HPC School - Beginner

S2 - Work on the ULHPC

High Performance Computing & Big Data Services

hpc.uni.lu

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@ULHPC

LUXEMBOURG
LET'S MAKE IT HAPPEN

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Outline

- When can the ULHPC help me?
- How a cluster works?
- Types of workers
- Types of jobs
- Partitions and QoS
- Modules
- Monitoring your jobs
- Storage
- Learn more by yourself

When can the ULHPC help me?

Embarrassingly parallel jobs

This is when you have a lot of similar jobs to run. Maybe running one job on your laptop is fine but 10000 jobs would take too long.

Multi threaded applications

Laptop / work machines usually have 2 to 16 cores. If what you run can take advantage (compute multiple things at the same time by distributing computation on the available cores), then you could benefit from our nodes, ranging from 28 to 128 cores.

When can the ULHPC help me?

Not enough memory on my machine

Laptop / work machines usually have between 8G to 32G or RAM. This may be too small for your experiments. We have nodes from 128G to 3000G of RAM.

Multi node (computer) application

Sometime, even one big node is not enough. Our cluster allows you to run jobs up to 64 nodes per job. On AION this means 8192 cores and 16T of RAM.

Not enough storage

The ULHPC benefits from several storage services for a total of 10PB (10 000 TB)

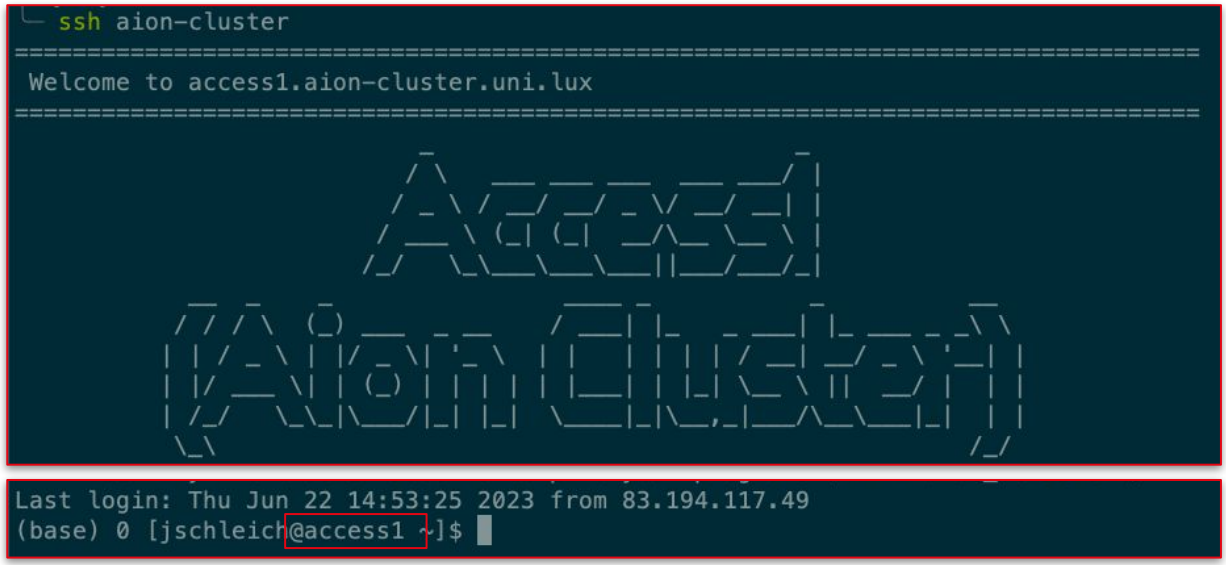
How a cluster works?

- You first access a cluster via its **access node**
- You then use **worker nodes** to compute your jobs
- Access nodes
  - Servers on which you “land” when you connect on the cluster
  - Can be used **to request resources**
  - **Should not be used to compute things**
  - Application programs via module are not available
- Worker nodes
  - Servers on which computation should be run
  - When you request some resources from the access nodes, the resources are from the worker nodes
  - Several types of worker nodes at ULHPC (discussed in detail later)

How a cluster works?

Example:

- **You connect on AION, you are now on an access node**
- For your work, you need 64 cores / 128G of RAM
- You request those resources from the access node
- When available, you land on the machine on which the resources you received are located



How a cluster works?

Example:

- You connect on AION, you are now on an access node
- **For your work, you need 64 cores / 128G of RAM**
- **You request those resources from the access node**
- **When available, you land on the machine on which the resources you received are located**

```
0 [jschleich@access1 ~]$ si -c64
# salloc -p interactive --qos debug -C batch  -c64
salloc: Granted job allocation 803494
salloc: Waiting for resource configuration
salloc: Nodes aion-0041 are ready for job
(base) 0 [jschleich@aion-0041 ~](803494 1N/T/1CN)$
```

Types of worker nodes at ULHPC

Currently the ULHPC offers the following types of resources:

CPU nodes

- Recommended for most usages
- Large number of nodes

GPU nodes

- Nodes with graphic card accelerators
- More and more tools take advantage of GPUs
- **Limited** number of nodes

Bigmem nodes

- Recommended when a tool has huge memory requirements which cannot be distributed over multiple nodes
- **Very limited** number of nodes

Types of worker nodes at ULHPC

Currently the ULHPC offers the following types of resources:

CPU nodes

- AION: **354 nodes**, each node has 128 cores and 256G of RAM
- IRIS: **168 nodes**, each node has 28 cores and 128G of RAM

GPU nodes

- IRIS: **18 nodes,** each node has 28 cores and 768G of RAM and 4 NVIDIA V100 with 16G
- IRIS: **6 nodes**, each node has 28 cores and 768G of RAM and 4 NVIDIA V100 with 32G

Bigmem nodes

- IRIS: **4 nodes**, each node has 112 cores and 3T RAM

Types of worker nodes at ULHPC - pricing

Currently the ULHPC offers the following types of resources:

CPU nodes

- AION (CPU - regular) : 0.0097€ per core-hour
- IRIS (CPU - small) : 0.0089€ per core-hour

GPU nodes

- IRIS (GPU): 1.25€ per GPU-hour

Bigmem nodes

- IRIS (CPU - big mem): 0.0535€ per core-hour

Documentation: https://hpc-docs.uni.lu/policies/usage-charging/#compute

Types of worker nodes at ULHPC - pricing

Note 1: core-hour and GPU-hour do not imply that we will charge one full hour at the first second of the job. We consider the job duration with a

Note 2: regarding the RAM of a job, if you do not override the default behaviour, you will receive a percentage of the RAM corresponding to the amount of requested cores, e.g, 128G of RAM for the 64 cores on an AION CPU node (50% of a CPU - regular node). If you override the default behaviour and request more RAM, we will re-compute the equivalent number of cores, e.g. if you request 256G of RAM and 64 cores, we will charge 128 cores.

Note 3: on GPU nodes, there are 4 GPUs, 28 cores and 768G of RAM. This means that for each GPU, you can have up to **7 cores** and 192G of RAM. If you request more than those default, we will re-compute the GPU equivalent, e.g. if you request 1 GPU and 8 cores, we will charge 2 GPUs.

Documentation: https://hpc-docs.uni.lu/policies/usage-charging/#compute

Types of jobs

Two types of jobs:

- interactive jobs
- batch jobs

Interactive: when you receive the resources you can type commands in an interactive fashion and see the results. This is adapted to debugging / trial and errors.

Batch: you submit the commands you wish to be executed and you specify the resources. When the resources are available, your commands are executed automatically. This type of job is adapted to run campaigns of experiments.

Interactive jobs

Request an interactive job

- `si` for CPU nodes
- `si-gpu` for GPU nodes (on the IRIS cluster only)
- `si-bigmem` for bigmem nodes (on the IRIS cluster only)

Important parameters

- `-t` to specify the duration. 30 min is the default, 120 min is the max
- `-c` to specify the number of cores. 1 by default.
- add `-A=your-project-name` to specify which project to charge

Example: `si -c8 -t120 -A=your-project-name` request a 2 hours interactive session with 8 cores on a CPU node

Note: if you use less than 120 minutes, you will not be charged for 120 but for the time you used your session

Interactive jobs

Multiple jobs can run on each node, from multiple users. How are the resources shared?

Example 1

- A user wants 64 cores on an AION node
- Reminder: each AION node has 128 cores and 256G of RAM
- If the user enters `si -c64`, that user will have half the available cores and will automatically receive half the RAM: 64 cores and 128G of RAM.
- It means 1 AION core → 2G of RAM

Example 2

- A user wants 1 core on an IRIS node:
- Reminder: each IRIS CPU node has 28 cores and 128G of RAM
- The user will receive 1/28th of 128G of RAM, roughly 4G

Note: IRIS and AION CPU nodes have a different RAM per core ratio

Interactive jobs

Multiple jobs can run on each node, from multiple users. How are the resources shared?

Example 3

- A user wants 1 GPU to run some experiment
- On a GPU node, you also have CPU cores and RAM
- **All of those resources are linked together**
- Reminder: each GPU node has
  - 28 cores
  - 768G of RAM
  - 4 NVIDIA V100
- `si-gpu -c7` will lead to: 1 GPU, 7 CPU cores and 7/28th (¼) of the 768G of RAM

Note: requesting more than 7 CPU cores could lead to some GPUs to not be allocable for other users by Slurm. Please think about this when using GPU nodes. In case of doubt, contact the support.

Batch jobs

Submit a batch job

- Use the sbatch command, usually, `sbatch some-script.sh`
- add `-A=your-project-name` to specify which project to charge or add the parameter in the script
- The script contains:
  - A first section containing Slurm parameters (what resources you want, for how long…).
  - A second section containing what your job should do with those resources
- This script is usually referred as the **launcher script**
- We maintain launcher script templates for various use cases, see documentation

Batch jobs

Submit a batch job

- First line is mandatory for scripts
- #SBATCH parameters specify your job characteristics. Here we request 16 cores for 5 minutes on the batch partition (CPU)
- Anything after #SBATCH is what should be executed on the allocated resources. Here, we execute a Python script.

```
1 #!/bin/bash -l
2 #SBATCH -c 16
3 #SBATCH --time=0-00:05:00
4 #SBATCH -p batch
5
6 module load lang/Python/3
7
8 python my-script.py
9
```

📚Documentation about SBATCH options: https://hpc-docs.uni.lu/slurm/#job-submission-options

Charge jobs to a projet

Terminology

- In the Slurm terminology, user can be associated to one or several accounts
- For LIST users, each account represent one project
- You can check to which project you can charge your jobs by using the `acct your-username`
- You can specify which project to charge with the `-A` or `--account` parameter
- If you do not specify it, your default project will be charged

```
0 [jschleich@access2 ~]$ acct jschleich
# sacctmgr show user where name="jschleich" format=user%15,account%20,DefaultAccount%20,share,qos%50 withassoc
           User              Account           Def Acct     Share                                                QOS
--------------- -------------------- -------------------- --------- --------------------------------------------------
      jschleich                ulhpc                ulhpc         1 admin,besteffort,debug,high,long,low,normal,urgen+
      jschleich       pascal.bouvry                ulhpc         1                   besteffort,debug,long,low,normal
      jschleich       pascal.bouvry                ulhpc         1                   besteffort,debug,long,low,normal
      jschleich                ulhpc                ulhpc         1 admin,besteffort,debug,high,long,low,normal,urgen+

# ==> jschleich Default account: ulhpc
```

Number of tasks and core per task

Slurm tasks?

- In our documentation you will come across the notion of Slurm task
- In our launcher templates you will see `-n` or `--n-tasks-per-node`
- For most use case, do not use it or set it to 1
- If your application does not support multi-node computation → 1 task
- There are exceptions, in case of doubt, please contact your support

Note: if your app is not fast enough, do not increase -n as an attempt to speed up the computation: it will allocate more resources but they will likely not be used

What are partitions?

Partitions

In Slurm multiple nodes can be grouped into partitions which are sets of nodes aggregated by shared characteristics.

You will find on ULHPC resources the following partitions:

- **batch** is intended for running parallel scientific applications as passive jobs on CPU nodes
- **gpu** is intended for running GPU-accelerated scientific applications as passive jobs on "gpu" nodes
- **bigmem** is dedicated for memory intensive data processing jobs on "bigmem" nodes
- **interactive**: a floating partition intended for interactive jobs

Partitions

Partitions

In Slurm multiple nodes can be grouped into partitions which are sets of nodes aggregated by shared characteristics.

Type	Default/MaxTime	MaxNodes (per job)
interactive	30min - 2h	2
batch (cpu)	2h-48h	64
gpu	2h-48h	4
bigmem	2h-48h	1

Question:

- What is the maximum amount of GPUs you can use for one single job?
- Can you use the interactive partition to test a program over 10 nodes?

QoS

QoS (Quality of Service)
Quality of Service or QOS is used to constrain or modify the characteristics that a job can have.
For example: l**onger run time** or a **high priority queue** for a given job

Interesting QoS

- **long**: for longer jobs, max **4** (running) jobs per user (simplification), up to **14** days
- **besteffort**: a preemptible (your jobs can be killed when the cluster is too busy with other normal jobs and restarted when resources are available again), max **100** (running) jobs per user (simplification), up to **50** days

You can type `sqos` to learn about all existing QoS and their restrictions

QoS

Type	Max # of running jobs	Max duration
normal	50	2 days
long	4 per users, 6 per user group	14 days
best effort	100	50 days

QoS

Example: submit a long job

```
sbatch --qos long my-script.sh
```

Example: submit a besteffort job

```
sbatch --qos besteffort my-script.sh
```

📚Documentation: https://hpc-docs.uni.lu/jobs/long/#long-jobs

Software on ULHPC

There are plenty of way to run software on the ULHPC:

- Modules (see next slides)
- Conda → check our tutorial
- Containers → check our tutorial
- Use Jupyter Notebook, Abaqus CAE, Matlab or Stata via a GUI → check our portal
- Compile your own program → too advanced for this tutorial

Note

The portal is only accessible from the UL network (or via the UL VPN)

Modules

Modules

- The ULHPC proposes and maintain software via modules.
- Pre-installed software, multiple version of the same software can co-exist
- Workflow: search modules, load them, use them
- **Only available on worker nodes**: you will see an error if you try to use the module command on an access node.

📚Documentation: https://hpc-docs.uni.lu/environment/modules/

Modules

Module search

`module av the-program-you-want`

On the right, we search with the keyword “Python”. The list of results contains various elements which are sorted by category (e.g. chem = Chemistry, lang = Programming languages, …)

We can see that two version of the Python language are available: 2.7.18 and 3.8.6. If no version is specified, the default choice (D) will be assumed, here 3.8.6.

```
[jschleich@iris-056 ~](3174323 1N/T/1CN)$ module av Python

-------------- /opt/apps/resif/iris-rhel8/2020b/broadwell/modules/all ----
 bio/TopHat/2.1.2-GCC-10.2.0-Python-2.7.18
 chem/spglib-python/1.16.0-foss-2020b
 chem/spglib-python/1.16.0-intel-2020b              (D)
 devel/flatbuffers-python/1.12-GCCcore-10.2.0
 devel/pkgconfig/1.5.1-GCCcore-10.2.0-python
 devel/protobuf-python/3.14.0-GCCcore-10.2.0
 lang/Python/2.7.18-GCCcore-10.2.0
 lang/Python/3.8.6-GCCcore-10.2.0                   (D)
 lang/SciPy-bundle/2020.11-foss-2020b-Python-2.7.18
 lib/Boost.Python/1.74.0-GCC-10.2.0

Where:
 D:  Default Module
```

📚Documentation: https://hpc-docs.uni.lu/environment/modules/

Modules

Module list

List the currently loaded modules

```
module list
```

Module load

```
module load the-program-you-want
```

Module purge

Unload all loaded modules

```
module purge
```

```
0 [jschleich@iris-056 ~](3174323 1N/T/1CN)$ module list
No modules loaded
0 [jschleich@iris-056 ~](3174323 1N/T/1CN)$ module load lang/Python
0 [jschleich@iris-056 ~](3174323 1N/T/1CN)$ module list

Currently Loaded Modules:
  1) compiler/GCCcore/10.2.0              7) lang/Tcl/8.6.10-GCCcore-10.2.0
  2) lib/zlib/1.2.11-GCCcore-10.2.0       8) devel/SQLite/3.33.0-GCCcore-10.2.0
  3) tools/binutils/2.35-GCCcore-10.2.0   9) tools/XZ/5.2.5-GCCcore-10.2.0
  4) tools/bzip2/1.0.8-GCCcore-10.2.0    10) math/GMP/6.2.0-GCCcore-10.2.0
  5) devel/ncurses/6.2-GCCcore-10.2.0    11) lib/libffi/3.3-GCCcore-10.2.0
  6) lib/libreadline/8.0-GCCcore-10.2.0  12) lang/Python/3.8.6-GCCcore-10.2.0



0 [jschleich@iris-056 ~](3174323 1N/T/1CN)$ module purge
0 [jschleich@iris-056 ~](3174323 1N/T/1CN)$ module list
No modules loaded
```

📚Documentation: https://hpc-docs.uni.lu/environment/modules/

Monitor your jobs

Why monitor your jobs?

- Check the status of your jobs
- For each job, check its progression
- Ensure ULHPC resources are used efficiently

Monitor your jobs

Monitor your jobs - check the status of your jobs

To see the full list of your jobs and their current status, you can use: `sq`

In this example you see jobs of random user. The ST column means status and you can see jobs which are PD (pending, i.e. not yet started) and jobs which are R (running).

```
(base) 0 [jschleich@access1 ~]$ squeue -u djoubaud
   JOBID PARTIT       QOS                NAME       USER NODE  CPUS ST         TIME    TIME_LEFT PRIORITY NODELIST(REASON)
846027_[  batch    normal   DatasetsGeneration   djoubaud    1     4 PD         0:00   1-23:59:00    11410 (QOSMaxJobsPerUserLimit)
846037_[  batch    normal   DatasetsGeneration   djoubaud    1     4 PD         0:00   1-23:59:00    11410 (QOSMaxJobsPerUserLimit)
846036_[  batch    normal   DatasetsGeneration   djoubaud    1     4 PD         0:00   1-23:59:00    11410 (QOSMaxJobsPerUserLimit)
846035_[  batch    normal   DatasetsGeneration   djoubaud    1     4 PD         0:00   1-23:59:00    11410 (QOSMaxJobsPerUserLimit)
846034_[  batch    normal   DatasetsGeneration   djoubaud    1     4 PD         0:00   1-23:59:00    11410 (QOSMaxJobsPerUserLimit)
846033_[  batch    normal   DatasetsGeneration   djoubaud    1     4 PD         0:00   1-23:59:00    11410 (QOSMaxJobsPerUserLimit)
846027_7  batch    normal   DatasetsGeneration   djoubaud    1     4  R         9:06   1-23:49:54    11408 aion-0163
846027_6  batch    normal   DatasetsGeneration   djoubaud    1     4  R        12:12   1-23:46:48    11407 aion-0113
846027_5  batch    normal   DatasetsGeneration   djoubaud    1     4  R        32:42   1-23:26:18    11403 aion-0078
846027_1  batch    normal   DatasetsGeneration   djoubaud    1     4  R        57:38   1-23:01:22    11398 aion-0163
846027_0  batch    normal   DatasetsGeneration   djoubaud    1     4  R        59:36   1-22:59:24    11398 aion-0163
844973_7  batch    normal   DatasetsGeneration   djoubaud    1     4  R   1-08:57:50     15:01:10    11375 aion-0019
```

Monitor your jobs

Monitor your jobs - check the progression of a job

By default, for a running job, there will be two files:

- An output file, containing the log of your job
- An error file, containing the errors of your job

By default, the files will be named `slurm-JOBID.out` and `slurm-JOBID.err`

You can check the content of those files with a variety of commands, from an access node:

- `cat filename`, `less filename` will display the current full content of the file
- `tail -f filename` will display the end of the file and keep waiting for new content until you close it via `CTRL+C`

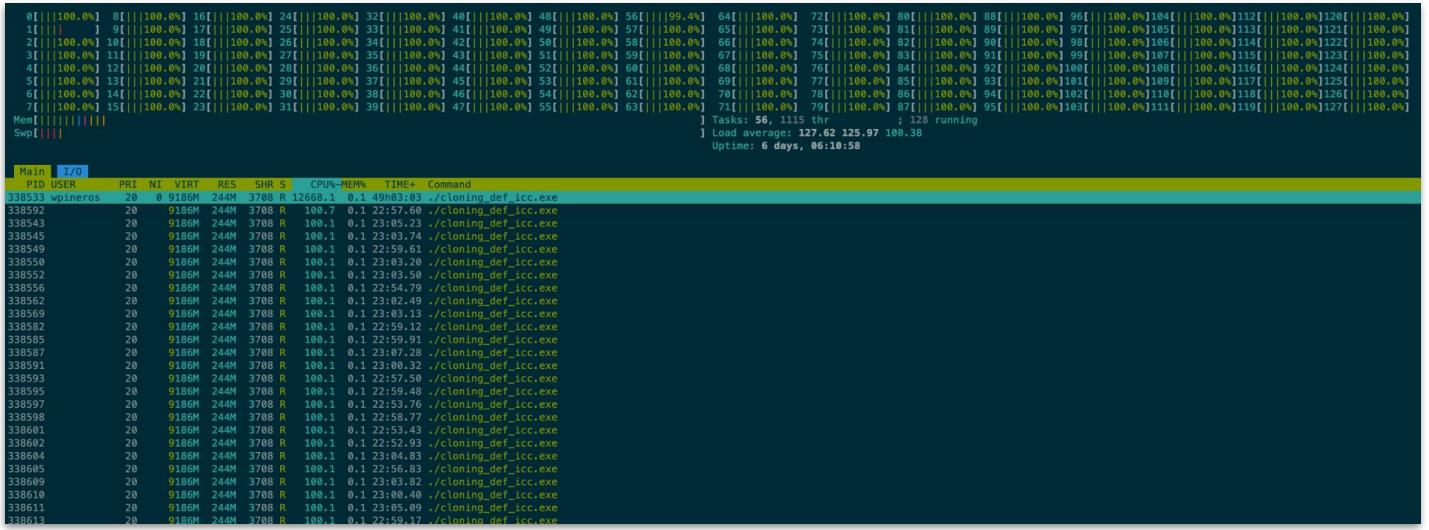
Monitor your jobs

Monitor your jobs - check the efficient usage of resources

1. Use the following command: `sjoin JOB-ID` to connect to your worker's job
2. Use the `htop` command, press u and select your user to see what is happening
3. Exit by pressing `q` or `CTRL+C`

Monitor your jobs

Monitor your jobs - check the efficient usage of resources



Monitor your jobs

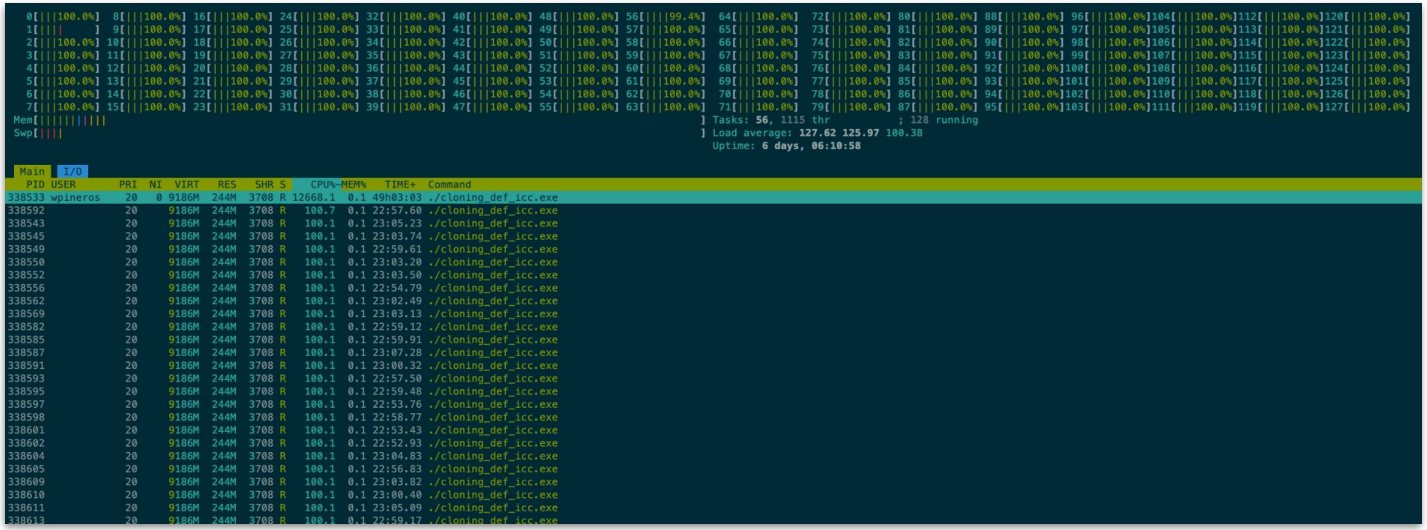
Monitor your jobs - cancel a job

1. Use the following command: `scancel JOB-ID` to cancel a specific job
2. Use the following command: `scancel -u username` to cancel all your jobs

Monitor your jobs

Example 1

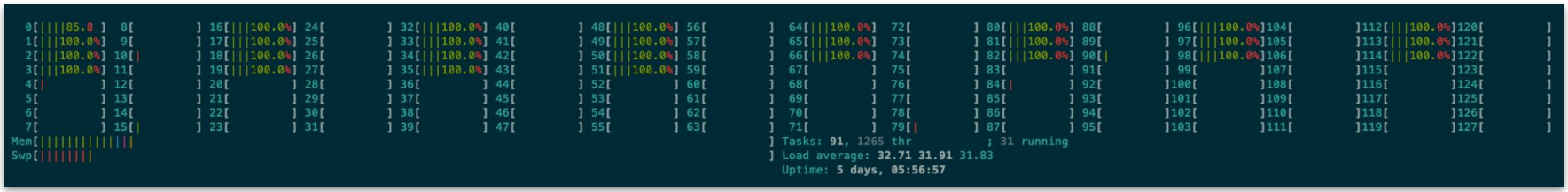
Here we can see that all 128 cores look very busy (100%) and we can see the load average is high. We can also see that the memory usage is quite low. Good usage of ULHPC resource for a CPU bound job.



Monitor your jobs

Example 2

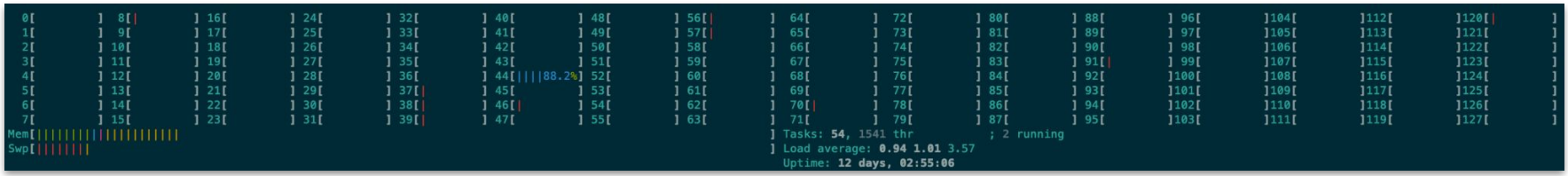
Here we can see that not all the cores are used and that the memory is not used much. It is likely that this job could be optimized. In case of doubt, please contact us [by opening a ticket](#).



Monitor your jobs

Example 3

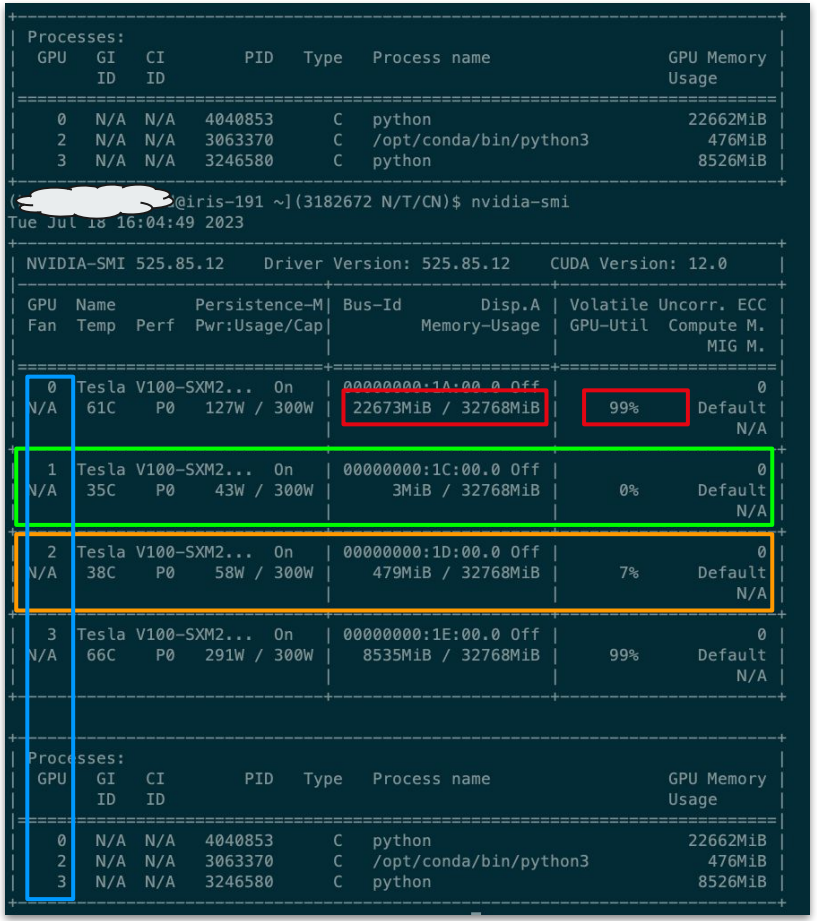
Don’t be that person :)



Monitor your jobs

Monitor your jobs - check the efficient usage of resources - GPU case

1. Use the following command: `sjoin JOB-ID` to connect to your worker's job
2. Type `nvidia-smi` to check the GPU usage (computing and memory)



Storage

- Types of storage
- Different storage quotas
- Pricing

Storage

We offer different storage services:

- Home: this storage is personal to each user. When connecting to the ULHPC, you land in your home storage. The location should look like this: `/home/users/your-username`
- Project: project storage are meant to store / share files for a specific project. Multiple users can have access to a project space. The location starts with `/work/projects/project-name`
- Scratch: special storage for temporary files. The location starts with `/scratch/users/your-username`.

Important note on storage

ULHPC storage is shared and costly. It is meant for running computation only and should not be used as a long term solution. We cannot backup everything and we do not guarantee the long term safety of your storage.

Storage - quota - price

Storage quota and pricing

- Home: free, 500G quota, no possible extension
- Scratch: free, 10T quota, no possible extension
- Project: 1T free, 0.02€ (excl. VAT) / GB / Month above the free 1T

Note

You can check your current quota usage with the following command `df-ulhpc`

Note 2

Additionally to the storage size quota, the is a number of files quota (referred as inodes quota), e.g., you cannot have as many files as you want. you can check this quota usage with the following command `df-ulhpc -i`

Storage - quota

Let's see an example of `df-ulhpc`

Your home and scratch

Your projects

```
df-u ~ df-ulhpc
Directory                 Used  Soft quota  Hard quota  Grace period
---------                 ----  ----------  ----------  ------------
/home/users/[redacted]    339.4G       500G        550G          none
/mnt/lscratch/             40.56G       10T         11T          none
/work/projects/adhoc           0      1000G      1.074T          none
/work/projects/cplex           0       16M         16M          none
/work/projects/hpcbenchs   6.011G       10T         10T          none
```

Storage - quota - price

Let's see an example of `df-ulhpc -i`

Your home and scratch

Your projects

```
~ df-ulhpc -i
Directory                 Used  Soft quota  Hard quota  Grace period
---------                 ----  ----------  ----------  ------------
/home/users/[redacted]    891633     1000000     1100000          none
/mnt/lscratch/            301644     1000000     1100000          none
/work/projects/adhoc           3     1000000     1100000          none
/work/projects/cplex           1           0           0          none
/work/projects/hpcbenchs   30283    30000000    31000000          none
```

Storage - quota

```
~ df-ulhpc -i
Directory                 Used  Soft quota  Hard quota  Grace period
---------                 ----  ----------  ----------  ------------
/home/users/[redacted]    891633     1000000     1100000          none
/mnt/lscratch/            301644     1000000     1100000          none
/work/projects/adhoc           3     1000000     1100000          none
/work/projects/cplex           1           0           0          none
/work/projects/hpcbenchs   30283    30000000    31000000          none
```

Soft quota is the quota you should respect

Hard quota is slightly above the soft quota, the system will prevent you to go above

Grace period is the remaining duration you have when you are between the soft and the hard quota.

Example: if the grace period states “1 day” you can still create / modify files while being above the soft quota. After the grace period is expired, you will be blocked until you fix the situation.

Storage - transfer

To transfer data from and to the ULHPC you can:

- Use MobaXterm file transfer feature, see our documentation
- Use rsync to synchronise a source directory with a destination directory, see our documentation

I want to know more

- Use virtual environments (R / Python / Conda)
  - Why? Compartmentalize your experimental setups, promotes reproducibility
  - R → try packrat
  - Python → try venv
  - Python things but also other non-Python stuffs → try conda
- Even more reproducibility? Containers
- If you use interactive job, use tmux to prevent losing your current terminal state
- Use GNU parallel to efficiently run embarrassingly parallel jobs, see tutorial
- Check our tutorials, maybe there is something that you need

Thank you