



Hands-on training on High Performance Computing

Workshop on UM6P's African Supercomputer (Toubkal)

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Overview

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2. Connection to the HPC
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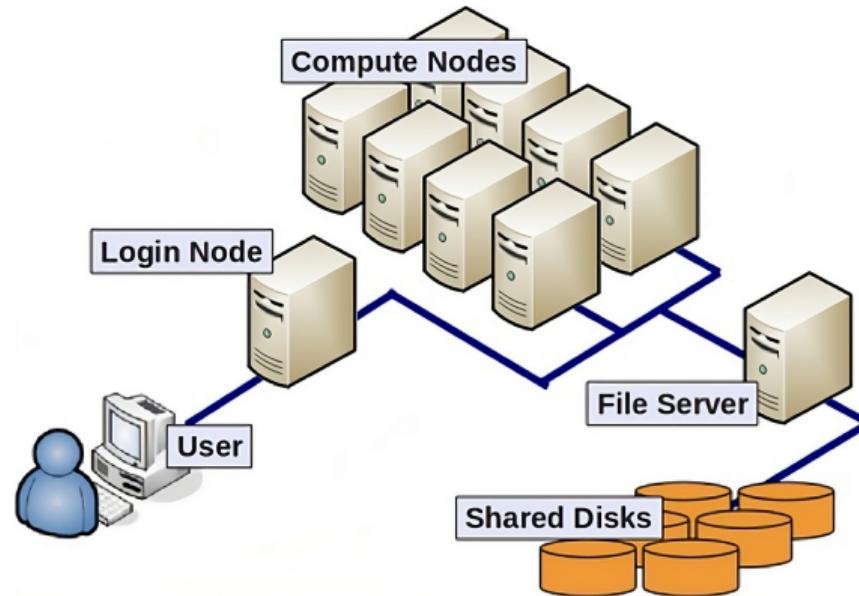
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¹Picture taken from: https://hbctraining.github.io/Intro-to-shell-fasrc-flipped/lessons/08_HPC_intro_and_terms.html

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Toubkal

Toubkal is a supercomputer acquired by UM6P in 2019. It is the fastest and most performant supercomputer in Africa!

Simlab

The SIMLAB is a supercomputer acquired by UM6P and aimed at providing HPC services to the research community in Morocco and the African continent.

Compute Resources:

- 69000 CPUs (Intel Xeon Platinium 8276)
- 5 servers with 4 Nvidia A100 each
- Servers have from 192GB to 1.5TB of RAM

Storage Resource:

- A LOT of Terabytes (20TB per team)
- Lustre Parallel file system to manage large volumes with high performance

Compute Resources:

- 784 CPUs
- 7 P40, 5 V100 & 1 Quadro P4000 (visu)
- Servers have from 128GB to 382GB of RAM

Storage Resource:

- Hundreds of Terabytes
- Beegfs Parallel file system to manage large volumes with high performance

Connection to the HPC

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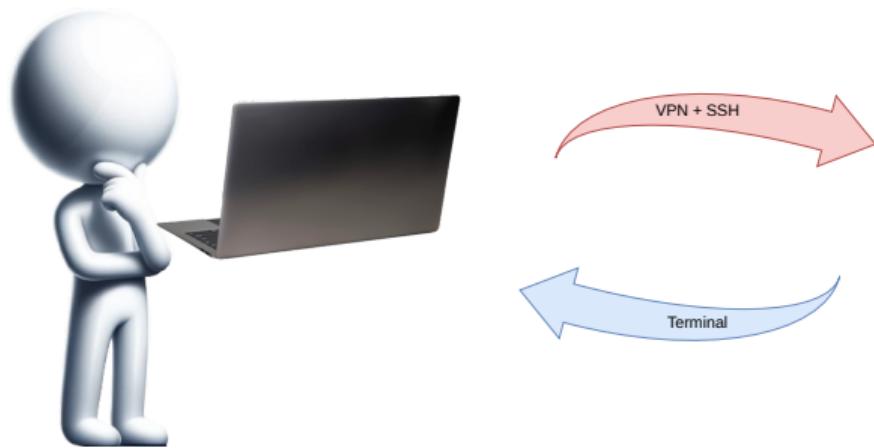
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```
user@Toubkal:~$ echo Hello Ai movement
```

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1 - Connect to the VPN



2 - SSH the cluster



3 - Access the required node



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1 - Connect to the VPN: vpn.um6p.ma

The screenshot shows the official website of the University Mohammed VI Polytechnic (UM6P). The header features the UM6P logo, the university's name, and a 'Logout' button. Below the header is a search bar. The main content area is titled 'Network Access' and contains a button labeled 'UM6P VPN Access' with a shield icon.

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2 - SSH the cluster:

Option 1: Via terminal with the SSH command:

```
usr@Laptop:~$ ssh name.lastname@toubkal.hpc.um6p.ma
```

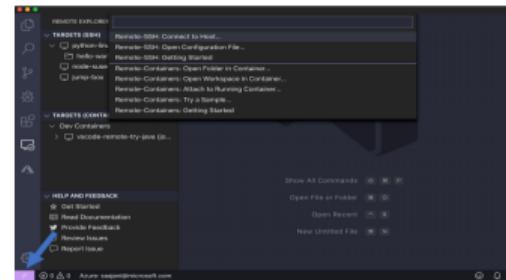
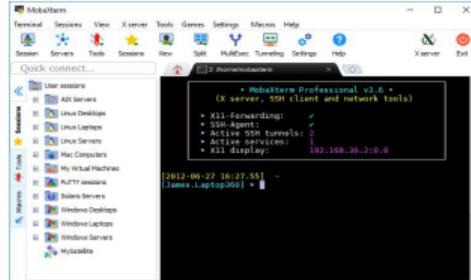
Option 2: Via your favourite ssh client



MobaXterm



Vs Code



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3 - Queue the selected node:

Simlab

Partition	Max Time	Nodes
defq	1 hour	7
shortq	4 hours	7
longq	30 days	7
special	30 minutes	17
visu	24 hours	1
gpu	48 hours	12

Toubkal

Partition	Max Time	Nodes
compute	48 hours	1219
himem	36 hours	5
gpu	24	5

Toubkal also has special QoS for each partition



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SLURM: Simple Linux Utility for Resource Management

SLURM is:

- free and open-source
- used to manage computing clusters
- used to allocate resources (e.g. processors, GPUs, memory, etc...) fairly
- used to run tasks smoothly and efficiently on multiple machines simultaneously.



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Some useful SLURM commands²:

- **sinfo:** Display all partitions information
- **squeue:** Display all the queued jobs
- **salloc:** This command is used to allocate resources to a job in real-time
- **sbatch:** This command is used to submit a job script for later execution. Typically, this is associated with other directives such as –job-name, –cpus-per-task etc
- **srun:** To submit a job for execution in real-time
- **scancel:** Used to cancel a submitted job

²Please refer to either Toubkal/SIMLAB, and SLURM documentation for a more comprehensive view

What *can* be done and *can't* be done in HPC



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Can be done

Almost everything you can do in a linux based system

Can't be done

- You can't run commands in sudo mode
- You can't install software as you would normally
 - No "sudo apt insall" or ".deb", not a debian based distro
 - No "sudo yum install" or ".rpm", for security/operability constraints

You can't run sudo commands and can't use packet managers to install software.
You either load a module for it if available or build it/ download the binaries.

Hands-on applications and examples

How to set your development environment

- Search for available modules:

```
$ module avail [wanted module {cuda}]
```

```
[ML] (base) [anass.grini@slurm-login-h23d5-u38-svn3 anass.grini]$ module avail cuda
-----
----- /srv/software/easybuild/modules/all -----
Arrow/0.17.1-fosscuda-2020b (D) CUDAcore/11.1.1 OpenMPI/4.0.5-gcccuda-2020b cuDNN/8.0.4.30-CUDA-11.1.1
CUDA/9.2.88-GCC-7.3.0-2.30 CUDAcore/11.2.1 (D) PyTorch/1.8.1-fosscuda-2020b cuDNN/8.1.1.33-CUDA-11.2.1
CUDA/11.1.1-GCC-10.2.0 GDRCopy/2.1-GCCcore-10.2.0-CUDA-11.1.1 (D) PyTorch/1.9.0-fosscuda-2020b (D) cuDNN/8.4.1.50-CUDA-11.7.0 (D)
CUDA/11.3.1 GROMACS/2021.3-foss-2021a-CUDA-11.3.1 (D) SciPy-bundle/2020.11-fosscuda-2020b fosscuda/2020b
CUDA/11.4.1 Horovod/0.22.0-fosscuda-2020b-PyTorch-1.8.1 (D) Spark/3.1.1-fosscuda-2020b (D) gcccuda/2018b
CUDA/11.7.0 NCCL/2.8.3-GCCcore-10.2.0-CUDA-11.1.1 UCX-CUDA/1.11.2-GCCcore-11.2.0-CUDA-11.4.1 gcccuda/2020b (D)
CUDA/12.1.0 (D) OpenCV/4.6.0-foss-2022a-CUDA-11.7.0-contrib UCX/1.9.0-GCCcore-10.2.0-CUDA-11.1.1 magma/2.5.4-fosscuda-2020b

Where:
D: Default Module
```

- Load Wanted module:

```
$ module load [module {CUDA/12.1.0}]
```

- Unload Specific module:

```
$ module unload [module {CUDA/12.1.0}]
```

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How to set your development environment

- Search for available Anaconda modules:

```
$ module avail conda
```

```
• (ML) (base) [anass.grini@slurm-login-h23d5-u38-svn3 anass.grini]$ module avail conda
```

```
Anaconda2/2019.10 Anaconda3/2020.11
```

```
----- /srv/software/easybuild/modules/all -----
```

- Load Anaconda module:

```
$ module load Anaconda3/2020.11
```

- Verify if Anaconda is correctly loaded:

```
$ conda -V
```

```
• (ML) (base) [anass.grini@slurm-login-h23d5-u38-svn3 anass.grini]$ conda -V  
conda 4.9.2
```

Hands-on applications and examples

How to set your development environment

- Create a Python Environment on Conda:

```
conda create -n "aim_env" python=3.8.0
```

- You continue the steps as displayed on the terminal

- Activate the created environment:

```
$ conda activate aim_env
```

```
▶ (ML) (base) [anass.grini@slurm-login-h23d5-u38-svn3 anass.grini]$ conda activate aim_env
▶ (aim_env) (base) [anass.grini@slurm-login-h23d5-u38-svn3 anass.grini]$ []
```

- Now you can install any python package using

```
$ conda install [package name]
```

or

```
$ pip install [package name]
```



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How to set your development environment

- Export your packages for *aim_env* as YAML file
`$ conda env export > aim_env.yml`
- You can create a conda environment from your local one using a YAML file
`$ conda env create -f aim_env.yml`

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Introduction to bash scripting for SLURM

```
1 #!/bin/bash
2 #SBATCH --job-name=test_job          # Name your job
3 #SBATCH --partition=gpu             # Setting the partition
4 #SBATCH --gres=gpu:1                # You need this for gpu, remove if not using the gpu
5 #SBATCH --account=XXXXX-XXXXXX      # GPU account: you can find it by running the command "mybalance" (only for Toubkal users)
6 #SBATCH --output=outputs.log        # Standard output/error log (%) to add date info to the log file name
7
8 pwd; hostname; date # Log the current working directory, hostname and date at the start of the execution
9
10 user="Name.lastName" #<<- Add your HPC username here
11
12 module load OpenMPI/3.1.1-GCC-8.3.0
13 module load PyQt5/5.15.4-GCCcore-11.2.0
14 module load Spark/3.1.1-Foss-2020a-Python-3.8.2
15
16 # Uncomment if you work with conda environments
17 # load modules or conda environments here (you can use your own conda environment)
18 module load Anaconda3
19
20 conda activate ML
21
22 nvidia-smi
23
24
25 # Run your python script (You copy-paste the .py file path)
26 python3.10 /home/anass.grini/anass.grini/aim_HPC_handsontrain_wandb.py
27
28 # Launch Sweep
29 # wandb agent anass-gr/wandb_test/c6z4lgly
30
31 date
```

SLURM required script to determine computation mode

Load necessary modules

Activate your conda environment

Run your python script or command

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Run your Python script in SLURM

- Obtaining a terminal on a GPU compute node

```
$ srun --pty --partition=gpu --nodes=1 --gres=gpu:1 [--other-options] bash
```

- Then load required modules manually using "module load [name-module]"

OR

- Create a *bash script* (as seen previously)
- Run your Python script from .sh file

```
$ sbatch run_train.sh
```



Weights & Biases

- WandB: A powerful experiment tracking, collaboration, and model management platform.
- Used by many companies and world's leading AI teams (Meta, Nvidia, Stanford University, OpenAI...)
- Track, compare, and visualize ML experiments to build **better models faster**.

Experiment Tracking with WandB

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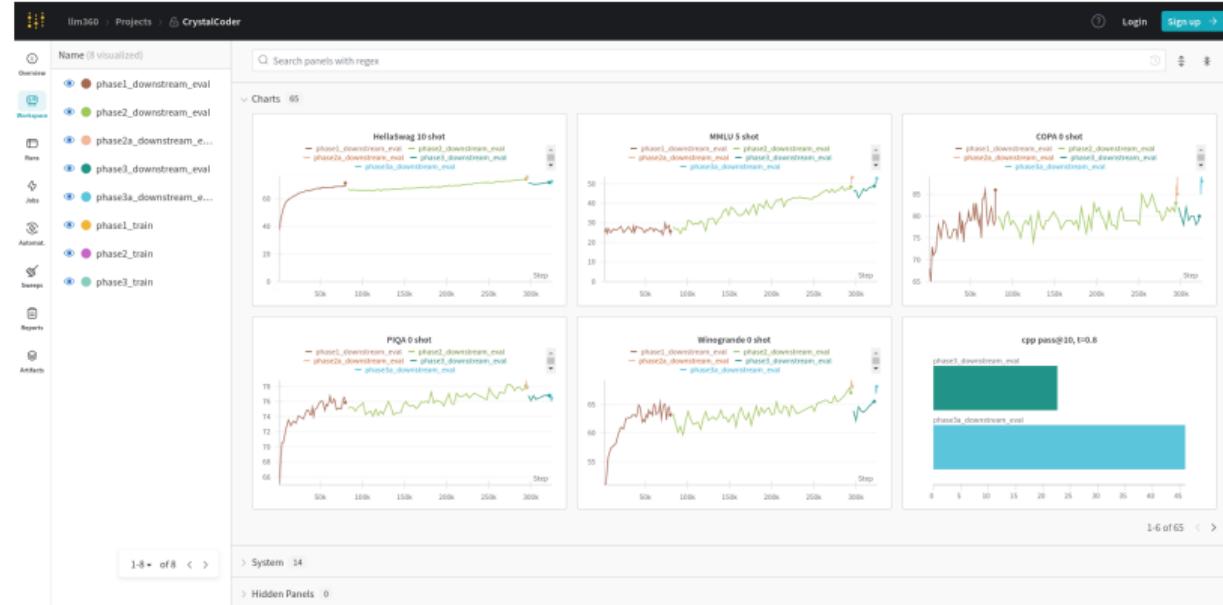


Figure 6.1: Overview on WandB's Dashboard

Sweeps: Automate hyperparameter optimization



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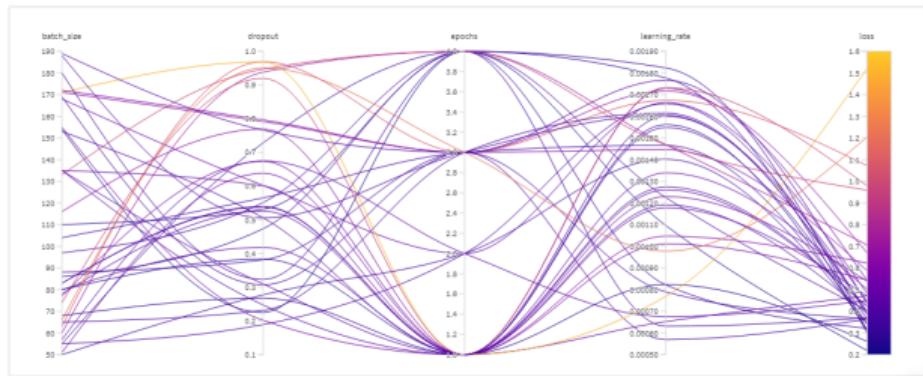
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- *Sweeps* in WandB is a feature that automates finding the best hyperparameters for your model.
- You provide a range of values for your hyperparameters, and WandB tests different combinations to identify the most effective setup.
- Saves time and effort in hyperparameter tuning, leading to better model performance.

Sweeps: Automate hyperparameter optimization

```
program: /home/USER/project/train.py
method: bayes
metric:
  goal: minimize
  name: Loss
parameters:
  lr:
    max: 0.01
    min: 1e-4
    distribution: uniform
  epochs:
    max: 30
    min: 10
    distribution: int_uniform
  batch_size:
    values:
      - 124
      - 32
    distribution: categorical
```

Figure 6.2: YAML script for sweep creation

Thank You.

Ai movement

