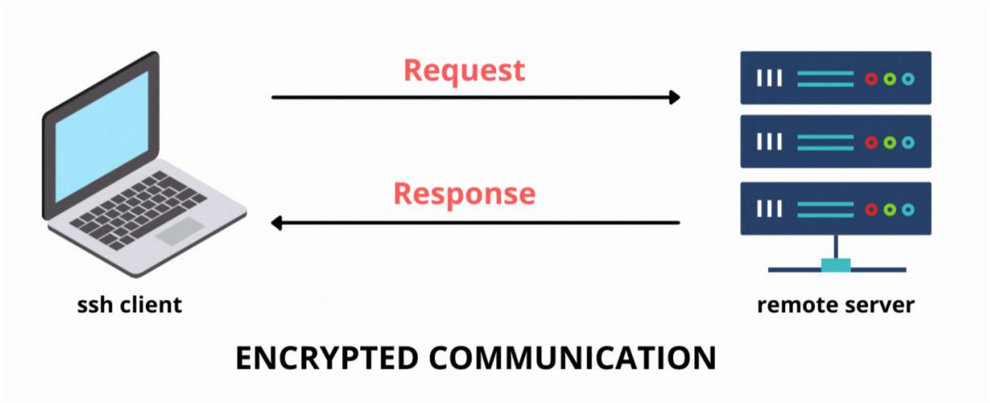
jmir@pc-ici02: ~/nautilus-tutorial

```
jmir@pc-ici02:~/nautilus-tutorial$ touch test_script.sh
jmir@pc-ici02:~/nautilus-tutorial$ vi test_script.sh
jmir@pc-ici02:~/nautilus-tutorial$ ./test_script.sh
bash: ./test_script.sh: Permission denied
jmir@pc-ici02:~/nautilus-tutorial$ chmod u+x test_script.sh
jmir@pc-ici02:~/nautilus-tutorial$ ./test_script.sh
Ciao
jmir@pc-ici02:~/nautilus-tutorial$ ls
cheat-sheet  new-dir  python  pytorch_geometric  test-dir  test_script.sh
jmir@pc-ici02:~/nautilus-tutorial$ 
```

SSH CONNECTIONS

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
  - Key,
  - Configuration,
  - Key/IP address known to the supercomputer

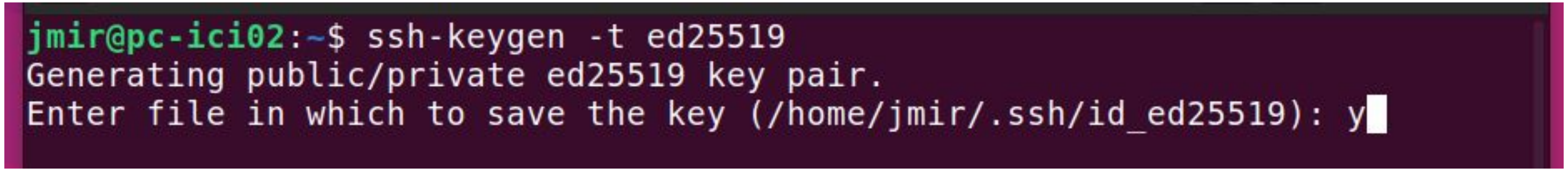


How to access GLiCID cluster?

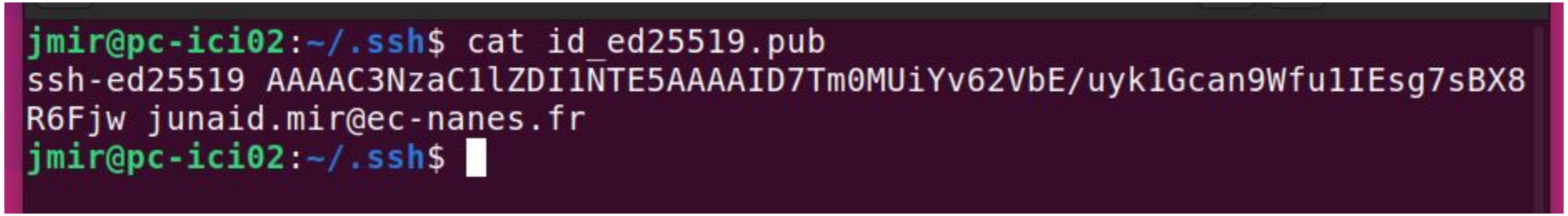
- Create an account on https://clam.glicid.fr
- Account validation by an administrator
- User uploads SSH key to CLAM portal (in profile's SSH Access tab)
- SSH connection configuration on local PC

How to configure SSH connection?

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



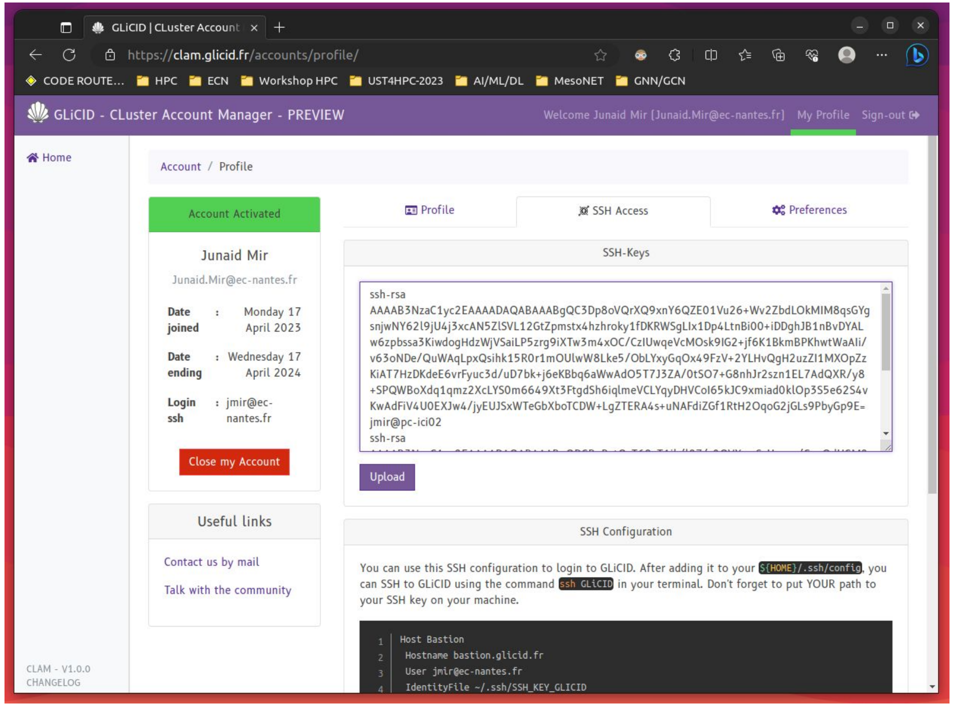
```
jmir@pc-ici02:~$ ssh-keygen -t ed25519
Generating public/private ed25519 key pair.
Enter file in which to save the key (/home/jmir/.ssh/id_ed25519): y
```



```
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



GLiCID | CLuster Account

https://clam.glicid.fr/accounts/profile/

CODE ROUTE... HPC ECN Workshop HPC UST4HPC-2023 AI/ML/DL MesoNET GNN/GCN

GLiCID - CLuster Account Manager - PREVIEW

Welcome Junaid Mir (Junaid.Mir@ec-nantes.fr) My Profile Sign-out

Home

Account / Profile

Account Activated

Junaid Mir

Junaid.Mir@ec-nantes.fr

Date joined	:	Monday 17 April 2023
Date ending	:	Wednesday 17 April 2024
Login ssh	:	jmir@ec-nantes.fr

Close my Account

Useful links

Contact us by mail

Talk with the community

Profile SSH Access Preferences

SSH-Keys

```
ssh-rsa
AAAAB3NzaC1yc2EAAAADAQABAAABgQC3Dp8oVQrXQ9xnY6QZE01Vu26+Wv2ZbdLOkMIM8qsGYg
snjwNY62l9jU4j3xcAN5ZlSVL12GtZpmstx4hzhroky1fDKRWSgLIx1Dp4LtnBi00+iDDghJB1nBvDYAL
w6zpbssa3KiwdogHdzWjVSaiLP5zrg9iXTw3m4xOC/CzIUwqeVcMOsk9IG2+jf6K1BkmBPKhwtWaAIi/
v63oNDe/QuWAqLpxQsihk15R0r1mOUlwW8Lke5/ObLYxyGqOx49FzV+2YLHvQgH2uzZI1MXOpZz
KiAT7HzDKdeE6vrFyuc3d/uD7bk+j6eKBbq6aWwAdO5T7J3ZA/0tSO7+G8nhJr2szn1EL7AdQXR/y8
+SPQWBoXdq1qmz2XcLYS0m6649Xt3FtgdSh6iqlmeVCLYqyDHVCoI65kJC9xmiad0klOp3S5e62S4v
KwAdFiV4U0EXJw4/jyEUJSxWTeGbXboTCDW+LgZTERA4s+uNAFdiZGf1RtH2OqoG2jGLs9PbyGp9E=
jmir@pc-ici02
ssh-rsa
```

Upload

SSH Configuration

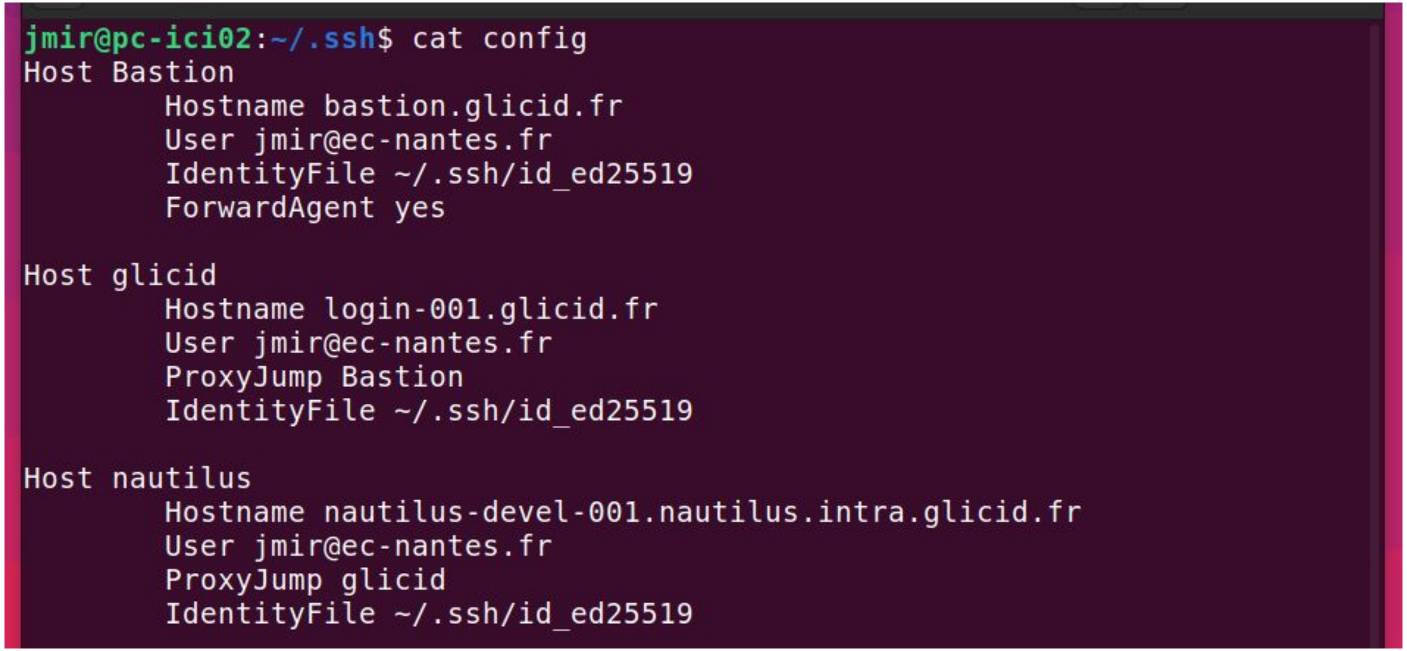
You can use this SSH configuration to login to GLiCID. After adding it to your `${HOME}/.ssh/config`, you can SSH to GLiCID using the command `ssh GLiCID` in your terminal. Don't forget to put YOUR path to your SSH key on your machine.

```
Host Bastion
 Hostname bastion.glicid.fr
 User jmir@ec-nantes.fr
 IdentityFile ~/.ssh/SSH_KEY_GLICID
```

CLAM - V1.0.0
CHANGELOG

How to configure SSH connection?

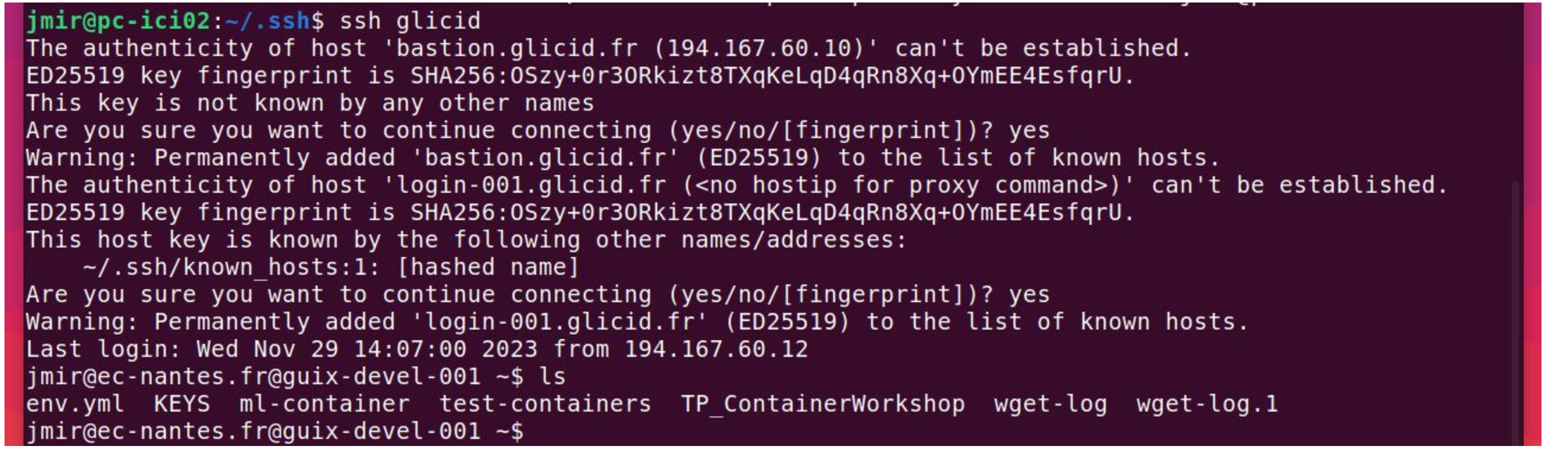
- Copy Contents to the config file and save it
- Replace <my_username> with your username



```
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
```

SSH to GLiCID Cluster

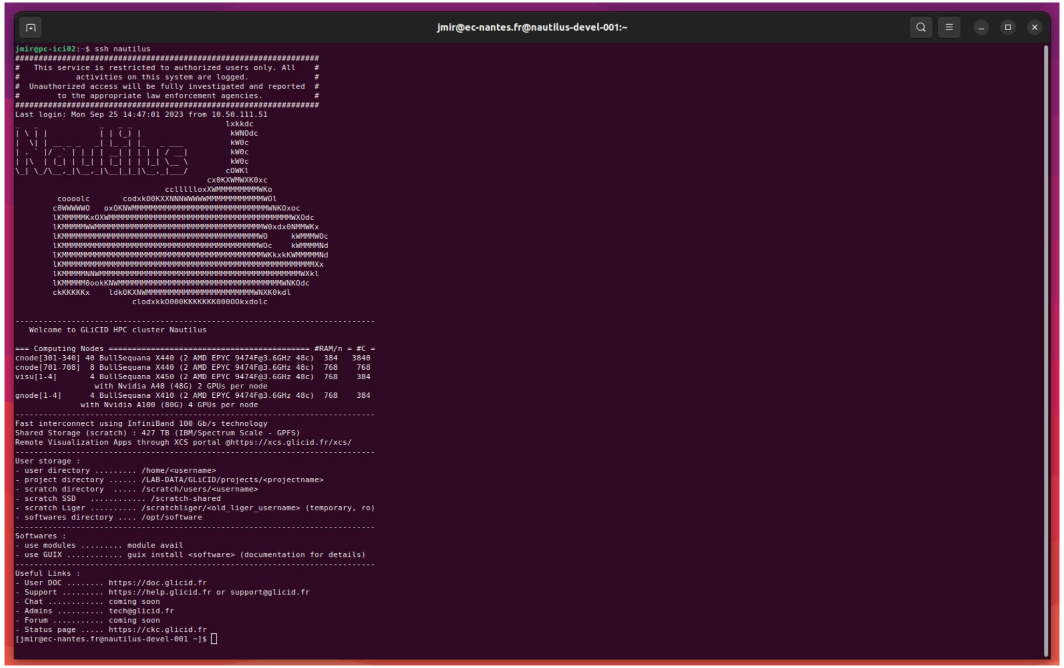
- Login using SSH by typing this command in the terminal
  - ssh glicid and then press <Enter>



```
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:OSzy+0r3ORkizt8TXqKeLqD4qRn8Xq+0YmEE4EsfqrU.
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:OSzy+0r3ORkizt8TXqKeLqD4qRn8Xq+0YmEE4EsfqrU.
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
jmir@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 ~$
```

SSH to GLiCID Cluster

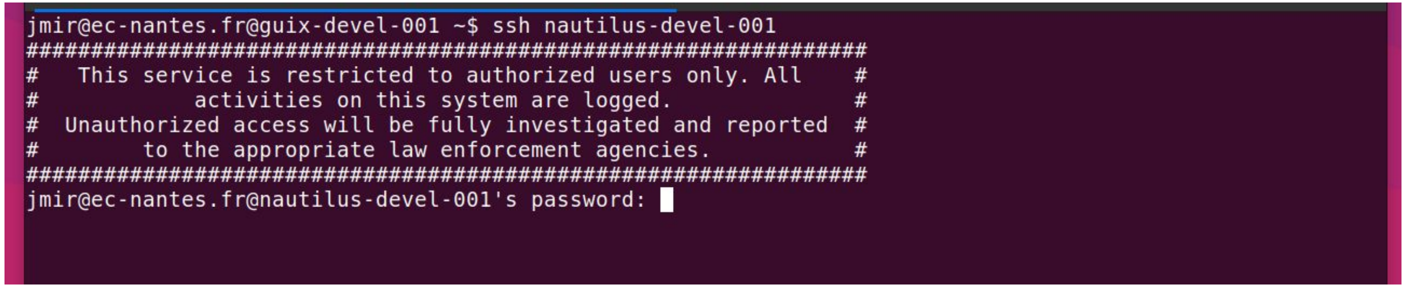
- Login directly to nautilus
  - ssh nautilus and then press <Enter>



```
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
| \ | |           | | (_) |                       kWNOdc
|  \| | __ _ _   _| |_ _| |_   _ ___              kW0c
| . ` |/ _` | | | | __| | | | | / __|             kW0c
| |\  | (_| | |_| | |_| | | |_| \__ \             kW0c
\_| \_/\__,_|\__,_|\__|_|_|\__,_|___/            cOWKl
                                             cx0KXWMWXK0xc
                                    ccllllloxXWMMMMMMMMMWKo
         coooolc       codxkO0KXXNNNWWWWWMMMMMMMMMMMMMWOl
        c0WWWWWO   oxOKNWMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWNKOxoc
        lKMMMMMKxOXWMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWXOdc
        lKMMMMMWWMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMW0xdx0NMMWKx
        lKMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWO     kWMMMWOc
        lKMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWOc    kWMMMMNd
        lKMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWKkxkKWMMMMMNd
        lKMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMXx
        lKMMMMMNNWMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWXkl
        lKMMMMM0ookKNWMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWNKOdc
        ckKKKKKx    ldkOKXNWMMMMMMMMMMMMMMMMMMMMMMMMMWNXK0kdl
                         clodxkkO000KKKKKKK0000Okxdolc

------------------------------------------------------------------------------
   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 BullSequana X450 (2 AMD EPYC 9474F@3.6GHz 48c)  768    384
                 with Nvidia A40 (48G) 2 GPUs per node
gnode[1-4]      4 BullSequana 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
- 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
[jmir@ec-nantes.fr@nautilus-devel-001 ~]$
```

SSH to GLiCID Cluster

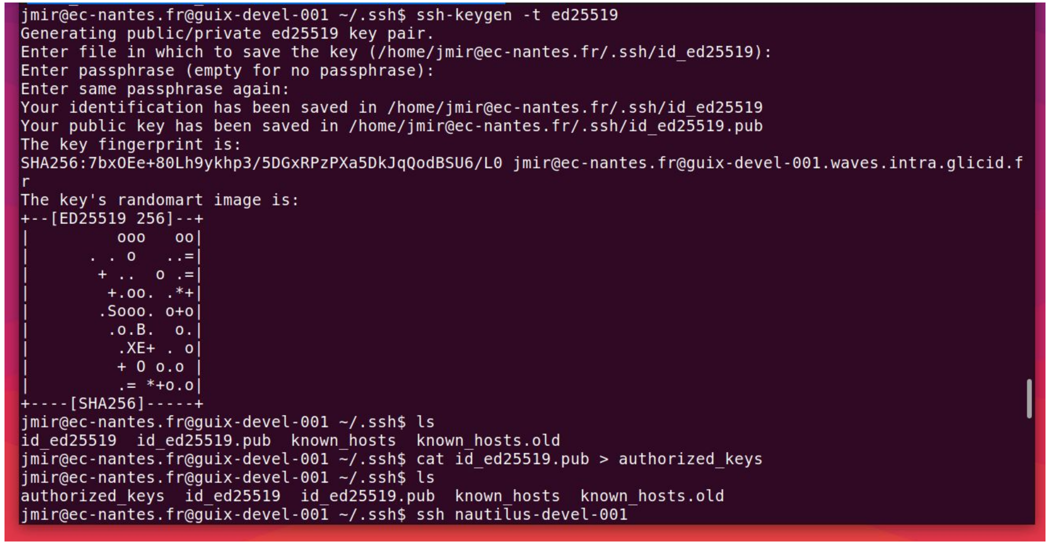
- Switch from glicid to nautilus
  - ssh nautilus-devel-001 and then press <Enter>
  - It will not work but ask for a password



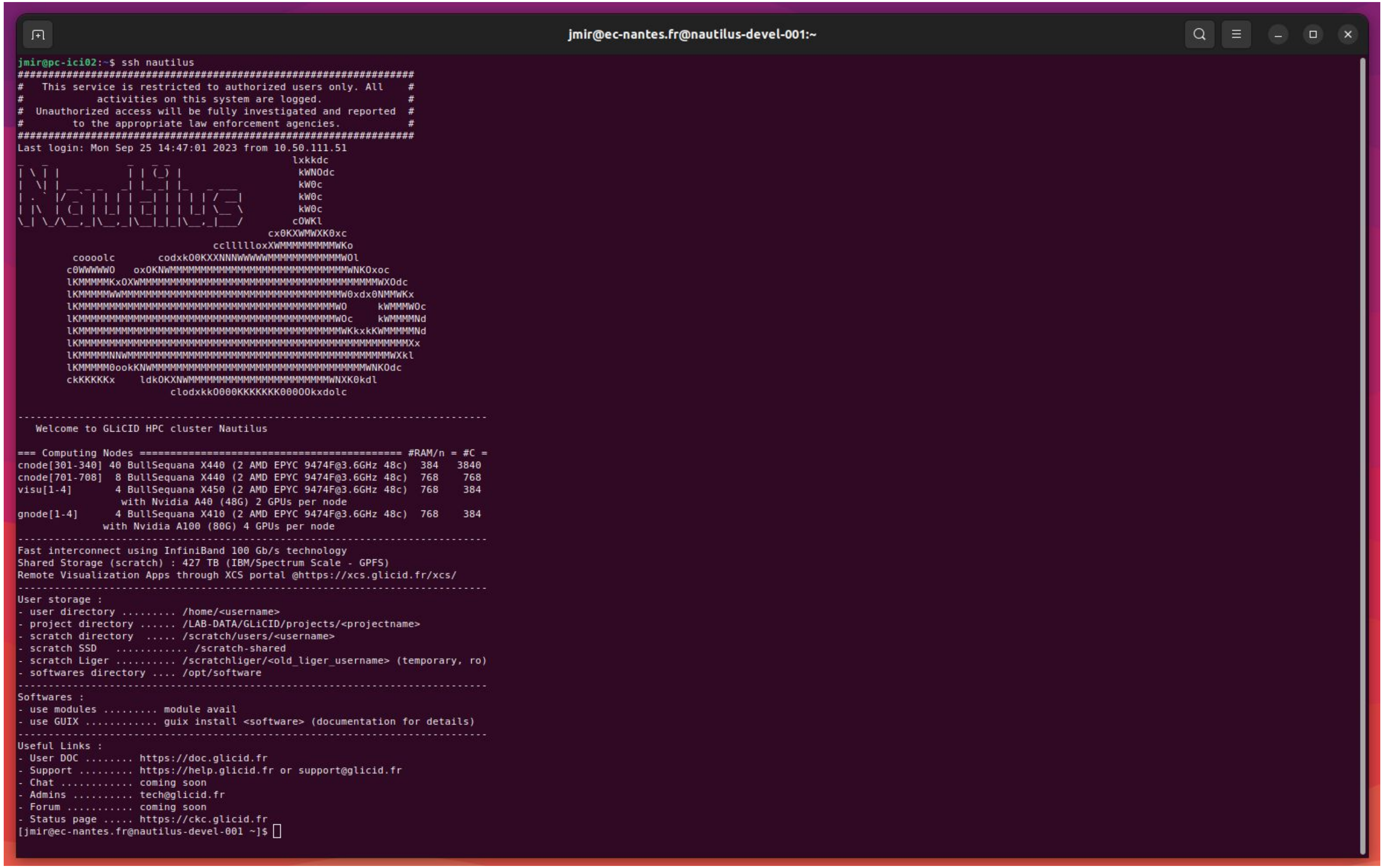
```
jmir@ec-nantes.fr@guix-devel-001 ~$ ssh nautilus-devel-001
#################################################################
#   This service is restricted to authorized users only. All    #
#            activities on this system are logged.              #
#  Unauthorized access will be fully investigated and reported  #
#        to the appropriate law enforcement agencies.           #
#################################################################
jmir@ec-nantes.fr@nautilus-devel-001's password:
```

SSH to GLiCID Cluster

- 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 (which is not a good idea)



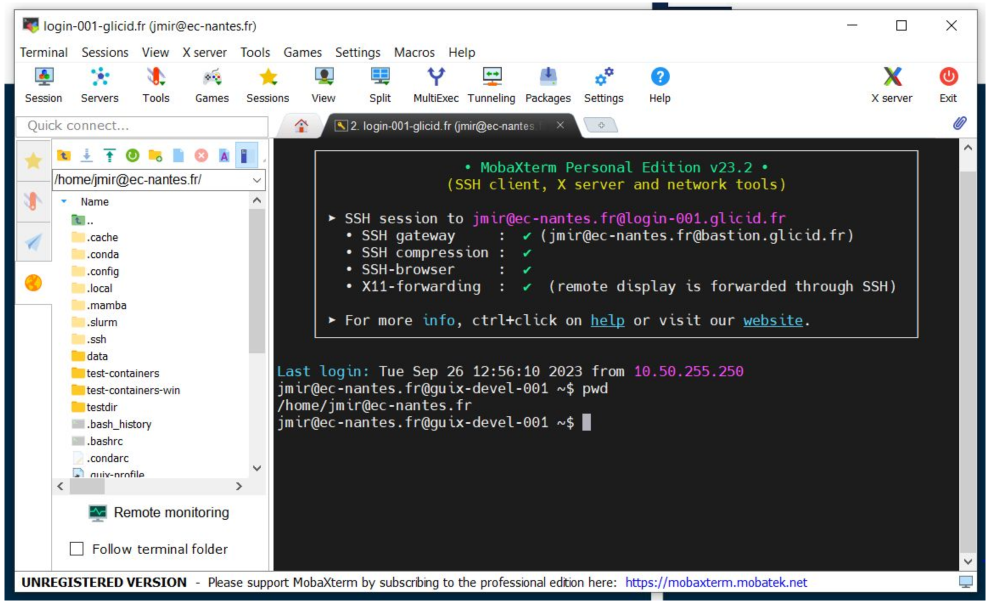
```
jmir@ec-nantes.fr@guix-devel-001 ~/.ssh$ ssh-keygen -t ed25519
Generating public/private ed25519 key pair.
Enter file in which to save the key (/home/jmir@ec-nantes.fr/.ssh/id_ed25519):
Enter passphrase (empty for no passphrase):
Enter same passphrase again:
Your identification has been saved in /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:
SHA256:7bxOEe+80Lh9ykhp3/5DGxRPzPXa5DkJqQodBSU6/L0 jmir@ec-nantes.fr@guix-devel-001.waves.intra.glicid.f
r
The key's randomart image is:
+--[ED25519 256]--+
|         ooo   oo|
|      . . o   ..=|
|       + ..  o .=|
|        +.oo. .*+|
|       .Sooo. o+o|
|        .o.B.  o.|
|         .XE+ . o|
|         + O o.o |
|         .= *+o.o|
+----[SHA256]-----+
jmir@ec-nantes.fr@guix-devel-001 ~/.ssh$ ls
id_ed25519  id_ed25519.pub  known_hosts  known_hosts.old
jmir@ec-nantes.fr@guix-devel-001 ~/.ssh$ cat id_ed25519.pub > authorized_keys
jmir@ec-nantes.fr@guix-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
| \ | |           | | (_) |                    kWNOdc
|  \| | __ _ _   _| |_ _| |_   _ ___          kW0c
| . ` |/ _` | | | | __| | | | | / __|         kW0c
| |\  | (_| | |_| | |_| | | |_| \__ \         kW0c
\_| \_/\__,_|\__,_|\__|_|_|\__,_|___/        cOWKl
                                         cx0KXWMWXK0xc
                                ccllllloxXWMMMMMMMMMWKo
         coooolc       codxkO0KXXNNNWWWWWMMMMMMMMMMMMWOl
        c0WWWWWO   oxOKNWMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWNKOxoc
        lKMMMMMKxOXWMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWXOdc
        lKMMMMMWWMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMW0xdx0NMMWKx
        lKMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWO     kWMMMWOc
        lKMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWOc    kWMMMMNd
        lKMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWKkxkKWMMMMMNd
        lKMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMXx
        lKMMMMMNNWMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWXkl
        lKMMMMM0ookKNWMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMWNKOdc
        ckKKKKKx    ldkOKXNWMMMMMMMMMMMMMMMMMMMMMMMWNXK0kdl
                         clodxkkO000KKKKKKK0000Okxdolc

-----------------------------------------------------------------------------
   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 BullSequana X450 (2 AMD EPYC 9474F@3.6GHz 48c)  768    384
                 with Nvidia A40 (48G) 2 GPUs per node
gnode[1-4]      4 BullSequana 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
- 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
[jmir@ec-nantes.fr@nautilus-devel-001 ~]$ 
```

SSH configuration on Windows

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


login-001-glicid.fr (jmir@ec-nantes.fr)
Terminal Sessions View X server Tools Games Settings Macros Help
Session Servers Tools Games Sessions View Split MultiExec Tunneling Packages Settings Help X server Exit
Quick connect...
2. login-001-glicid.fr (jmir@ec-nantes
/home/jmir@ec-nantes.fr/
Name
..
.cache
.conda
.config
.local
.mamba
.slurm
.ssh
data
test-containers
test-containers-win
testdir
.bash_history
.bashrc
.condarc
.guix-profile
Remote monitoring
Follow terminal folder

```
    • MobaXterm Personal Edition v23.2 •
  (SSH client, X server and network tools)

 ➤ SSH session to jmir@ec-nantes.fr@login-001.glicid.fr
   • SSH gateway     : ✔ (jmir@ec-nantes.fr@bastion.glicid.fr)
   • SSH compression : ✔
   • SSH-browser     : ✔
   • X11-forwarding  : ✔  (remote display is forwarded through SSH)

 ➤ For more info, ctrl+click on help or visit our website.

Last login: Tue Sep 26 12:56:10 2023 from 10.50.255.250
jmir@ec-nantes.fr@guix-devel-001 ~$ pwd
/home/jmir@ec-nantes.fr
jmir@ec-nantes.fr@guix-devel-001 ~$
```

UNREGISTERED VERSION - Please support MobaXterm by subscribing to the professional edition here: https://mobaxterm.mobatek.net

SSH configuration on Windows

- 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)

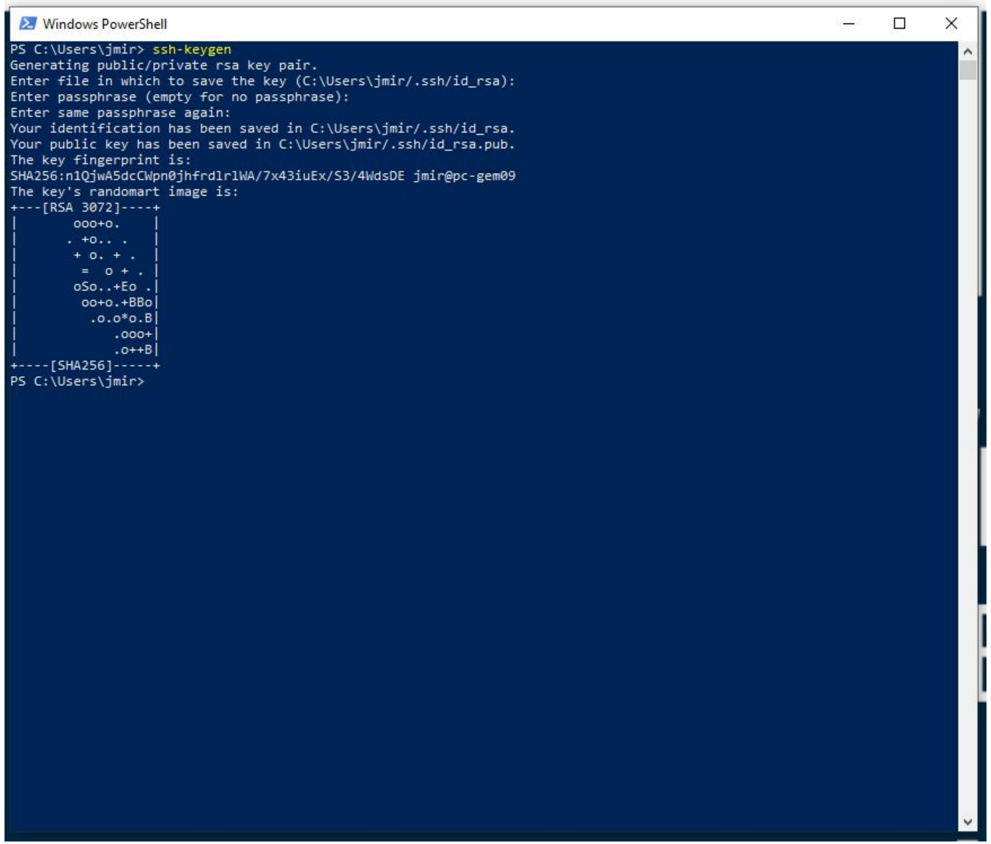
SSH configuration on Windows

- 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

SSH configuration on Windows

- Open PowerShell

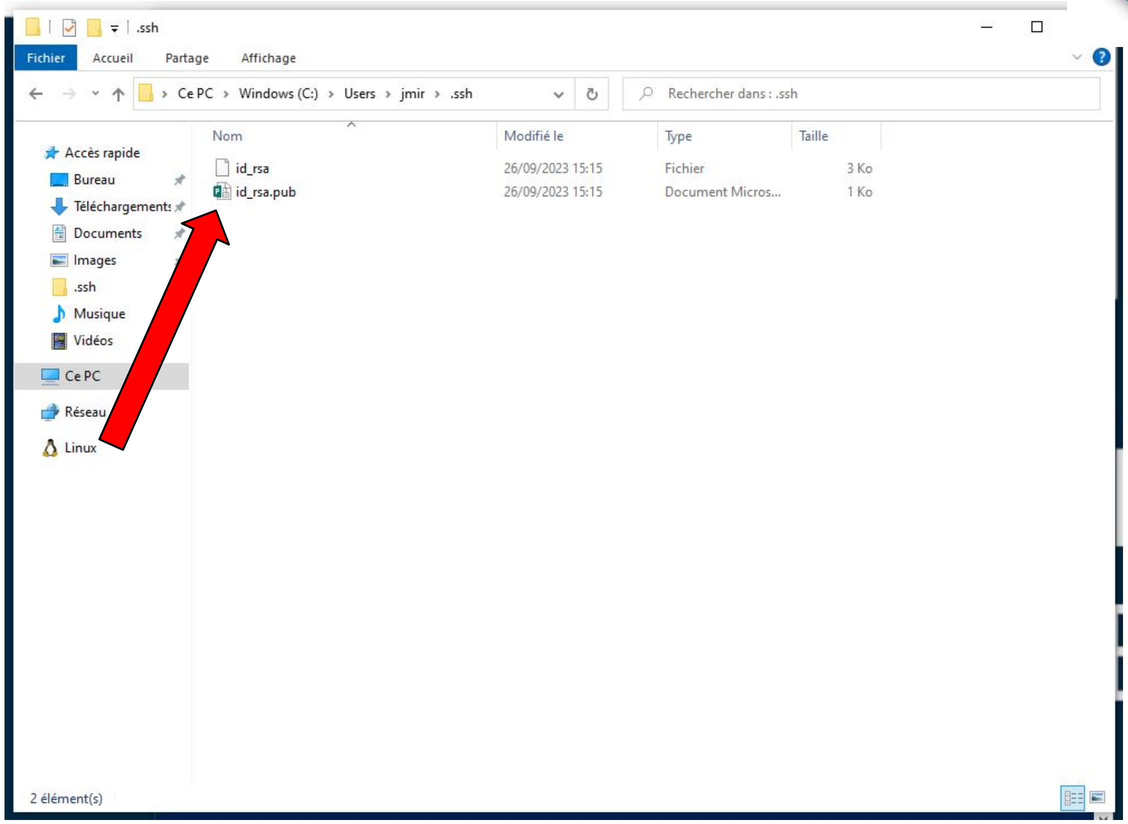
  ssh-keygen



```
PS C:\Users\jmir> ssh-keygen
Generating public/private rsa key pair.
Enter file in which to save the key (C:\Users\jmir/.ssh/id_rsa):
Enter passphrase (empty for no passphrase):
Enter same passphrase again:
Your identification has been saved in C:\Users\jmir/.ssh/id_rsa.
Your public key has been saved in C:\Users\jmir/.ssh/id_rsa.pub.
The key fingerprint is:
SHA256:n1QjwA5dcCWpn0jhfrdlrlWA/7x43iuEx/S3/4WdsDE jmir@pc-gem09
The key's randomart image is:
+---[RSA 3072]----+
|       ooo+o.    |
|      . +o.. .   |
|       + o. + .  |
|        =  o + . |
|       oSo..+Eo .|
|        oo+o.+BBo|
|         .o.o*o.B|
|            .ooo+|
|            .o++B|
+----[SHA256]-----+
PS C:\Users\jmir>
```

SSH configuration on Windows

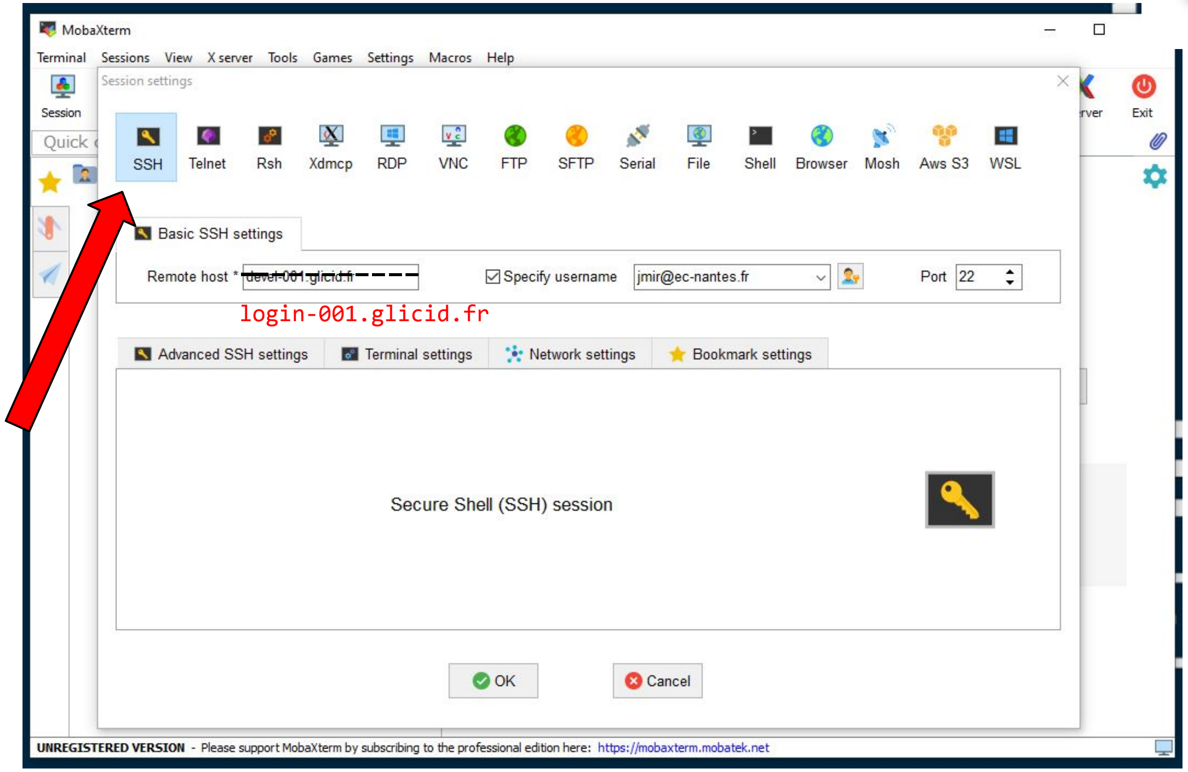
- Keys generated
  - Private key
  - Public key



Nom	Modifié le	Type	Taille
id_rsa	26/09/2023 15:15	Fichier	3 Ko
id_rsa.pub	26/09/2023 15:15	Document Micros...	1 Ko

SSH configuration on Windows

- Open a session
- Configure SSH


MobaXterm
Terminal Sessions View X server Tools Games Settings Macros Help
Session
Session settings
SSH Telnet Rsh Xdmcp RDP VNC FTP SFTP Serial File Shell Browser Mosh Aws S3 WSL
Basic SSH settings
Advanced SSH settings
Terminal settings
Network settings
Bookmark settings
Secure Shell (SSH) session
OK
Cancel
Exit

Remote host * ~~devel-001.glicid.fr~~ login-001.glicid.fr

☑ Specify username jmir@ec-nantes.fr

Port 22

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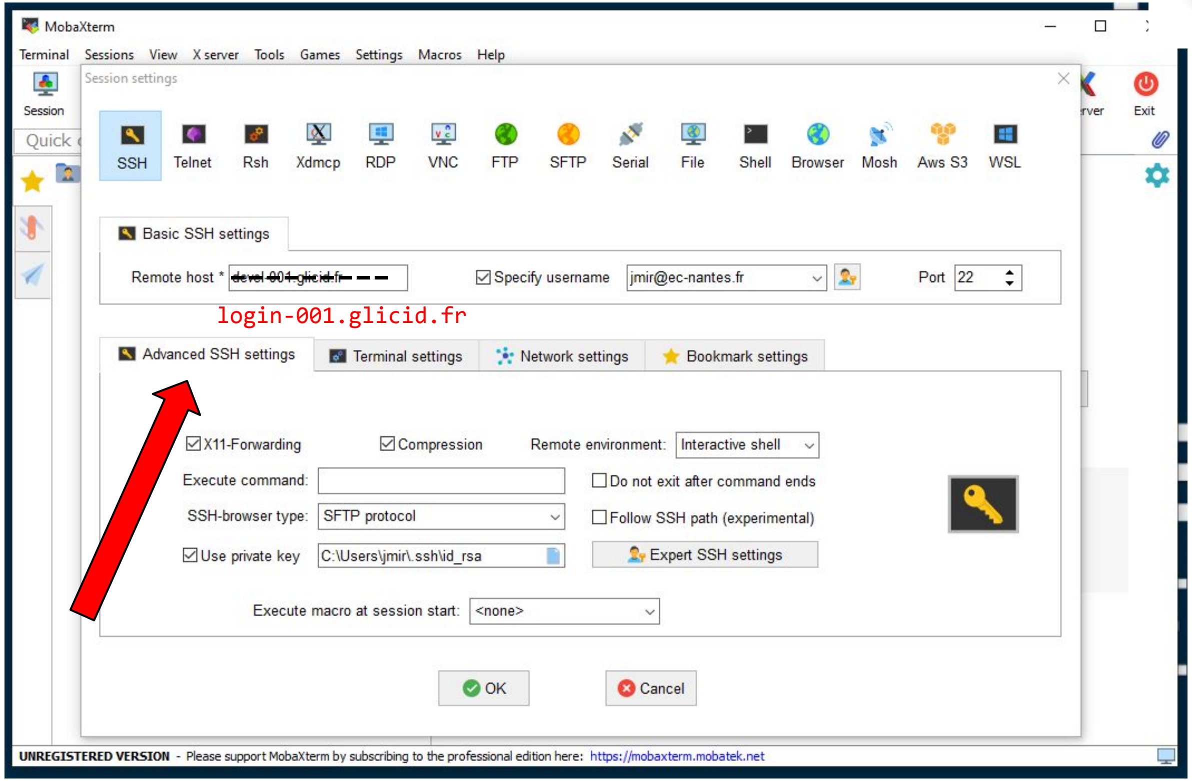
SSH configuration on Windows

- Advanced SSH
  - Upload id_rsa



Remote host * ~~devel-001-glicid.fr~~ — —

☑ Specify username jmir@ec-nantes.fr

Port 22

login-001.glicid.fr

☑ X11-Forwarding

☑ Compression

Remote environment: Interactive shell

Execute command:

☐ Do not exit after command ends

SSH-browser type: SFTP protocol

☐ Follow SSH path (experimental)

☑ Use private key C:\Users\jmir\.ssh\id_rsa

Execute macro at session start: <none>

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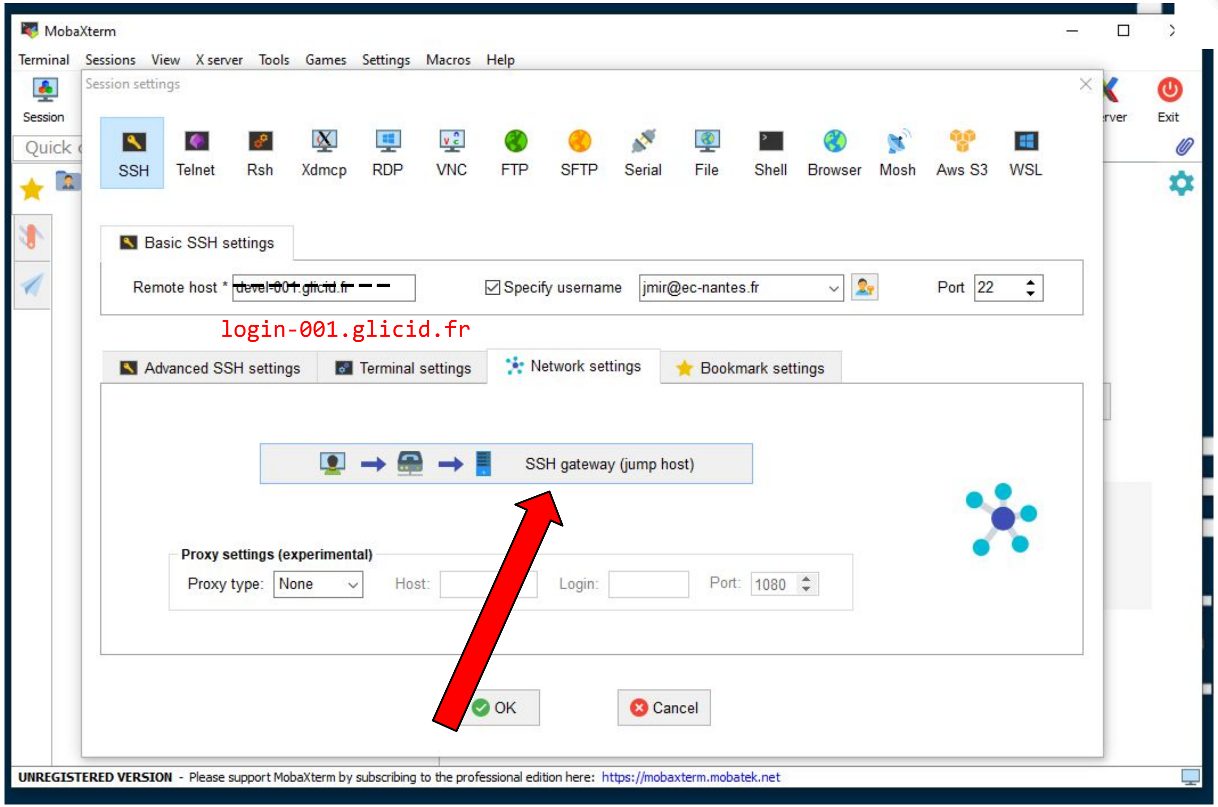
SSH configuration on Windows

- SSH Gateway



Basic SSH settings

Remote host * ~~devel-001.glicid.fr~~ — — —

login-001.glicid.fr

☑ Specify username jmir@ec-nantes.fr

Port 22

Proxy settings (experimental)

Proxy type: None Host: Login: Port: 1080

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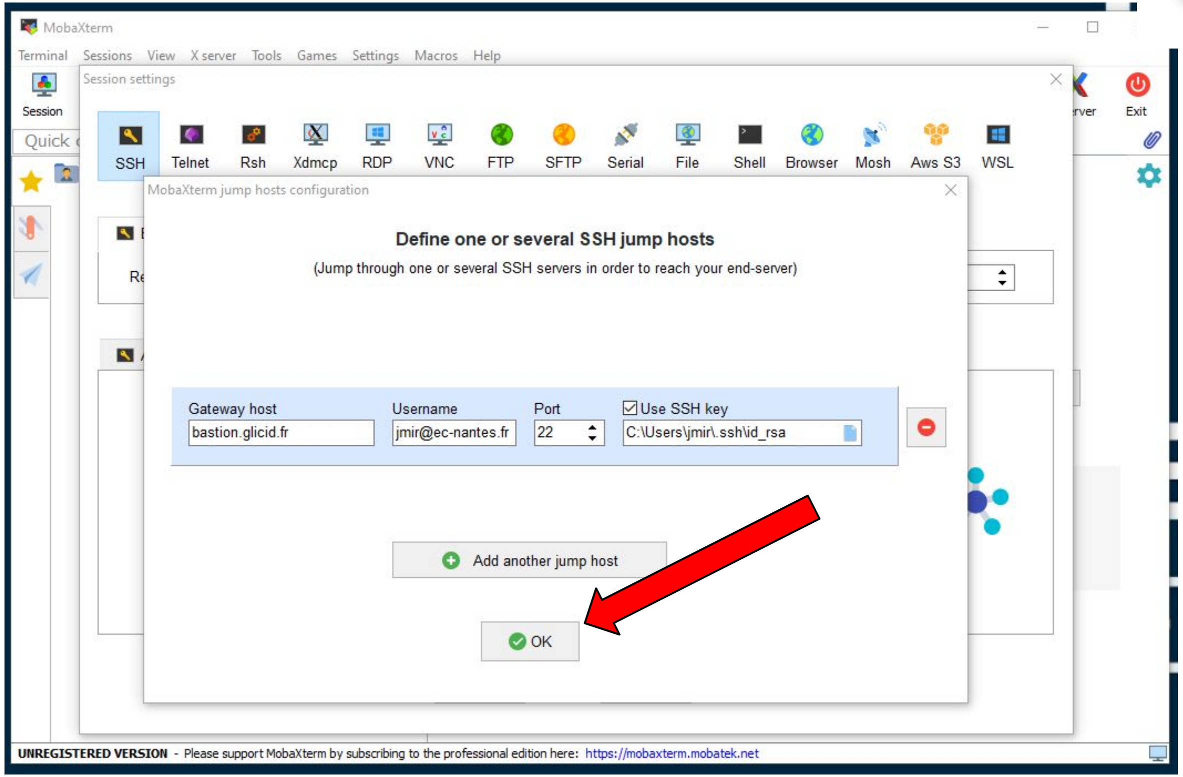
SSH configuration on Windows

- SSH Gateway
  - Upload id_rsa



Define one or several SSH jump hosts

(Jump through one or several SSH servers in order to reach your end-server)

Gateway host	Username	Port	☑ Use SSH key
bastion.glicid.fr	jmir@ec-nantes.fr	22	C:\Users\jmir\.ssh\id_rsa

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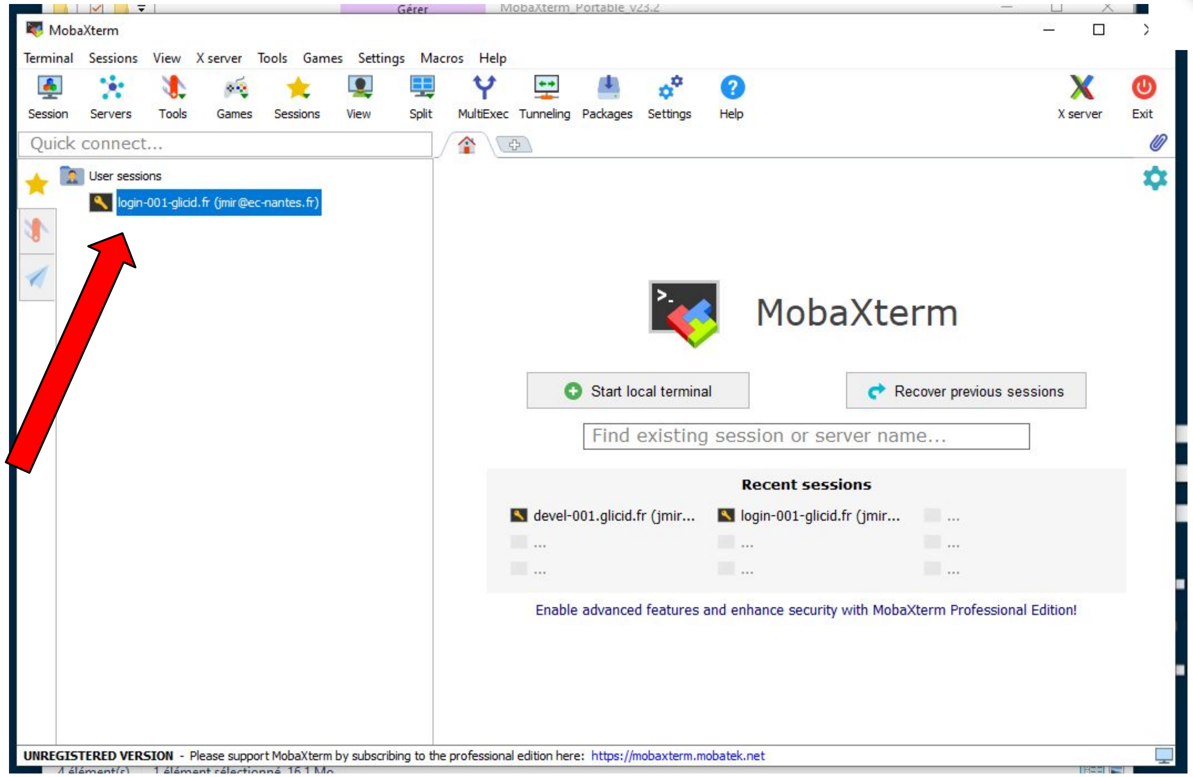
SSH configuration on Windows

- Execute Session


MobaXterm
Terminal Sessions View X server Tools Games Settings Macros Help
Session Servers Tools Games Sessions View Split MultiExec Tunneling Packages Settings Help X server Exit
Quick connect...
User sessions
login-001-glicid.fr (jmir@ec-nantes.fr)
Start local terminal
Recover previous sessions
Find existing session or server name...
Recent sessions
devel-001.glicid.fr (jmir...
login-001-glicid.fr (jmir...

Enable advanced features and enhance security with MobaXterm Professional Edition!

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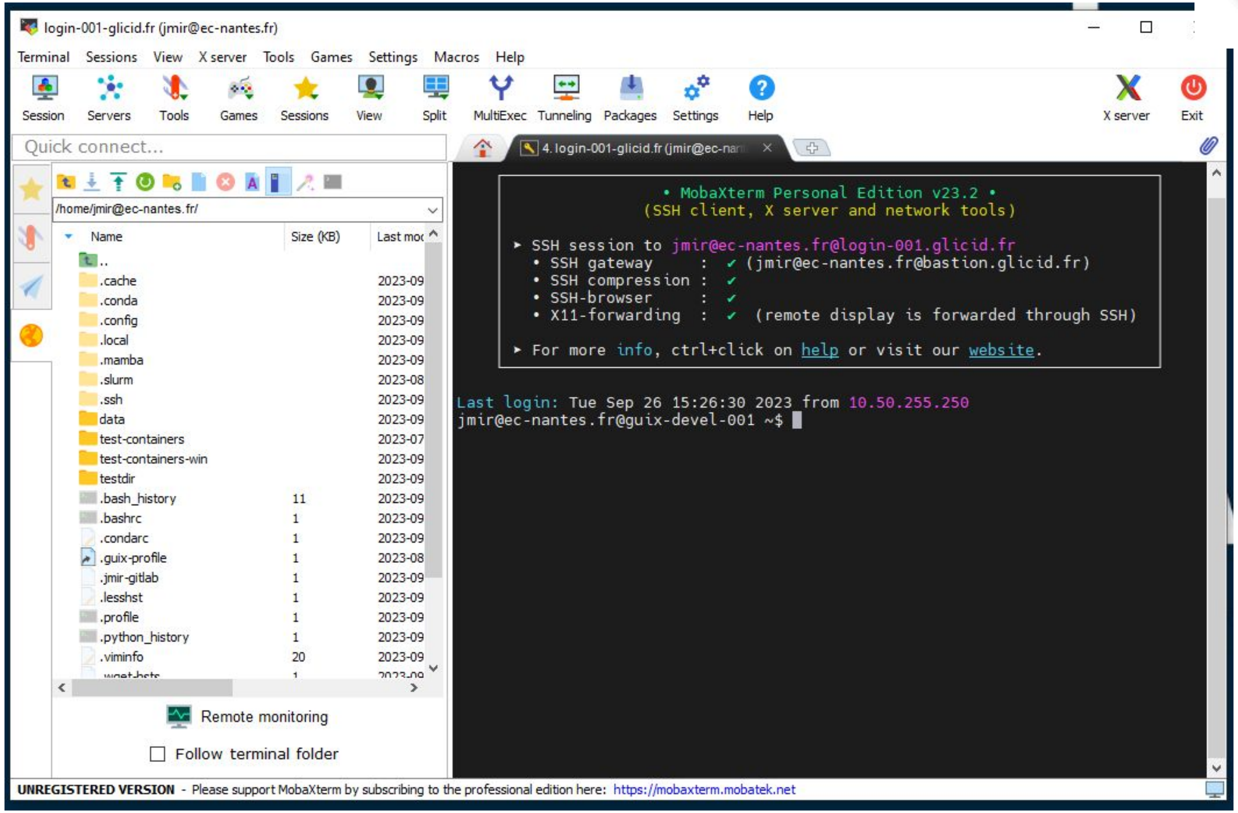
SSH configuration on Windows

- Here you go…



login-001-glicid.fr (jmir@ec-nantes.fr)
Terminal Sessions View X server Tools Games Settings Macros Help
Session Servers Tools Games Sessions View Split MultiExec Tunneling Packages Settings Help X server Exit
Quick connect...
4. login-001-glicid.fr (jmir@ec-nan
/home/jmir@ec-nantes.fr/
Remote monitoring
Follow terminal folder

Name	Size (KB)	Last mod
..		
.cache		2023-09
.conda		2023-09
.config		2023-09
.local		2023-09
.mamba		2023-09
.slurm		2023-08
.ssh		2023-09
data		2023-09
test-containers		2023-07
test-containers-win		2023-09
testdir		2023-09
.bash_history	11	2023-09
.bashrc	1	2023-09
.condarc	1	2023-09
.guix-profile	1	2023-08
.jmir-gitlab	1	2023-09
.lesshst	1	2023-09
.profile	1	2023-09
.python_history	1	2023-09
.viminfo	20	2023-09
.wget-hsts	1	2023-09

```
                  • MobaXterm Personal Edition v23.2 •
                (SSH client, X server and network tools)

 ➤ SSH session to jmir@ec-nantes.fr@login-001.glicid.fr
   • SSH gateway     :  ✔ (jmir@ec-nantes.fr@bastion.glicid.fr)
   • SSH compression :  ✔
   • SSH-browser     :  ✔
   • X11-forwarding  :  ✔  (remote display is forwarded through SSH)

 ➤ For more info, ctrl+click on help or visit our website.

Last login: Tue Sep 26 15:26:30 2023 from 10.50.255.250
jmir@ec-nantes.fr@guix-devel-001 ~$
```

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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 :(

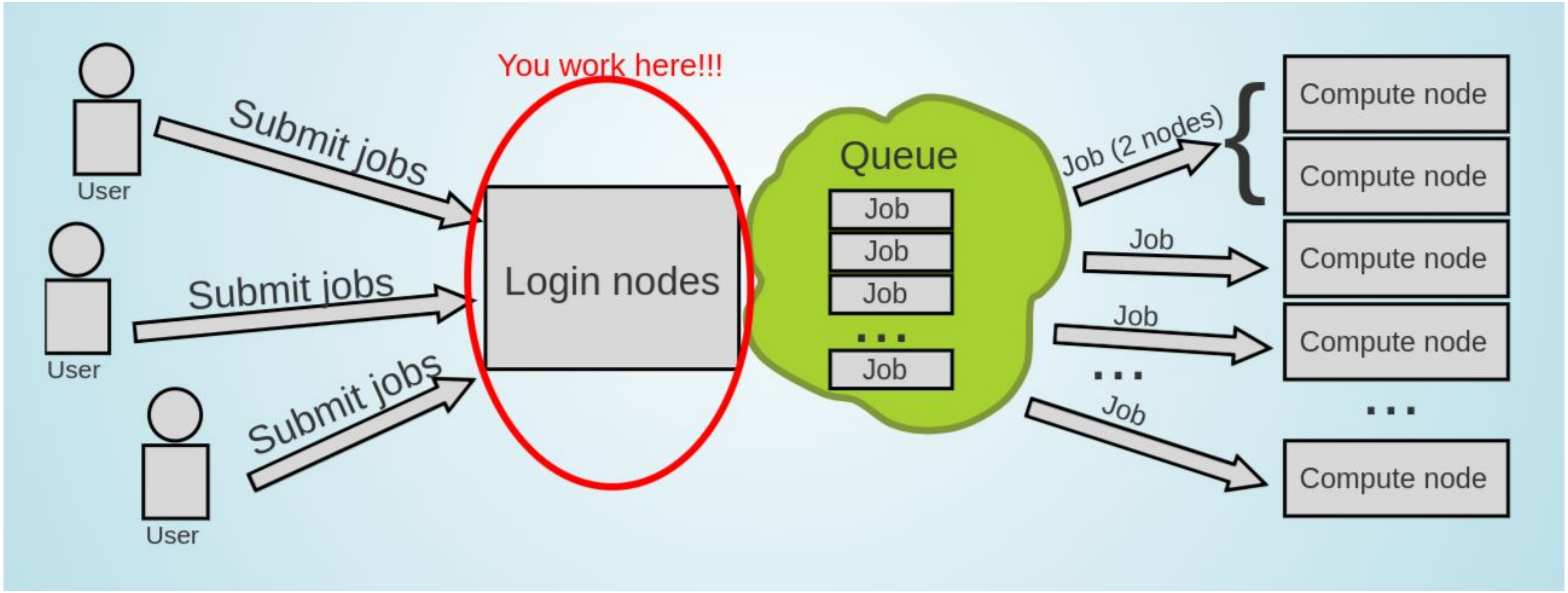
Get Your Hands Dirty

slurm

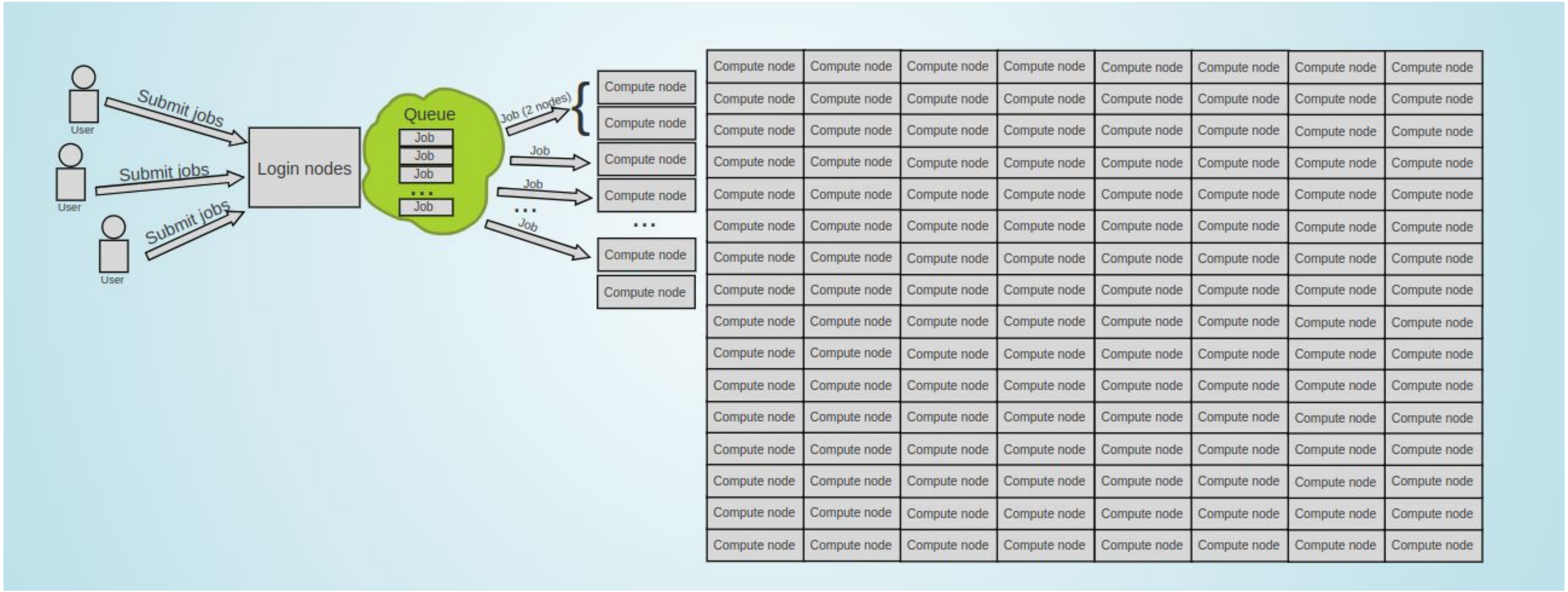
workload manager

Bringing Order To Chaos

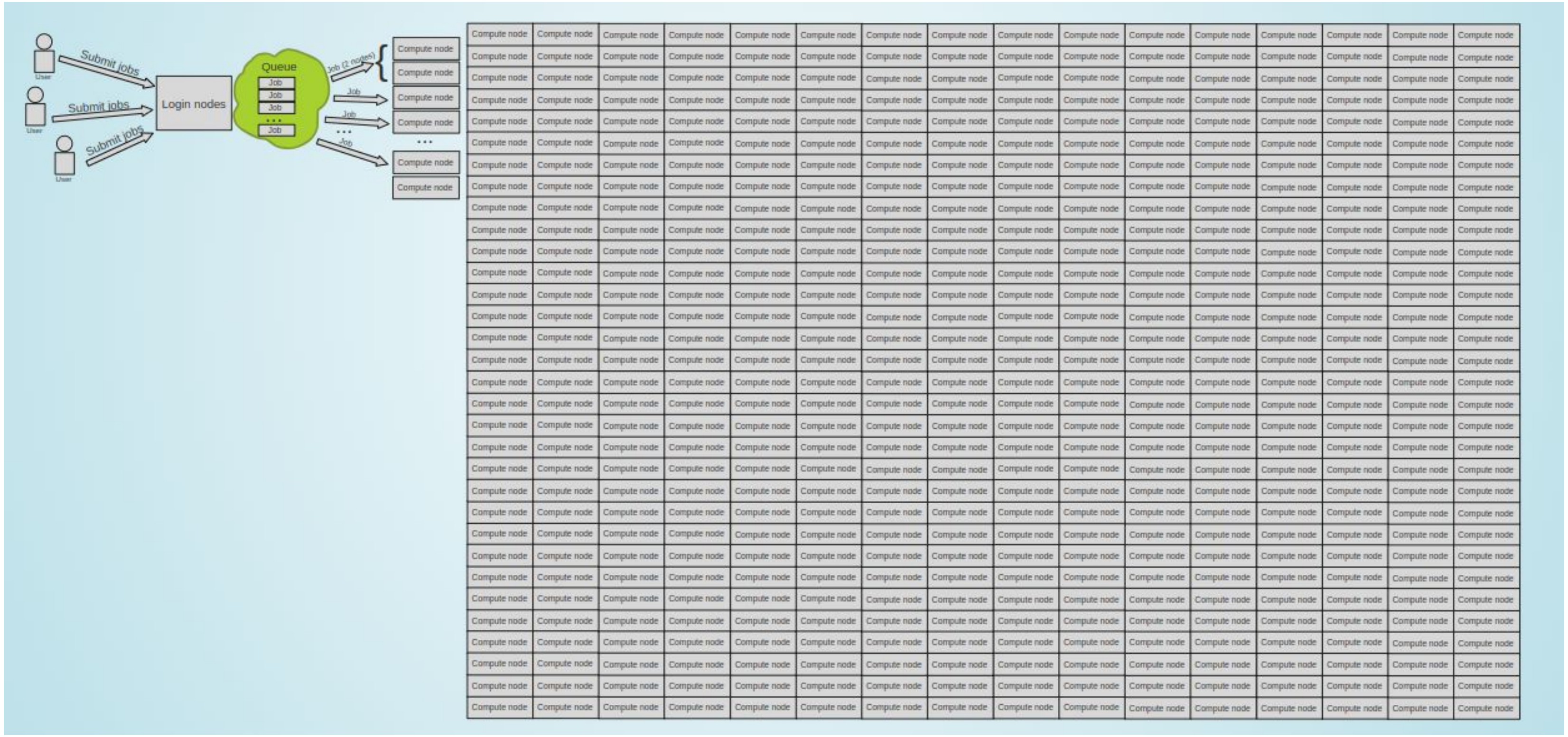
You submit jobs



But you don't use the whole Supercomputer



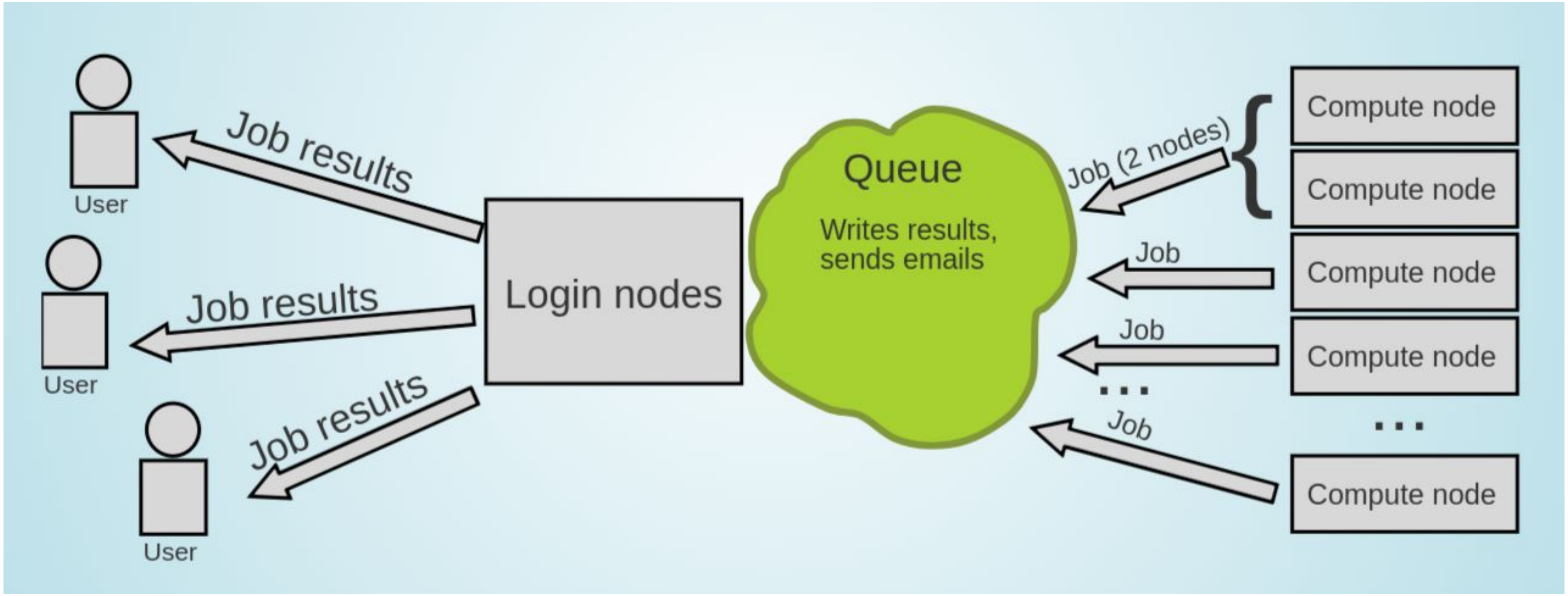
There are many more users



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

Results


User
Job results
User
Job results
User
Job results
Login nodes
Queue
Writes results, sends emails
Job (2 nodes)
Job
Job
...
Job
Compute node
Compute node
Compute node
Compute node
...
Compute node

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

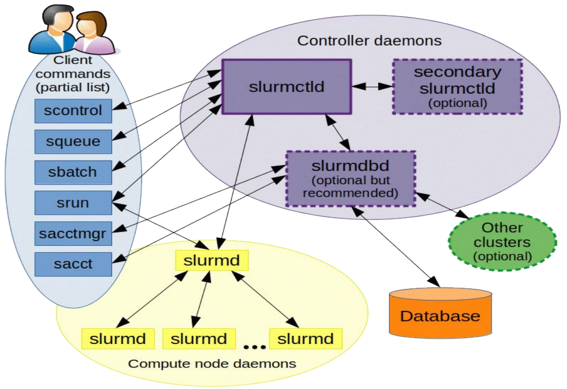
Who will manage this workload?

- 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

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.



Client commands (partial list)
scontrol
squeue
sbatch
srun
sacctmgr
sacct
Controller daemons
slurmctld
secondary slurmctld (optional)
slurmdbd (optional but recommended)
Other clusters (optional)
Database
slurmd
slurmd
slurmd
...
slurmd
Compute node daemons

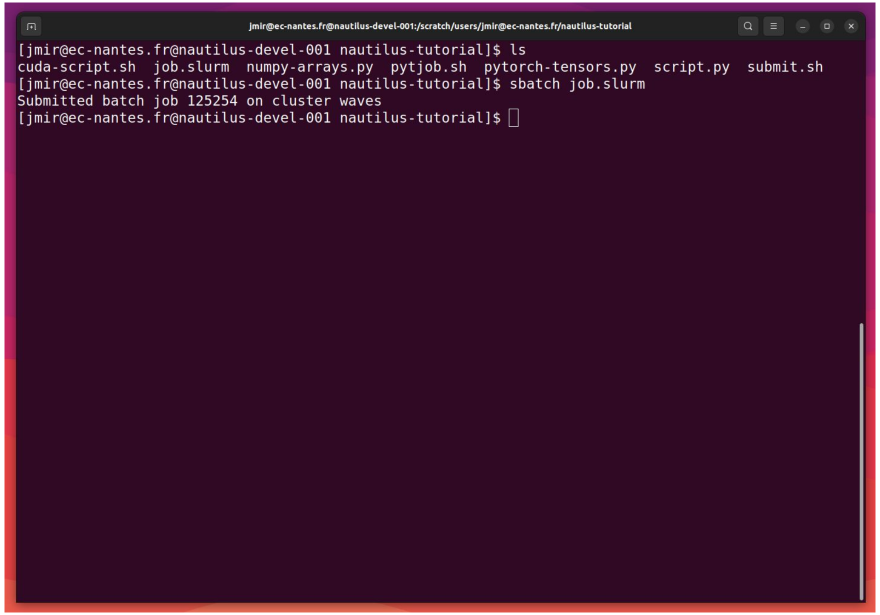
Basic Slurm Commands

Command	Syntax	Description
sbatch	sbatch <job_id>	To submit job script for later execution (batch mode)
sinfo	sinfo	Get information about available nodes
squeue	squeue -u	Show information about jobs
scancel	scancel <job-id>	To terminate queued or running jobs
srun	srun <resource-parameters>	To run jobs interactively
sacct	sacct	Show information about current and previous jobs

Basic Slurm Commands

- To submit a job

  `sbatch job.slurm`



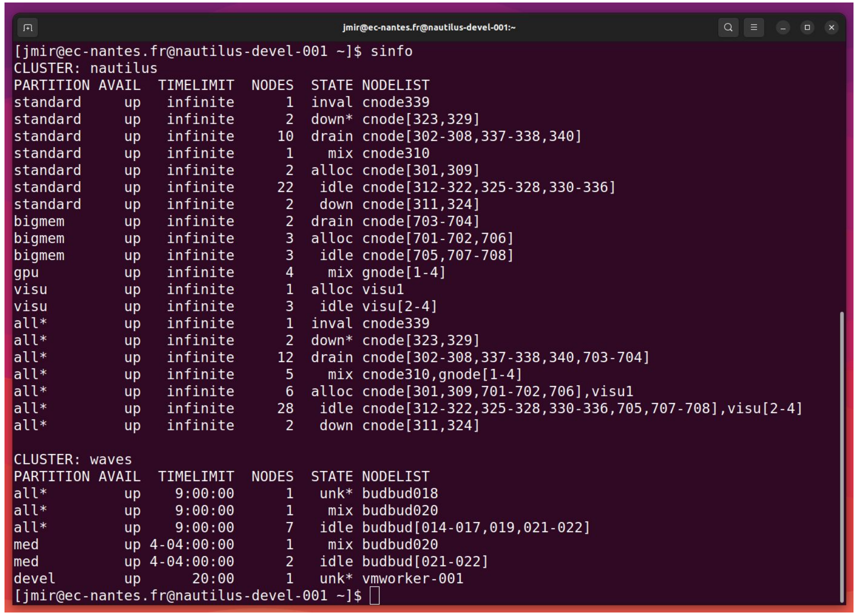
jmir@ec-nantes.fr@nautilus-devel-001:/scratch/users/jmir@ec-nantes.fr/nautilus-tutorial

```
[jmir@ec-nantes.fr@nautilus-devel-001 nautilus-tutorial]$ ls
cuda-script.sh  job.slurm  numpy-arrays.py  pytjob.sh  pytorch-tensors.py  script.py  submit.sh
[jmir@ec-nantes.fr@nautilus-devel-001 nautilus-tutorial]$ sbatch job.slurm
Submitted batch job 125254 on cluster waves
[jmir@ec-nantes.fr@nautilus-devel-001 nautilus-tutorial]$ 
```

Basic Slurm Commands

- Get information about available nodes

  `sinfo`

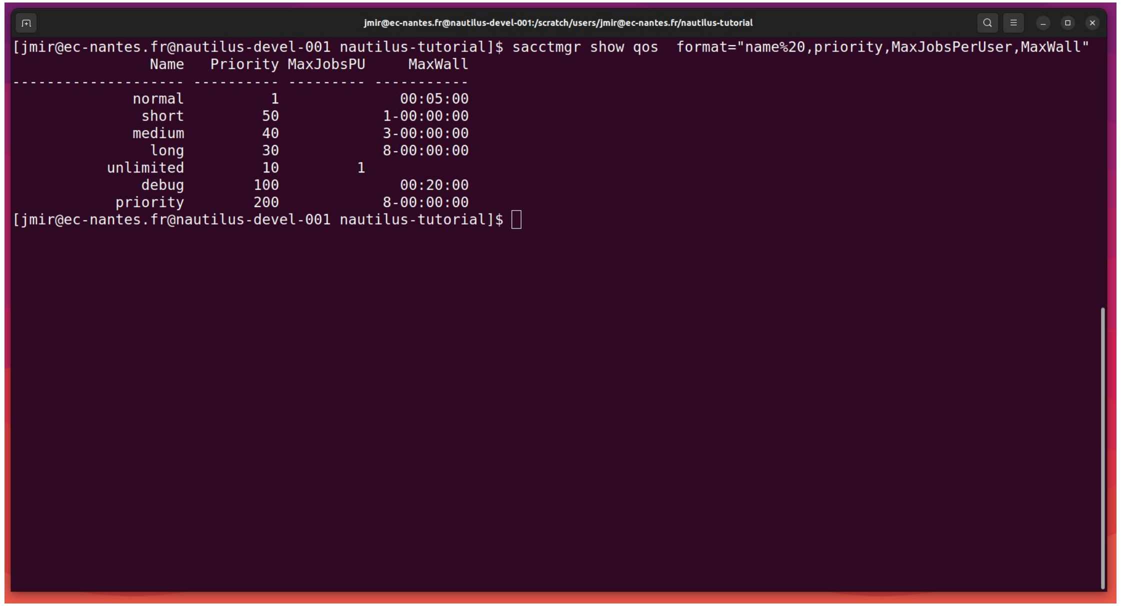


```
[jmir@ec-nantes.fr@nautilus-devel-001 ~]$ sinfo
CLUSTER: nautilus
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
standard     up   infinite      1  inval cnode339
standard     up   infinite      2  down* cnode[323,329]
standard     up   infinite     10  drain cnode[302-308,337-338,340]
standard     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]
gpu          up   infinite      4    mix gnode[1-4]
visu         up   infinite      1  alloc visu1
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    9:00:00      7   idle budbud[014-017,019,021-022]
med          up 4-04:00:00      1    mix budbud020
med          up 4-04:00:00      2   idle budbud[021-022]
devel        up      20:00      1   unk* vmworker-001
[jmir@ec-nantes.fr@nautilus-devel-001 ~]$ 
```

Basic Slurm Commands

- To check Priority and MaxWall Time

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



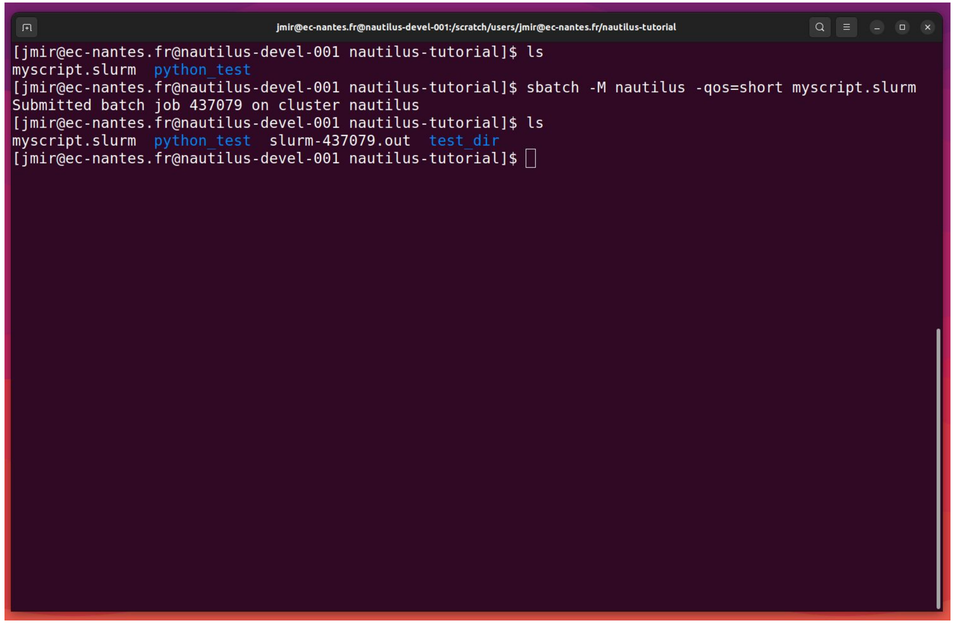
jmir@ec-nantes.fr@nautilus-devel-001:/scratch/users/jmir@ec-nantes.fr/nautilus-tutorial

```
[jmir@ec-nantes.fr@nautilus-devel-001 nautilus-tutorial]$ sacctmgr show qos  format="name%20,priority,MaxJobsPerUser,MaxWall"
                Name   Priority MaxJobsPU     MaxWall
-------------------- ---------- --------- -----------
              normal          1              00:05:00
               short         50            1-00:00:00
              medium         40            3-00:00:00
                long         30            8-00:00:00
           unlimited         10         1
               debug        100              00:20:00
            priority        200            8-00:00:00
[jmir@ec-nantes.fr@nautilus-devel-001 nautilus-tutorial]$ 
```

Basic Slurm Commands

- Submit your slurm script

```
sbatch -M nautilus -p standard -qos=short <script-name>.slurm
```



jmir@ec-nantes.fr@nautilus-devel-001:/scratch/users/jmir@ec-nantes.fr/nautilus-tutorial

```
[jmir@ec-nantes.fr@nautilus-devel-001 nautilus-tutorial]$ ls
myscript.slurm  python_test
[jmir@ec-nantes.fr@nautilus-devel-001 nautilus-tutorial]$ sbatch -M nautilus -qos=short myscript.slurm
Submitted batch job 437079 on cluster nautilus
[jmir@ec-nantes.fr@nautilus-devel-001 nautilus-tutorial]$ ls
myscript.slurm  python_test  slurm-437079.out  test_dir
[jmir@ec-nantes.fr@nautilus-devel-001 nautilus-tutorial]$ 
```

Slurm - Batch Script

Sample script to run python code using conda environment

```
#!/bin/bash
#SBATCH --job-name=myjob            # create a short name for your job
#SBATCH --nodes=1                   # node count
#SBATCH --ntasks=1                  # total number of tasks across all nodes
#SBATCH --cpus-per-task=1           # cpu-cores per task
#SBATCH --mem-per-cpu=2G            # memory per cpu-core
#SBATCH --gres=gpu:4                # number of gpus per node
#SBATCH --time=00:05:00             # total run time limit (HH:MM:SS)


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

hostname

python myscript.py
```

Software Modules

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

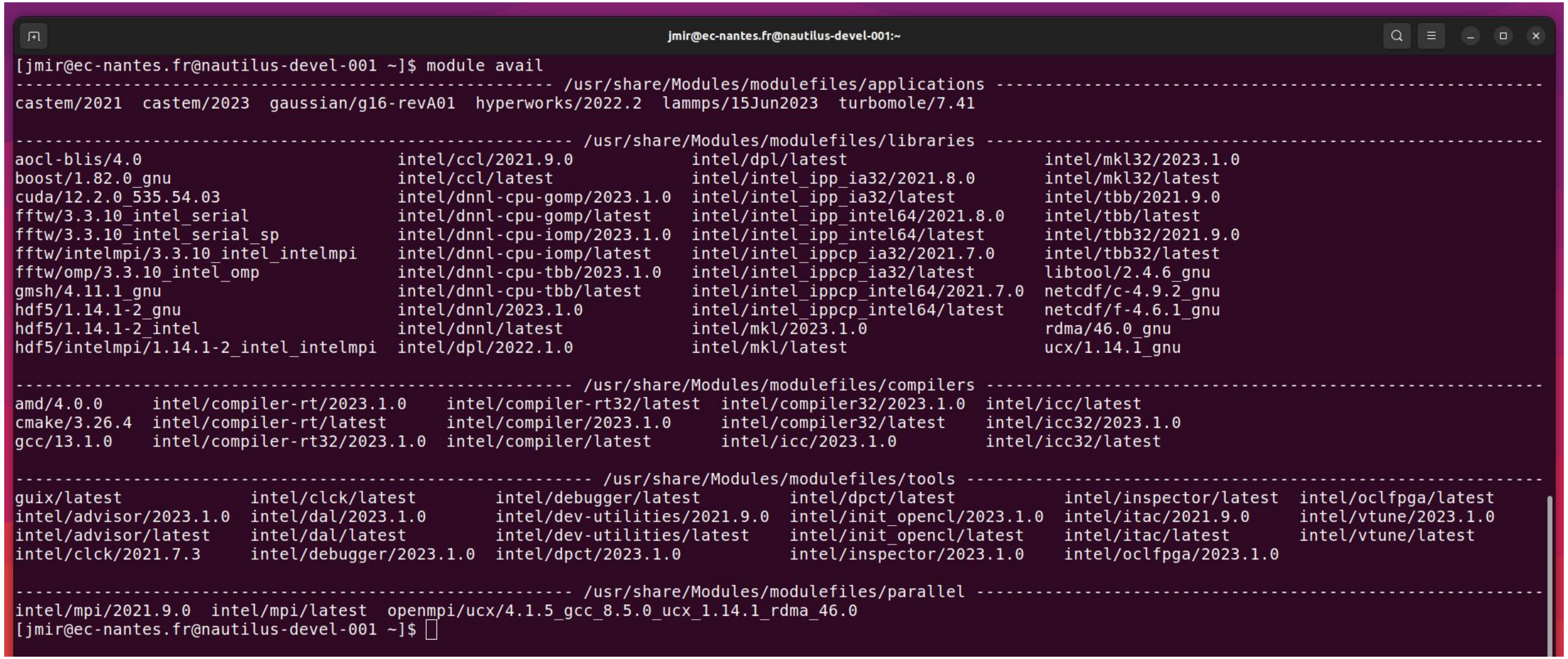
How to use Modules?

- Useful commands

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

How to use Modules?

```
$module avail
```



```
[jmir@ec-nantes.fr@nautilus-devel-001 ~]$ module avail
------------------------------------------------------- /usr/share/Modules/modulefiles/applications -------------------------------------------------------
castem/2021  castem/2023  gaussian/g16-revA01  hyperworks/2022.2  lammps/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/intel_ipp_ia32/latest          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           intel/dnnl-cpu-iomp/2023.1.0   intel/intel_ipp_intel64/latest       intel/tbb32/2021.9.0
fftw/intelmpi/3.3.10_intel_intelmpi   intel/dnnl-cpu-iomp/latest     intel/intel_ippcp_ia32/2021.7.0      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            intel/intel_ippcp_intel64/latest     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/2023.1.0    intel/compiler-rt32/latest  intel/compiler32/2023.1.0  intel/icc/latest
cmake/3.26.4  intel/compiler-rt/latest      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/share/Modules/modulefiles/tools -----------------------------------------------------------
guix/latest             intel/clck/latest         intel/debugger/latest         intel/dpct/latest            intel/inspector/latest  intel/oclfpga/latest
intel/advisor/2023.1.0  intel/dal/2023.1.0        intel/dev-utilities/2021.9.0  intel/init_opencl/2023.1.0   intel/itac/2021.9.0     intel/vtune/2023.1.0
intel/advisor/latest    intel/dal/latest          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 ----------------------------------------------------------
intel/mpi/2021.9.0  intel/mpi/latest  openmpi/ucx/4.1.5_gcc_8.5.0_ucx_1.14.1_rdma_46.0
[jmir@ec-nantes.fr@nautilus-devel-001 ~]$
```

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

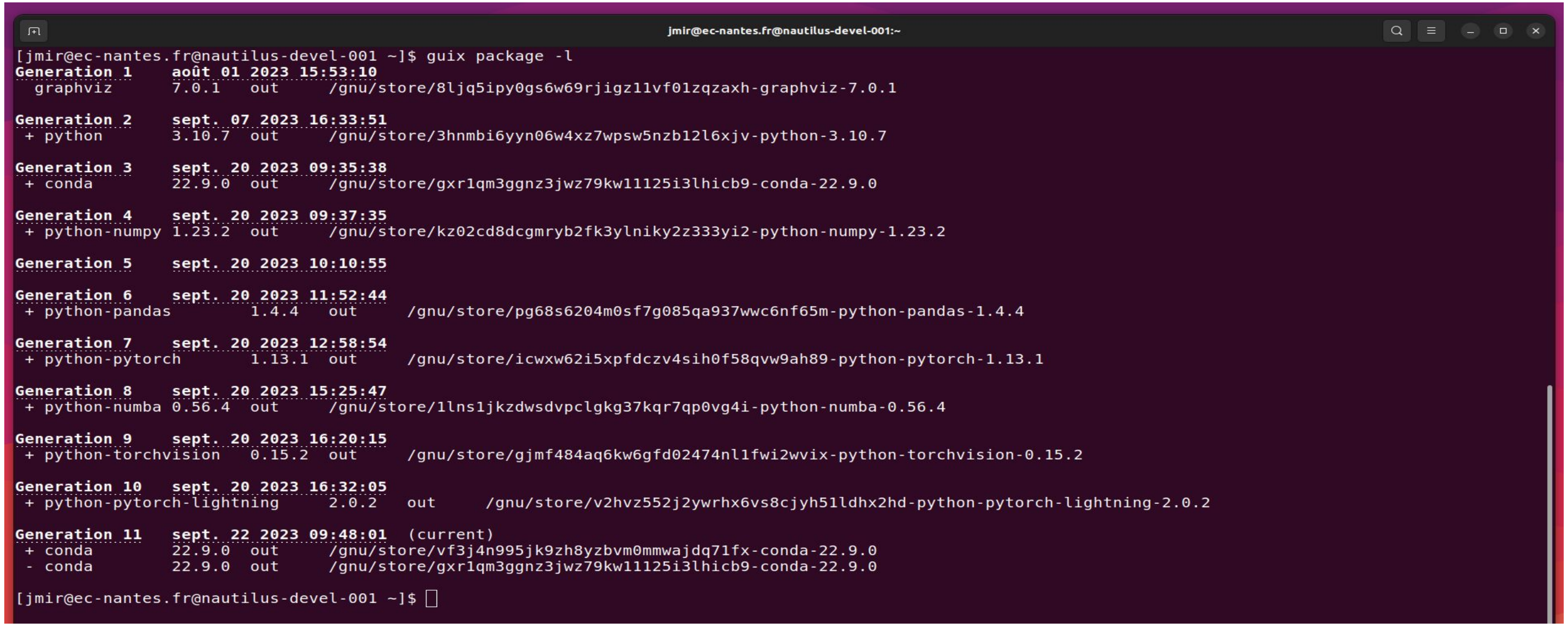
Guix Package Manager

- Useful commands

Command	Description
`guix pull`	You need to run this at least once(maybe weekly :p)
`guix search <package_name>`	Look for a package to install
`guix install <package_name>`	To install a package
`guix remove <package_name>`	To remove a package
`guix package -l`	List of installed packages

How to use Guix?

```
$guix package -l
```

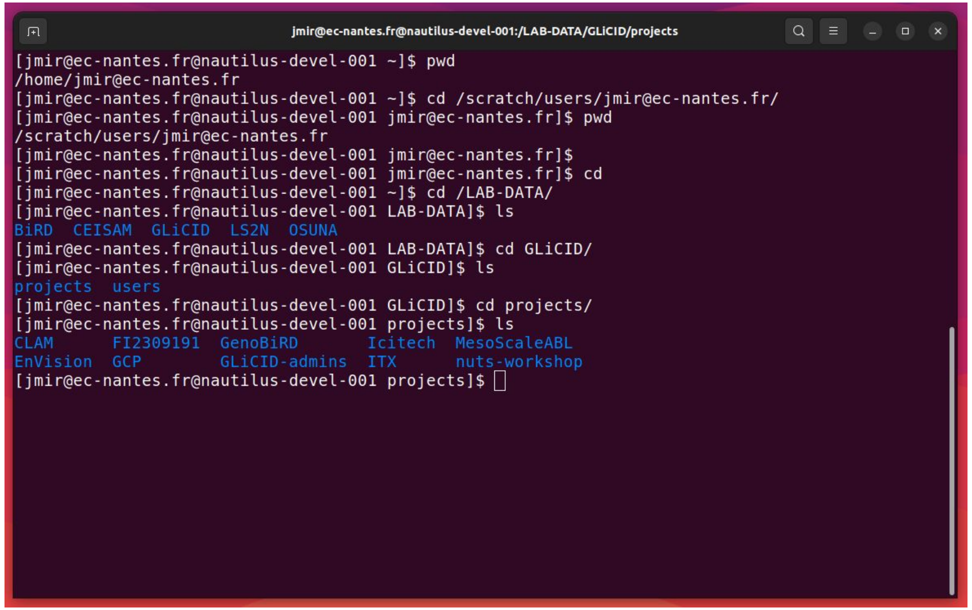


```
[jmir@ec-nantes.fr@nautilus-devel-001 ~]$ guix package -l
Generation 1    août 01 2023 15:53:10
  graphviz      7.0.1   out     /gnu/store/8ljq5ipy0gs6w69rjigz11vf01zqzaxh-graphviz-7.0.1

Generation 2    sept. 07 2023 16:33:51
 + python       3.10.7  out     /gnu/store/3hnmbi6yyn06w4xz7wpsw5nzb12l6xjv-python-3.10.7

Generation 3    sept. 20 2023 09:35:38
 + conda        22.9.0  out     /gnu/store/gxr1qm3ggnz3jwz79kw11125i3lhicb9-conda-22.9.0

Generation 4    sept. 20 2023 09:37:35
 + python-numpy 1.23.2  out     /gnu/store/kz02cd8dcgmryb2fk3ylniky2z333yi2-python-numpy-1.23.2

Generation 5    sept. 20 2023 10:10:55

Generation 6    sept. 20 2023 11:52:44
 + python-pandas        1.4.4   out     /gnu/store/pg68s6204m0sf7g085qa937wwc6nf65m-python-pandas-1.4.4

Generation 7    sept. 20 2023 12:58:54
 + python-pytorch       1.13.1  out     /gnu/store/icwxw62i5xpfdczv4sih0f58qvw9ah89-python-pytorch-1.13.1

Generation 8    sept. 20 2023 15:25:47
 + python-numba 0.56.4  out     /gnu/store/1lns1jkzdwsdvpclgkg37kqr7qp0vg4i-python-numba-0.56.4

Generation 9    sept. 20 2023 16:20:15
 + python-torchvision   0.15.2  out     /gnu/store/gjmf484aq6kw6gfd02474nl1fwi2wvix-python-torchvision-0.15.2

Generation 10   sept. 20 2023 16:32:05
 + python-pytorch-lightning     2.0.2   out     /gnu/store/v2hvz552j2ywrhx6vs8cjyh51ldhx2hd-python-pytorch-lightning-2.0.2

Generation 11   sept. 22 2023 09:48:01  (current)
 + conda        22.9.0  out     /gnu/store/vf3j4n995jk9zh8yzbvm0mmwajdq71fx-conda-22.9.0
 - conda        22.9.0  out     /gnu/store/gxr1qm3ggnz3jwz79kw11125i3lhicb9-conda-22.9.0

[jmir@ec-nantes.fr@nautilus-devel-001 ~]$ 
```

Data Management

Data management

- HOME (Personal Space/But don't train your neural network here)
- SCRATCH (Train it here)
    - HDD
    - SDD
- LAB-DATA
    - Users
    - Projects


jmir@ec-nantes.fr@nautilus-devel-001:/LAB-DATA/GLiCID/projects

```
[jmir@ec-nantes.fr@nautilus-devel-001 ~]$ pwd
/home/jmir@ec-nantes.fr
[jmir@ec-nantes.fr@nautilus-devel-001 ~]$ cd /scratch/users/jmir@ec-nantes.fr/
[jmir@ec-nantes.fr@nautilus-devel-001 jmir@ec-nantes.fr]$ pwd
/scratch/users/jmir@ec-nantes.fr
[jmir@ec-nantes.fr@nautilus-devel-001 jmir@ec-nantes.fr]$
[jmir@ec-nantes.fr@nautilus-devel-001 jmir@ec-nantes.fr]$ cd
[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]$ cd GLiCID/
[jmir@ec-nantes.fr@nautilus-devel-001 GLiCID]$ ls
projects  users
[jmir@ec-nantes.fr@nautilus-devel-001 GLiCID]$ cd projects/
[jmir@ec-nantes.fr@nautilus-devel-001 projects]$ ls
CLAM      FI2309191  GenoBiRD      Icitech  MesoScaleABL
EnVision  GCP        GLiCID-admins  ITX      nuts-workshop
[jmir@ec-nantes.fr@nautilus-devel-001 projects]$ 
```

Get Your Hands Dirty Again

Thank you. Any questions?

Please answer the survey if you haven't yet
https://forms.gle/B4dto4axGm4EVPwaA

Useful links:

User Doc: https://doc.glicid.fr

Support: https://help.glicid.fr or support@glicid.fr

Chat: On CLAM website

Admins: tech@glicid.fr

Forum: Coming soon

Status page: https://ckc.glicid.fr