Getting Started With GLiCID: Advanced Session

Mir Junaid

January 11, 2024

OUTLINE

- Why HPC?
- Guix Package Manager
- Modules
- SLURM Workload Manager
  - Why do we need Slurm?
  - Slurm Configuration Options
  - Example Slurm Script
  - TP
    - Basic Slurm Script
    - Slurm for Parallel Programming
    - Install Conda/Micromamba
    - Fortran: Hello World

Why HPC?

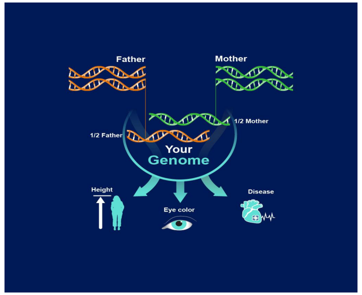
Q. Why would I be interested in High Performance Computing (HPC)?

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**.

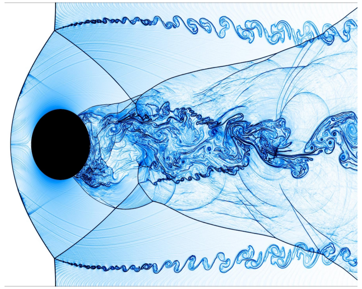
Why HPC?



Use Case 2: Genomics

- A genomics researcher has been using small datasets of sequence data, but some type of sequencing datasets 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.

Why HPC?



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.

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

Guix Package Manager

What is Guix?

- Package building system/Package manager
- Why Guix? Why is it better than modules?
    - 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

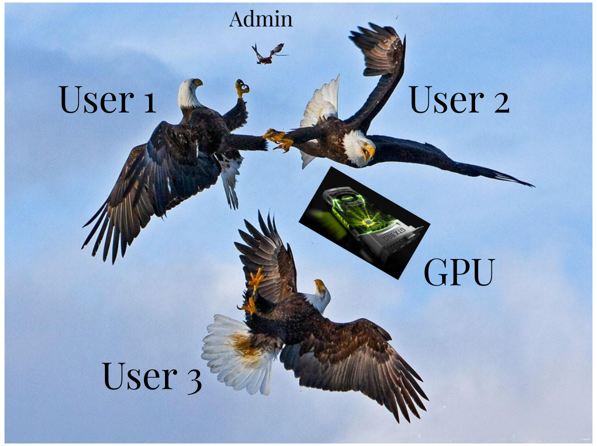
Search packages here https://packages.guix.gnu.org/

Note: To use Guix on Nautilus, load the guix module (module load guix) slurm

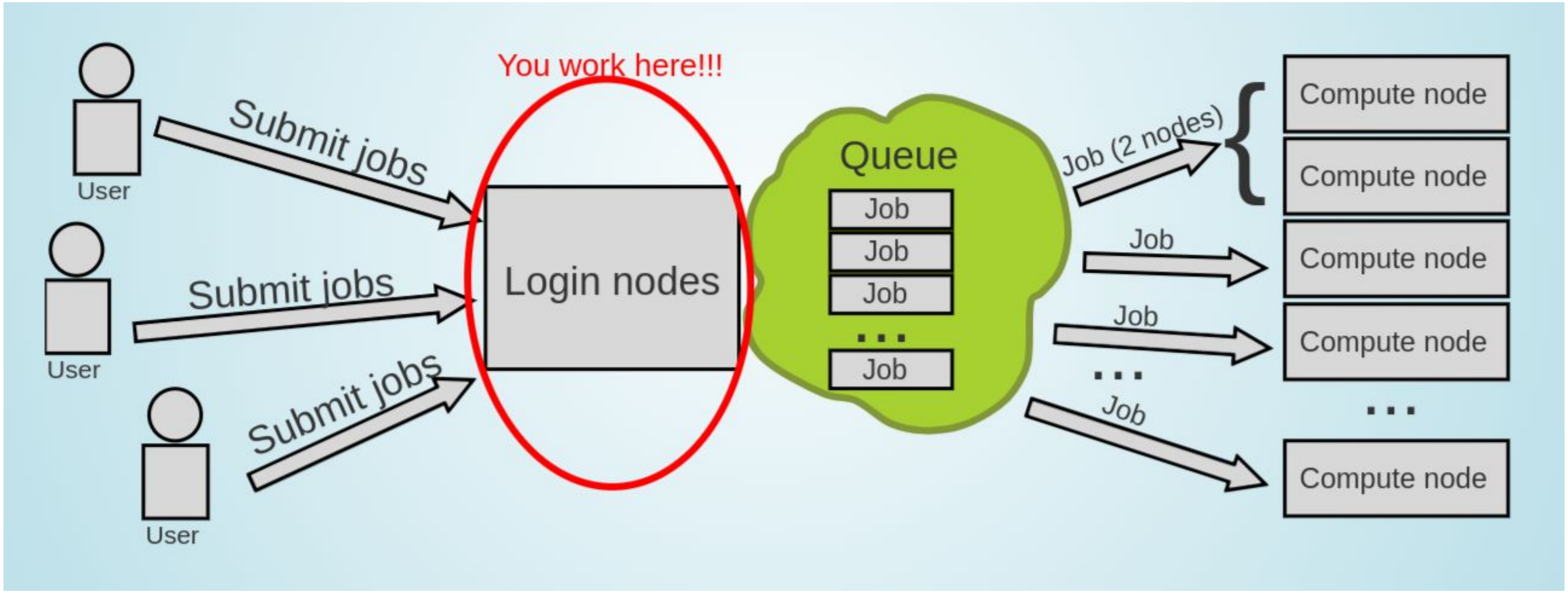
workload manager

Competition for limited resources

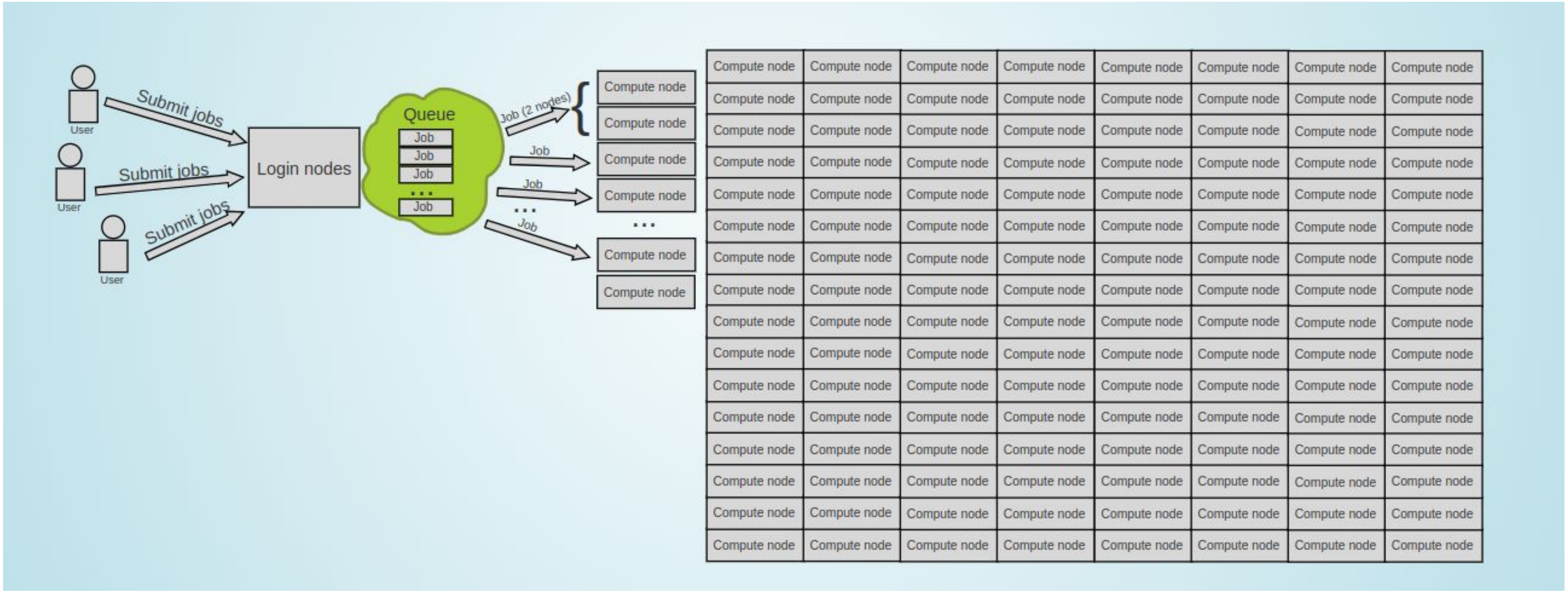
- On computing cluster, people compete to use a finite set of resources (CPUs/GPUs/RAM)
- If everyone just starts running code, then everyone will have a bad time as resources are shared
- To solve this problem, computing centers use resource manager and job scheduler called Slurm
- With Slurm, you can submit jobs and tell Slurm what resources you need
- Slurm will allocate those resources to your job and then schedule your job



This is how it works



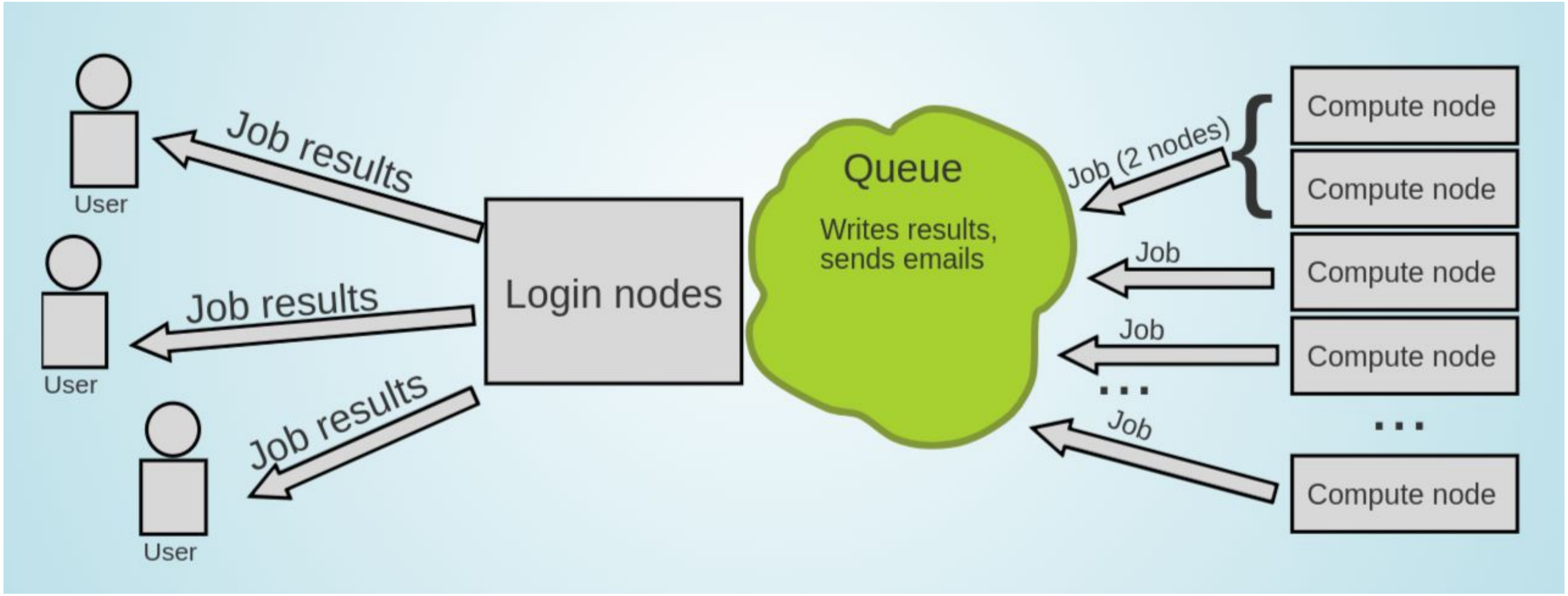
But you don’t use the whole Supercomputer



Enter the queue, and wait

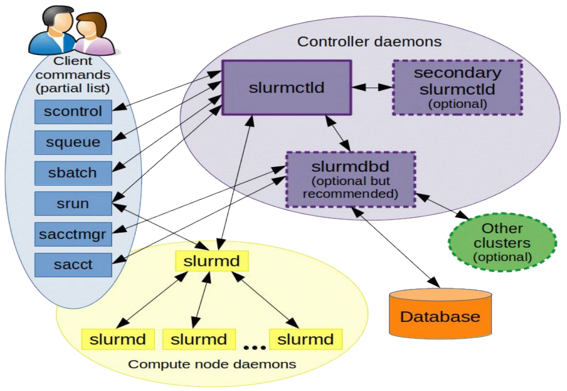
- Your job(s) enter the queue, and wait for its turn
- When there are enough resources for that job, it runs

Results


User
User
User
Job results
Job results
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

SLURM - Workload Manager/Job Scheduler

- **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

Getting Started with Slurm

- To tell Slurm what resources you need, you will have to create an sbatch script/ Slurm script
- The sbatch scripts generally follow this format:

```
#!/bin/bash

# Declaring Slurm Configuration Options

# Loading Software/Libraries

# Running Code
```

- Note: #!/bin/bash above tells our terminal what program to run this file with. In this case, bash.
- You can write an sbatch script in any language as long as #SBATCH doesn't result in errors
- Examples: Ruby, Python, Bash, R.

Configuration Options for Slurm

- There are many configuration options for Slurm
- Some options are cluster specific and may not work
- We can help you find the best set of configurations for your computing needs
- Configuration options are specified in your sbatch script like this:

```
#SBATCH <option_1>=<value>
#SBATCH <option_2>=<value>
...
#SBATCH <option_3>=<value>
```

- Note the pound sign(#) is not the comment here.
- Slurm looks for lines starting with #SBATCH so it can find configuration options

Accounting Configurations

- **Job Name**: `#SBATCH --job-name=<job_name>`
  - First thing you need to do is give your job a name and it should be descriptive
  - Example: `#SBATCH --job-name=RandomWalk`
  - The point of the job name is to remind yourself what you are doing
  - If it is not descriptive, you can easily get confused

- **Comment**: `#SBATCH --comment=<comment>`
  - To extend the description of your job, add a comment
  - Example: `#SBATCH --comment=“To explore the nodes.”`

- **Account**: `#SBATCH --account=<account_name>`
  - You need to tell Slurm which account to run your job under
  - This is not user account, but your project account
  - Example: `#SBATCH --account=glicid`

Accounting Configurations

- **Partition**: `#SBATCH --partition=<Partition_name>`
  - Slurm needs to know which partition to run your job on
  - Example: `#SBATCH --partition=standard`
  - Each partition has access to different resources and has a specific use case

- **Time Limit**: `#SBATCH --time=D-HH:MM:SS`
  - You need to tell Slurm how long your job needs to run
  - The format is Days-Hours:Minutes:Seconds
  - Example: `#SBATCH --time=1-12:30:00` (1 Day, 12 Hours, 30 Minutes, 0 Seconds)

Job Output Configurations

- **Output File**: `#SBATCH --output=%x_%j.out`
  - Any output from your compute job will be saved to the output file that you specify
  - %x is a variable that fills in your job name. %j is a variable that filles in your job ID number
  - Example: `#SBATCH --output=logs/%x_%j.out`

- **Error File**: `#SBATCH --error=%x_%j.err`
  - Any errors from your compute job will be saved to the error file that you specify
  - %x is a variable that fills in your job name. %j is a variable that filles in your job ID number
  - Example: `#SBATCH --error=logs/%x_%j.err`

Node Configurations

- A node is just a computer in a cluster
- Most of the time, it probably makes sense to only use one node

- **Nodes**: `#SBATCH --nodes=<num_nodes>`
  - The default is 1 node, so if you're using 1 node, you don't need to specify it in configuration
  - We recommend that you include it to remind yourself what resources your job is using
  - Example: `#SBATCH --nodes=4`

- **Excluding Nodes**: `#SBATCH --exclude=<node1, node2, …>`
  - If for some reason you want to make sure your job does not run a specific node
  - Example: `#SBATCH --exclude=cnode301`

- **Exclusive Access to a Node**: `#SBATCH --exclusive`
  - If your job can utilize all of the resources on a single node, you can specify it

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

Note: Other than Nautilus, we have Waves and (Philias)MesoNET cluster as well.

Task Configurations

- In the context of computing, a "**job**" and a "**task**" refer to different entities and have distinct meanings

- **Job**:
  - A job is a higher-level unit of work or a computational task that you submit to a cluster
  - It represents a specific computational workload, which can consist of one or more tasks
  - When you submit a job, you provide information about the resources it needs, such as the number of nodes, CPU cores, memory, runtime, etc.
- **Task**:
  - A task is a lower-level unit of work that is part of a job
  - It represents a specific computational operation or process
  - These tasks are typically parallelized to take advantage of the cluster's computing power

For example, if you have a job that needs to perform a large-scale simulation, you might divide the simulation into multiple tasks, each of which can be run on a separate compute node or cores to expedite the computation. Tasks within a job can be parallel or distributed, and they often communicate with each other to complete the overall workload.

Task Configurations

- **Number of Tasks**: `#SBATCH --ntasks=<num_tasks>`
  - By default, Slurm will assign one task per node
  - These tasks can run on the same node or the different nodes
  - Example: `#SBATCH --ntasks=2`

- **Number of Tasks per Node**: `#SBATCH --ntasks-per-node=<num_tasks>`
  - If your job is using multiple nodes, you can specify the number of tasks per node
  - Example: `#SBATCH --ntasks-per-node=2`
  - For instance, if your job is allocated four compute nodes, each node will run two tasks, resulting in a total of eight tasks running in parallel
  - This option is used when you want to control how many tasks are executed on each individual node in your cluster

CPU and GPU Configurations

- **CPUs per Tasks**: `#SBATCH --cpus-per-task=<num_cpus>`
  - By default, Slurm will assign 1 CPU per task if you do not specify in the configuration
  - Slurm needs to know how many CPUs your job needs
  - Example: `#SBATCH --cpus-per-task=4`

- **GPUs per Job**: `#SBATCH --gres=gpu:<gpu_num>`
  - By default, **Slurm will not assign any GPU** to your job
  - You need to specify how many GPUs your job needs
  - Example: `#SBATCH --gres=gpu:4`

Memory Configurations

- **Memory per Node**: `#SBATCH --mem=<memory>`
    - You need to tell Slurm how much memory you need per node
    - Example: To get 10 GB of memory per node, use `#SBATCH --mem=10g`
    - Default is megabytes(MB), so if you specify `#SBATCH --mem=10`, you will be assigned only 10 MB

- **Memory per CPU**: `#SBATCH --mem-per-cpu=<memory>`
    - You can also specify a memory required per CPU core
    - Example: To get 10 GB of memory per CPU, use `#SBATCH --mem-per-cpu=10g`
    - You need to make sure `--mem` and `--mem-per-cpu` don't conflict with each other
    - Default value is 4 GB for cnode301 to cnode340
    - 8 GB for cnode701 to cnode708

Job Scheduling

- When you submit your job, Slurm checks #SBATCH configurations and finds a time/place to run your job
- Four things that impact when you run your job
  - The resources you request
  - The frequency that you submit jobs
  - The other jobs in the queue
  - The maintenance windows (sometimes)

- Note
  - If you request a lot of resources, you'll have to wait until those resources are available
  - If you submit a lot of jobs with a small amount of resources, they'll likely execute quickly

Job Speed

- **Using GPUs may or may not result in a speedup for your job**
- There are a lot of factors in play when it comes to GPUs
  - Your code needs to be able to use GPUs
  - Not all libraries can leverage GPUs, make sure you read the documentation of libraries/frameworks
  - If using multiple GPUs, make sure your code can use GPUs on different nodes
  - Some code can leverage GPUs, but not in an impactful way
  - Some code just isn't doing enough computations to make it with the overhead of communicating between CPUs and GPUs, it may actually slow down your job

Example Slurm Script

```
#!/bin/bash

#SBATCH --job-name=myjob              # Name for your job
#SBATCH --comment="Run My Job"        # Comment for your job
#SBATCH --output=%x_%j.out            # Output file
#SBATCH --error=%x_%j.err             # Error file

#SBATCH --time=0-00:05:00             # Time limit
#SBATCH --nodes=1                     # How many nodes to run on
#SBATCH --ntasks=2                    # How many tasks per node
#SBATCH --cpus-per-task=2             # Number of CPUs per task
#SBATCH --mem-per-cpu=10g             # Memory per CPU
#SBATCH --qos=short                   # priority/quality of service

hostname                              # Run the command hostname
```

- Submitting Your Job

```
$ sbatch my-job.slurm
$ sbatch -M nautilus --reservation=training my-job.slurm
Submitted batch job 1411747 on cluster nautilus
```

So, in this example, we have requested a job with the following dimensions:

- **Max Run Time:** 5 Minutes
- **Number of Nodes:** 1
- **Number of Tasks Per Node:** 2
- **Number of CPUs Per Task:** 2
- **Memory Per CPU:** 10GB

Monitoring Your Job

- Monitoring Your Job

```
$ ls
myjob_1411747.err  myjob_1411747.out  my-job.slurm
```

```
$ scontrol show job 1411747 -M nautilus
```

```
$ scancel 1411747
```

Monitoring Your Job

- Monitoring Your Job

```
$ squeue -u $USER
```

```
CLUSTER: nautilus
    JOBID PARTITION                                NAME         USER ST             TIME  NODES QOS         PRIORITY NODELIST(REASON)

CLUSTER: waves
    JOBID PARTITION                                NAME         USER ST             TIME  NODES QOS         PRIORITY NODELIST(REASON)
```

Data Management - Compress/Decompress Large Files

- Compress

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

- Decompress

```
$ tar -xzvf <folder_name.tar.gz>
```

Data Management: File Transfer

- 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.

Hands-on: TP 1

- Submit your first job!
  - Download “nautilus-tutorial” → https://indico.mathrice.fr/event/498/manage/attachments/
  - Compress and transfer this folder to this location using SCP → /scratch/nautilus/users/username
  - Connect to cluster
  - Open a text editor and write a slurm script that will run the “hostname” command
  - Submit the job
  - Monitor your job

Reference: https://mirjunaid26.github.io/docs/tutorial-basics/slurm

Monitoring Your Job

- squeue
    - The squeue command will show what jobs are currently scheduled

```
$ squeue
CLUSTER: nautilus
    JOBID PARTITION                           NAME         USER ST         TIME  NODES QOS         PRIORITY
NODELIST(REASON)
  1443980       all                Exchange_Second nassaad2017@ PD         0:00      1 short          37307 (Dependency)
1443979_[       all                      Advection nassaad2017@ PD         0:00      1 short          37307 (Dependency)
  1443978       all                 Exchange_First nassaad2017@  R         0:05      1 short          37307 cnode321
  1439197       all                       edw_wave adermatis202  R        25:12      1 medium         37026 cnode324
  1439000       all                       edw_wave adermatis202  R        26:02      1 medium         37026 cnode321
  1430806       all                       edw_wave adermatis202  R      1:09:23      1 medium         37026 cnode323
  1440954       all                     SnappyMesh ahernandez20  R        16:05      1 medium         36825 cnode325
  1441150       all diff_284_29_Tdiv580_moreRefin_ sakkari2022@  R        15:15      1 medium         36624 cnode325
  1406284       all      diff_300_46_Tdiv600_check sakkari2022@  R      3:24:53      1 medium         36624 cnode324
  1349601       all  diff_284_29_Tdiv580_moreRefin sakkari2022@  R     18:39:15      1 medium         36624 cnode322
  1308984       all      diff_400_46_Tdiv800_check sakkari2022@  R   1-03:07:33      1 medium         36624 cnode321
  1405888       all                    train_model melaarabi202  R      3:26:58      1 long           27508 gnode1
  1404124  standard                 test_stability jlopez@ec-na  R      4:00:14      1 long           23725 cnode323

CLUSTER: waves
    JOBID PARTITION                           NAME         USER ST         TIME  NODES QOS         PRIORITY
NODELIST(REASON)
```

Monitoring Your Job

- The squeue command gives us the following information:
    - JOBID: The unique ID for your job
    - PARTITION: The partition your job is running on (or scheduled to run on)
    - NAME: The name of your job
    - USER: The username for whomever submitted the job
    - ST: The status of the job. The typical status codes you may see are:
        - CD (Completed): Job completed successfully
        - CG (Completing): Job is finishing, Slurm is cleaning up
        - PD (Pending): Job is scheduled, but the requested resources aren’t available yet
        - R (Running): Job is actively running TIME: How long your job has been running
    - TIME: How long your job has been running
    - NODES: How many nodes your job is using
    - QOS: Quality of Service
    - PRIORITY: Priority of your job
    - NODELIST(REASON): List of nodes and which nodes your job is running on (or scheduled to run on). If your job is not running yet, you will also see reason

Partition Information

- sinfo
  - available partitions on the cluster and partitions time limit
  - how many nodes are available on the partition and what is the state of those nodes

```
$ sinfo
CLUSTER: nautilus
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
standard     up   infinite      5    mix cnode[321-325]
standard     up   infinite     35   idle cnode[301-320,326-340]
bigmem       up   infinite      1  down* cnode707
bigmem       up   infinite      7   idle cnode[701-706,708]
gpu          up   infinite      1    mix gnode1
gpu          up   infinite      3   idle gnode[2-4]
visu         up   infinite      4   idle visu[1-4]
all*         up   infinite      1  down* cnode707
all*         up   infinite      6    mix cnode[321-325],gnode1
all*         up   infinite     49   idle cnode[301-320,326-340,701-706,708],gnode[2-4],visu[1-4]

CLUSTER: waves
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
all*         up    9:00:00      1   unk* budbud018
all*         up    9:00:00      8   idle budbud[014-017,019-022]
med          up 4-04:00:00      3   idle budbud[020-022]
devel        up      20:00      1   unk* vmworker-001
```

- Try `sinfo -N`

Track Your Jobs

- sacct
  - Track your recent jobs to find their job IDs and other details

```
$ sacct
JobID           JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
1404103           myjob   standard     glicid          1  COMPLETED      0:0
1404103.bat+      batch                glicid          1  COMPLETED      0:0
1404103.ext+     extern                glicid          1  COMPLETED      0:0
1419267           myjob        all     glicid          4  COMPLETED      0:0
1419267.bat+      batch                glicid          4  COMPLETED      0:0
1419267.ext+     extern                glicid          4  COMPLETED      0:0
```

- To view a specific job

```
$ sacct --jobs=1411747
JobID           JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
1419267           myjob        all     glicid          4  COMPLETED      0:0
1419267.bat+      batch                glicid          4  COMPLETED      0:0
1419267.ext+     extern                glicid          4  COMPLETED      0:0
```

Check Job State

- scontrol
    - To check job state, start time/end time, command, workdir, stderr, stdout

```
$ scontrol show job 1411747 -M nautilus
JobId=1446614 JobName=myjob
   UserId=jmir@ec-nantes.fr(8000019) GroupId=jmir@ec-nantes.fr(8000019) MCS_label=N/A
   Priority=45942 Nice=0 Account=glicid QOS=short
   JobState=COMPLETED Reason=None Dependency=(null)
   Requeue=1 Restarts=0 BatchFlag=1 Reboot=0 ExitCode=0:0
   RunTime=00:00:00 TimeLimit=00:05:00 TimeMin=N/A
   SubmitTime=2023-10-17T14:40:47 EligibleTime=2023-10-17T14:40:47
   AccrueTime=2023-10-17T14:40:47
   StartTime=2023-10-17T14:40:47 EndTime=2023-10-17T14:40:47 Deadline=N/A
   SuspendTime=None SecsPreSuspend=0 LastSchedEval=2023-10-17T14:40:47 Scheduler=Backfill
   Partition=all AllocNode:Sid=nautilus-devel-001:883696
   ReqNodeList=(null) ExcNodeList=(null)
   NodeList=cnode321
   BatchHost=cnode321
   NumNodes=1 NumCPUs=4 NumTasks=2 CPUs/Task=2 ReqB:S:C:T=0:0:*:*
   TRES=cpu=4,node=1,billing=4
   Socks/Node=* NtasksPerN:B:S:C=0:0:*:* CoreSpec=*
   MinCPUsNode=2 MinMemoryCPU=10G MinTmpDiskNode=0
   Features=(null) DelayBoot=00:00:00
   OverSubscribe=OK Contiguous=0 Licenses=(null) Network=(null)
   Command=/scratch/users/jmir@ec-nantes.fr/nautilus-tutorial/task_1/my-job.slurm
   WorkDir=/scratch/users/jmir@ec-nantes.fr/nautilus-tutorial/task_1
   Comment=Run My Job
   StdErr=/scratch/users/jmir@ec-nantes.fr/nautilus-tutorial/task_1/myjob_1446614.err
   StdIn=/dev/null
   StdOut=/scratch/users/jmir@ec-nantes.fr/nautilus-tutorial/task_1/myjob_1446614.out
   Power=
```

Job Priority Factors

- Slurm takes into account two different factors when scheduling jobs:
  - Requested Resources and Priority
  - If you request a lot of resources, your job may take longer to start than someone who requests very few resources because Slurm needs to wait for the resources you requested to be available
  - If you are constantly submitting and running jobs, Slurm may assign your jobs a lower priority than someone who rarely submits jobs.

```
Job_priority =
site_factor +
(PriorityWeightAge) * (age_factor) +
(PriorityWeightAssoc) * (assoc_factor) +
(PriorityWeightFairshare) * (fair-share_factor) +
(PriorityWeightJobSize) * (job_size_factor) +
(PriorityWeightPartition) * (priority_job_factor) +
(PriorityWeightQOS) * (QOS_factor) +
SUM(TRES_weight_cpu * TRES_factor_cpu,
    TRES_weight_<type> * TRES_factor_<type>,
    ...) - nice_factor
```

Job Priority Factors

- Nine factors in the Multifactor Job Priority plugin that influence job priority:
  - **Age**: the length of time a job has been waiting in the queue, eligible to be scheduled
  - **Association**: a factor associated with each association
  - **Fair-share**: the difference between the portion of the computing resource that has been promised and the amount of resources that has been consumed
  - **Job size**: the number of nodes or CPUs a job is allocated
  - **Nice**: a factor that can be controlled by users to prioritize their own jobs
  - **Partition**: a factor associated with each node partition
  - **QOS**: a factor associated with each Quality Of Service
  - **Site**: a factor dictated by an administrator or a site-developed job_submit or site_factor plugin
  - **TRES**: each TRES Type has its own factor for a job which represents the number of requested/allocated TRES Type in a given partition

Priorities in GLiCID Cluster

- sacctmgr
  - To view or modify Slurm account information

```
$ 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
```

Different Resource Scenarios

Here is a summary of different resource utilization scenarios:

- **RAM**:
  - Request too little: Job will die when it runs out of RAM
  - Request too much: Lots of RAM will sit idle and no one else can use it
  - *Ideal:* Request slightly more RAM than you need
  - Recommendation: Try to keep idle RAM at less than 10% of the total RAM you requested
- **CPUs**:
  - Request too little: Your job will trip over itself because of kernel scheduling; your job will take a massive performance hit as a result
  - Request too much: Lots or CPUs will sit idle and no one else can use them
  - *Ideal:* Request exactly the number of CPUs that your job can use

Different Resource Scenarios

- **GPUs**:
  - Request too little: You may not actually see a speedup (due to communication overhead between CPUs and GPUs)
  - Request too much: Your code may not be able to use multiple GPUs; idle GPUs cannot be used by anyone else until your job finishes
  - *Ideal:* Request exactly the number of GPUs that your job can use
  - Recommendation: Get your job working with one GPU, and make sure you're actually using the GPU before trying to use more
- **Time**:
  - Request too little: Your job will not finish before the time limit runs out; lots of time will be wasted
  - Request too much: Slurm may give your job a lower priority to let smaller jobs go first. If a maintenance window is coming up, your job may not schedule until after the maintenance window
  - *Ideal:* Request slightly more time than you need, but not too much

Parallel Programming Examples using Slurm

Parallel programming on a cluster can be challenging, but it is a powerful technique for harnessing the computational resources of a cluster effectively.

- Some reasons why parallel programming can be tricky on a cluster:
  - Distributed computing, load balancing, synchronization, communication overhead, debugging and troubleshooting, scalability, heterogeneous resources
- To overcome these challenges, developers often use parallel programming libraries,
  - such as MPI (Message Passing Interface) for distributed memory systems and
  - OpenMP for shared memory systems
- These libraries provide abstractions and tools for handling parallelism, communication, and synchronization
- Additionally, understanding the architecture of the cluster and the specifics of the job scheduler (e.g., Slurm) can be crucial for resource allocation and job management

Example 1: Intel/IntelMPI

Sample Script: `job-intel.slurm`

```
#!/bin/bash
#SBATCH --job-name=HelloWorldMpi
#SBATCH --partition=standard
#SBATCH --ntasks=4

module purge
module load intel/compiler intel/mpi

export I_MPI_PMI_LIBRARY=/lib64/libpmi2.so
export I_MPI_COLL_EXTERNAL=0
export I_MPI_ADJUST_BCAST=0
export I_MPI_FABRICS=shm:ofi
export FI_PROVIDER=psm3

srun --mpi=pmi2 hello-mpi
```

Example 1: Intel/IntelMPI

- Intel Compiler and IntelMPI

```
$ module load intel/compiler intel/mpi
$ mpicxx -cxx=icpx -O3 -o hello-mpi hello-mpi.cpp
```

- Submit your slurm script

```
$ sbatch -M nautilus -p standard -q short job-intel.slurm
```

Example 2: GNU/OpenMPI

Sample script: `job-mpi.slurm`

```
#!/bin/bash
#SBATCH --job-name=HelloWorldMpi
#SBATCH --partition=standard
#SBATCH --ntasks=4

module purge
module load gcc openmpi/ucx/4.1.5_gcc_8.5.0_ucx_1.14.1_rdma_46.0

export UCX_WARN_UNUSED_ENV_VARS=n
export OMPI_MCA_btl=^openib
export UCX_NET_DEVICES=mlx5_2:1

srun ./hello-openmpi
```

Example 2: GNU/OpenMPI

- GNU Compiler and OpenMPI
  - `module load gcc openmpi/ucx/4.1.5_gcc_8.5.0_uxc_1.14.1_rdma_46.0`
  - `mpicxx -O3 -o hello-openmpi hello-mpi.cpp`

- Submit your slurm script

```
$ sbatch -M nautilus -p standard -q short job-mpi.slurm
```

Example 3: GNU/OpenMP

Sample script → job-omp.slurm

```
#!/bin/bash
#SBATCH --job-name=HelloWorldOmp
#SBATCH --partition=standard
#SBATCH --cpus-per-task=12

module purge
module load gcc

if [[ "${SLURM_CPUS_PER_TASK}" ]]
then
  c=${SLURM_CPUS_PER_TASK}
else
  c=1
fi

export OMP_NUM_THREADS=$c
srun ./hello-omp
```

Example 3: GNU/OpenMP

- GNU Compiler and OpenMP
  - `module load gcc`
  - `g++ -fopenmp -o hello-omp hello_omp.cpp`

- Submit your slurm script

```
$ sbatch -M nautilus -p standard -q short job-omp.slurm
```

Example 4: GNU/hybrid OpenMPI/OpenMP

Sample script: job-hybrid.slurm

```
#!/bin/bash
#SBATCH --job-name=HelloWorldHybrid
#SBATCH --partition=standard
#SBATCH --cpus-per-task=6
#SBATCH --ntasks=16

module purge
module load gcc openmpi/ucx/4.1.5_gcc_8.5.0_ucx_1.14.1_rdma_46.0

export UCX_WARN_UNUSED_ENV_VARS=n
export OMPI_MCA_btl=^openib
export UCX_NET_DEVICES=mlx5_2:1

if [[ "${SLURM_CPUS_PER_TASK}" ]]
then
  c=${SLURM_CPUS_PER_TASK}
else
  c=1
fi

export OMP_NUM_THREADS=$c
srun ./hello-hybrid
```

Example 4: GNU/OpenMP

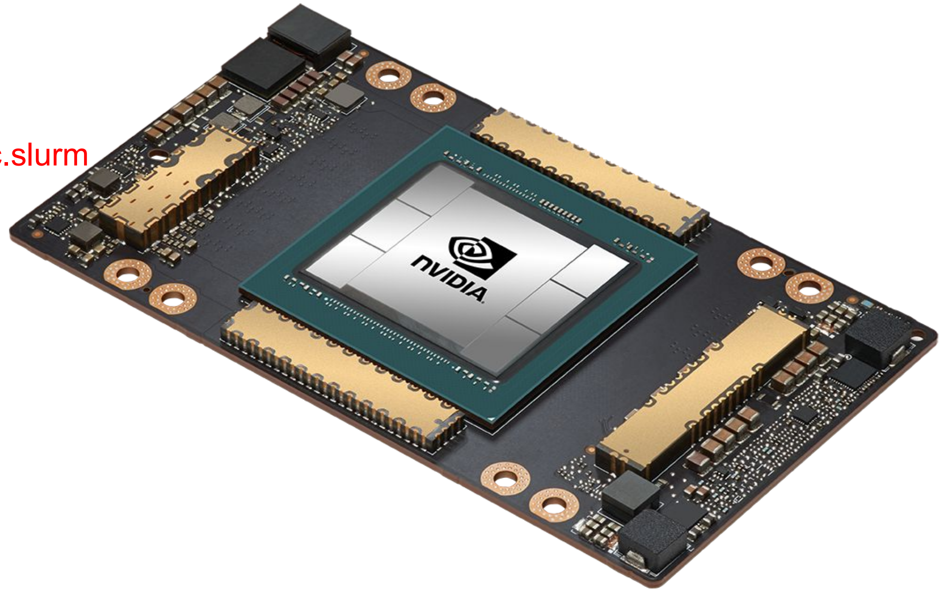
- GNU Compiler and OpenMP
  - `module load gcc openmpi/ucx/4.1.5_gcc_8.5.0_uxc_1.14.1_rdma_46.0`
  - `mpicxx -fopenmp -o hello-hybrid hello-mpi-omp.cpp`

- Submit your slurm script

```
$ sbatch -M nautilus -p standard -q short job-hybrid.slurm
```

Test GPU: Vector Multiplication of 2 billion elements

- Test Example Demo (commands for this particular session only as we have reserved GPU)
- Load Module
  - `module load nvhpc/23.9`
- To compile
  - `nvc++ -o dp_acc -O3 -acc  dp_acc.cpp`
- To submit job
  - `sbatch -M nautilus --reservation=training run_acc.slurm`
- To monitor
  - `ssh gnode1`
  - `nvidia-smi -l 1`



Hands-on: TP 2

- Create a Slurm script for any of the above 4 examples
  - Submit your job
  - Monitor your job

Micromamba/Anaconda

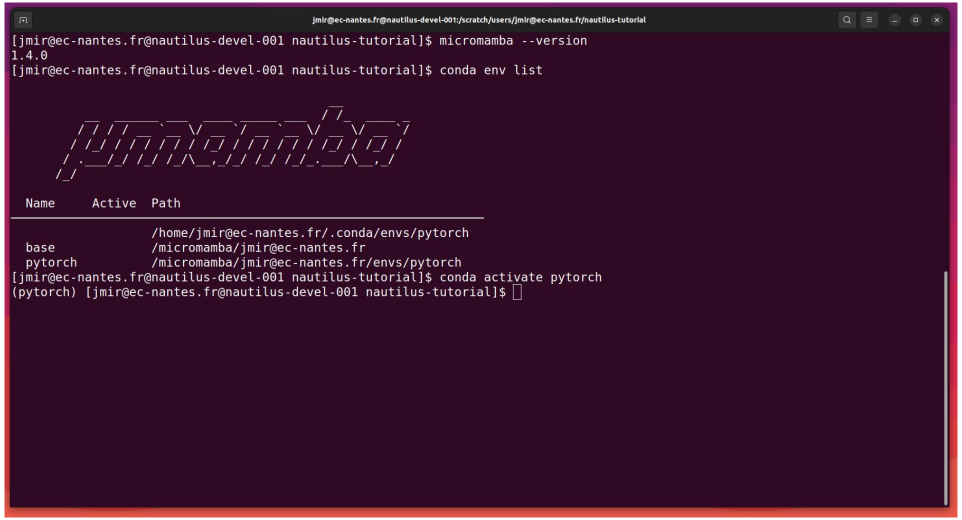
- No Anaconda module for now
- But you can use Micromamba - lighter version of conda

```
# Download micromamba
mkdir -p $HOME/.local/bin
wget -P $HOME/.local/bin https://s3.glicid.fr/pkgs/micromamba
chmod u+x $HOME/.local/bin/micromamba

# Initilize micromamba
$HOME/.local/bin/micromamba -r /micromamba/$USER/ shell init --shell=bash
--prefix=/micromamba/$USER/

# [OPTIONAL] Add a `conda` alias
echo -e '\n\n#Alias conda with micromamba\nalias conda=micromamba' >> ~/.bashrc

# Recharger le .bashrc
source ~/.bashrc
```

- Source: https://doc.glicid.fr/GLiCID-PUBLIC/0/logiciels/logiciels.html

Micromamba/Anaconda

```
$ micromamba --version
$ conda create --name myenv
$ conda env list
$ conda activate myenv
$ conda install numpy
$ conda list
$ conda deactivate
```


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

```
[jmir@ec-nantes.fr@nautilus-devel-001 nautilus-tutorial]$ micromamba --version
1.4.0
[jmir@ec-nantes.fr@nautilus-devel-001 nautilus-tutorial]$ conda env list

                                           __
          __  ______ ___  ____ _____ ___  / /_  ____ _
         / / / / __ `__ \/ __ `/ __ `__ \/ __ \/ __ `/
        / /_/ / / / / / / /_/ / / / / / / /_/ / /_/ /
       / .___/_/ /_/ /_/\__,_/_/ /_/ /_/_.___/\__,_/
      /_/

  Name      Active  Path
────────────────────────────────────────────────────────────────
                    /home/jmir@ec-nantes.fr/.conda/envs/pytorch
  base              /micromamba/jmir@ec-nantes.fr
  pytorch           /micromamba/jmir@ec-nantes.fr/envs/pytorch
[jmir@ec-nantes.fr@nautilus-devel-001 nautilus-tutorial]$ conda activate pytorch
(pytorch) [jmir@ec-nantes.fr@nautilus-devel-001 nautilus-tutorial]$ 
```

Hands-on: TP 3

- Install Micromamba and check version
- Create a Conda environment and check environment list
- Try to install numpy and check installed packages

Hands-on: TP4_Fortan

- Load gcc compiler and compile

```
$ module load gcc/13.1.0
$ gfortran hello-fortran.f90 -o hello
```

- Submit your slurm script

```
$ sbatch -M nautilus -p standard -q short my-job.slurm
```

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 help@glicid.fr

Chat: On CLAM website

Admins: tech@glicid.fr

Forum: Coming soon

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