An introduction to UL HPC-supercomputers

Performances, functionalities and accessibility

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February 1, 2023

BACKGROUND

High Performance Computing (HPC) most generally refers to the practice of aggregating computing power in a way that delivers much higher performance than one could get out of a typical desktop computer or workstation in order to solve large problems in science, engineering, or business."
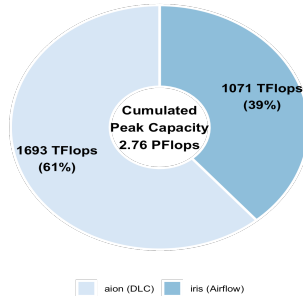
▶ The HPC is an infrastructure of the University of Luxembourg (UL) that starts operating in 2007

▶ Is the second largest HPC facility of the country. The first is Euro-HPC Luxembourg supercomputer "MeluXina"

▶ Installed in the premises of the University's Centre de Calcul (CDC), Belval

▶ The UL-HPC platform has kept growing over time thanks to the continuous efforts of the core HPC / Digital Platform team. Contact them via `hpc-team@uni.lu`

▶ To get a full overview of UL-HPC, visit the website `https://hpc.uni.lu/`
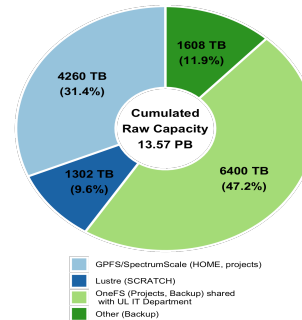
PERFORMANCES
SUPERCOMPUTING AND STORAGE RESOURCES AT A GLANCE

ULHPC Computing and Storage Capacity (2022)

UL HPC Supercomputers (2022)

- 1071 TFlops (39%)
- 1693 TFlops (61%)
- Cumulated Peak Capacity 2.76 PFlops
- aion (DLC)
- iris (Airflow)

UL HPC Storage FileSystems (2022)

- 1608 TB (11.9%)
- 4260 TB (31.4%)
- 1302 TB (9.6%)
- 6400 TB (47.2%)
- Cumulated Raw Capacity 13.57 PB
- GPFS/SpectrumScale (HOME, projects)
- Lustre (SCRATCH)
- OneFS (Projects, Backup) shared with UL IT Department
- Other (Backup)

How big is 1 PetaFlops? 1 PetaByte?

▶ 1 PetaFlops = 10^{15} floating-point operations per second (Flops), corresponds to the cumulative performance of more than **3510** Macbook Pro 13" laptops, or **7420** iPhone XS

▶ 1 PetaByte = 10^{15} bytes, corresponding to the cumulative raw capacity of more than 1950 Solid-state-drive with 512GB.

PERFORMANCES
IRIS VS AION

IRIS

- In production since June 2017, peak performance of 1071 TFlop/s-
- 196 computing nodes (totalling 5824 computing cores) and 96 GPU accelerators
- CPU (central processing units) vs GPU (graphics processing unit)
  1. Runs processes serially (CPU) vs in parallel (GPU)
  2. Better at processing one big task at a time (CPU) vs Better at processing several smaller tasks at a time (GPU)
- For more information, visit `https://hpc-docs.uni.lu/systems/iris/`

AION

- In production since October 2020, peak performance of 1692 TFlop/s
- 318 compute nodes (totaling 40704 compute cores) but. No GPU
- For more information, visit `https://hpc-docs.uni.lu/systems/iris/`

FUNCTIONALITIES
SOFTWARES

The UL HPC platform offers a modern software environment matching the evolving computing requirements of University of Luxembourg's researchers and students.

- ▶ Stata - `https://hpc-docs.uni.lu/software/maths/stata/`
- ▶ R - `https://ulhpc-tutorials.readthedocs.io/en/latest/maths/R/`
- ▶ Julia - `https://hpc-docs.uni.lu/software/maths/julia/`
- ▶ Python - `https://ulhpc-tutorials.readthedocs.io/en/latest/python/basics/`
- ▶ Full list of software - `https://hpc-docs.uni.lu/software/swsets/all_softwares/`

ACCESSIBILITY
THE THREE WISE (WEB)PAGES

All official and helpful information could be found from webpages below.

1. ULHPC Technical Documentation - link
2. UL HPC Tutorials - link
3. UL HPC homepage - link

ACCESSIBILITY
THE THREE WISE PAGES

Also I have written three documents providing guidance to people who are new to HPC.

Please use the LISER MS Teams account to get the document.

1. UL HPC fuzzy guideline - link
2. Hands-on HPC guide - link
3. ojv_hpc_data_transfer_guideline - link

ACCESSIBILITY
OVERALL WORKFLOW

The overall workflow of gaining access to the HPC is as follows:

1. Requesting a HPC account - link
2. Configuring your account - please check the 2. Hands-on HPC guide
   - Generate a SSH key
   - Store it in your account details
3. Configuring your login method on MobaXterm - please check the 2. Hands-on HPC guide

ACCESSIBILITY
SWITCHING FROM AION TO IRIS

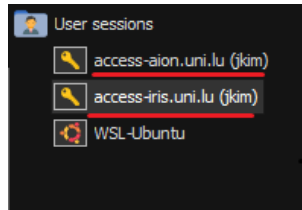You have to create a separate session for each cluster.

Figure. Two separate sessions for each cluster

PRACTICAL EXAMPLES

In this illustration you will learn how to:

1. Create new project folder in the MobaXterm Console
2. Upload data-sets from your local computer
3. Create Python virtual environments
4. Create bash files to run your scripts
5. Install new libraries or see which libraries are already installed in the virtual environment
6. Run scripts in other programming language, e.g. from Python to R/Stata
7. Extract the output from the MobaXterm Console in your local machine

PRACTICAL EXAMPLES
INTERACTIVE JOBS, HTTPS://HPC−DOCS.UNI.LU/JOBS/INTERACTIVE/

The interactive partition is to be used for code development, testing, and debugging.

► Start interactive jobs, with and without the requirement of GPU
► Run interactive jobs with R and Stata