
LUX
PROVIDE
SCynergy 2026
Getting Started with MeluXina
https://luxprovide.github.io/SCynergy2026-GettingStartedWithMeluXina/
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EPICURE
Unlocking European-level HPC Support
MADE IN
LUXEMBOURG

Getting Started with MeluXina

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High Performance Computing

- What is HPC?

HPC Platforms

- Hardware view
- Software view

Using an HPC platform

- User Interfaces
- Interactive vs batch job
- Job scheduler
- Software environment

MeluXina in practice

- User and project accounts
- Data storage
- Authentication
- Shell & web-portal access

Hands-on!

- Configuration
- Urban wind simulation
- Deep learning with PyTorch

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What is

High-Performance Computing?

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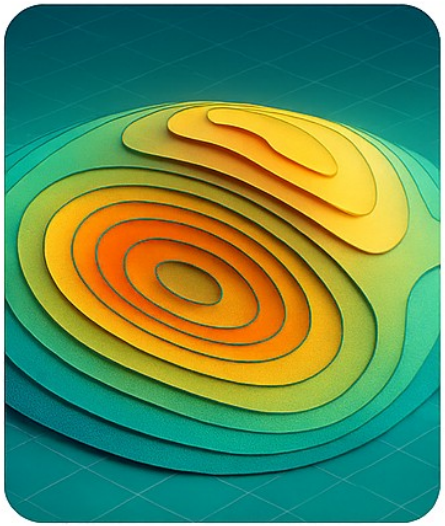
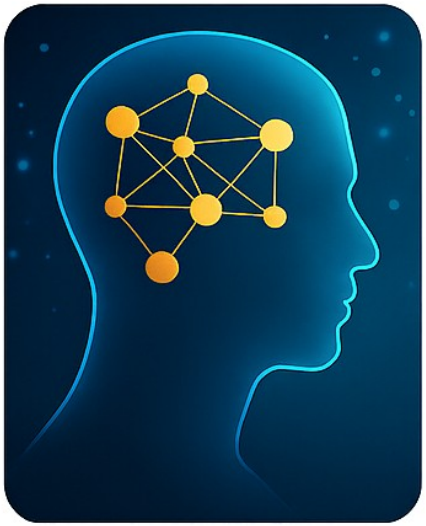
HPC is everywhere



Simulations & modeling



AI / ML training & inference

Large-scale data analytics

Engineering, science & industrial R & D

What is High Performance Computing?

High Performance Computing (HPC)

- Use of **parallel and distributed computers with fast interconnects**
- To execute an application quickly and efficiently

Why parallel computers?

- Performance of single CPU core is getting limited (power, physics)
- Multiple cores are used to increase the computing capacity

HPC is challenging

- Active research domain
- Provides tools for industry and research

How to get faster with HPC?

~~Build faster processors~~

- Moore's law continues but ***The free lunch is over!***
- CPU serial-processing speed is reaching its physical limit

→ **Multi-cores processor architectures**

→ **Accelerators and specialized processors** (GPU, TPU, FPGA, etc.)

Combine multiple computers

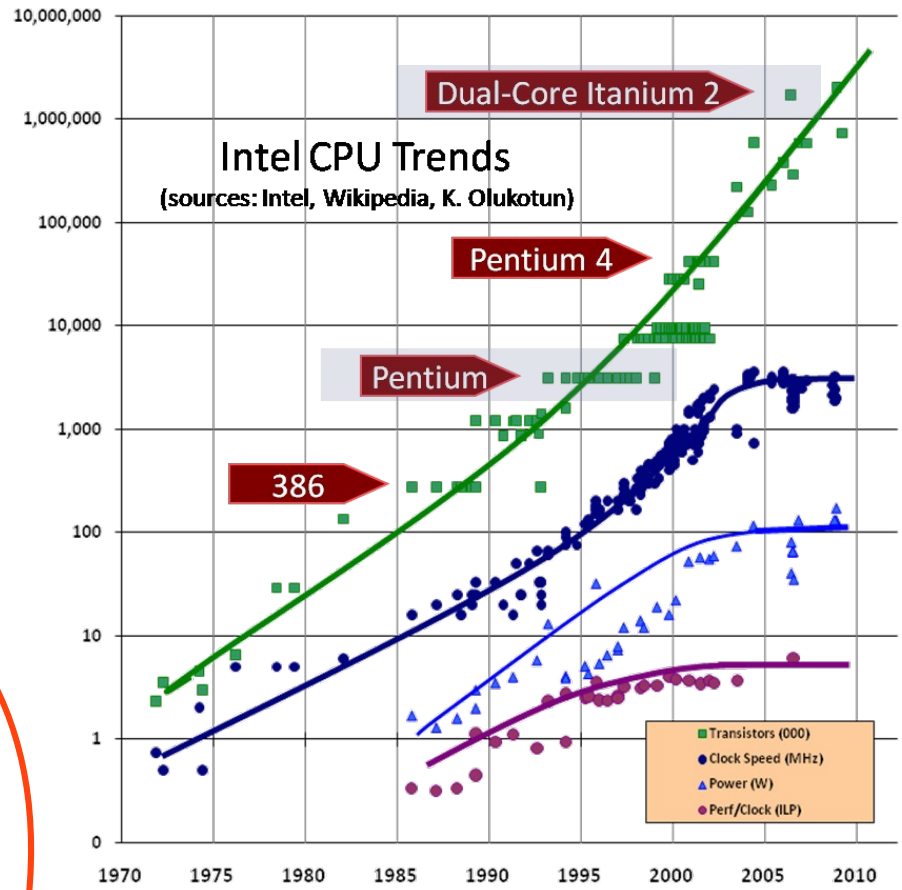
→ **HPC Clusters and Supercomputers**

Better use of the hardware

→ **Identify the actual bottleneck** (CPU, memory, network, etc.)

→ **Vectorization (SIMD)**

Not to forget: **Better algorithms**



H. Sutter. *The Free Lunch Is Over*. 2005

Parallel programming

How much faster is HPC?

Your laptop

shared with other users

MeluXina

shared with other users

EL CAPITAN

	Your laptop	MeluXina	EL CAPITAN
CPU	8 cores	89,984 cores	1,051,392 cores
Memory	32 **G**B	488 **T**B	5.44 **P**B
Storage	1 **T**B	12.6 **P**B	TBA
Network	Ethernet 10 Gb/s	Infiniband 200 Gb/s	Slingshot 200 Gb/s
Accelerators	1 GPU	800 GPUs	43,808 GPUs
Theoretical Performance	350 **G**flops	18 **P**flops	2.82 **E**flops

HPC Platforms

Hardware and Software Views

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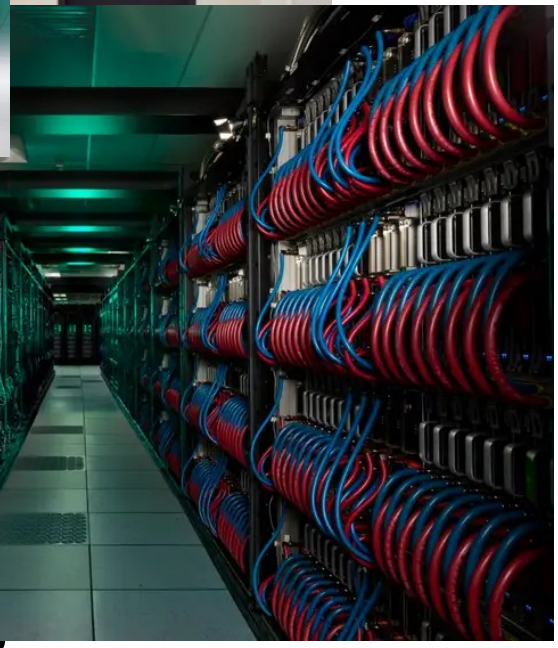
What does an HPC platform look like?

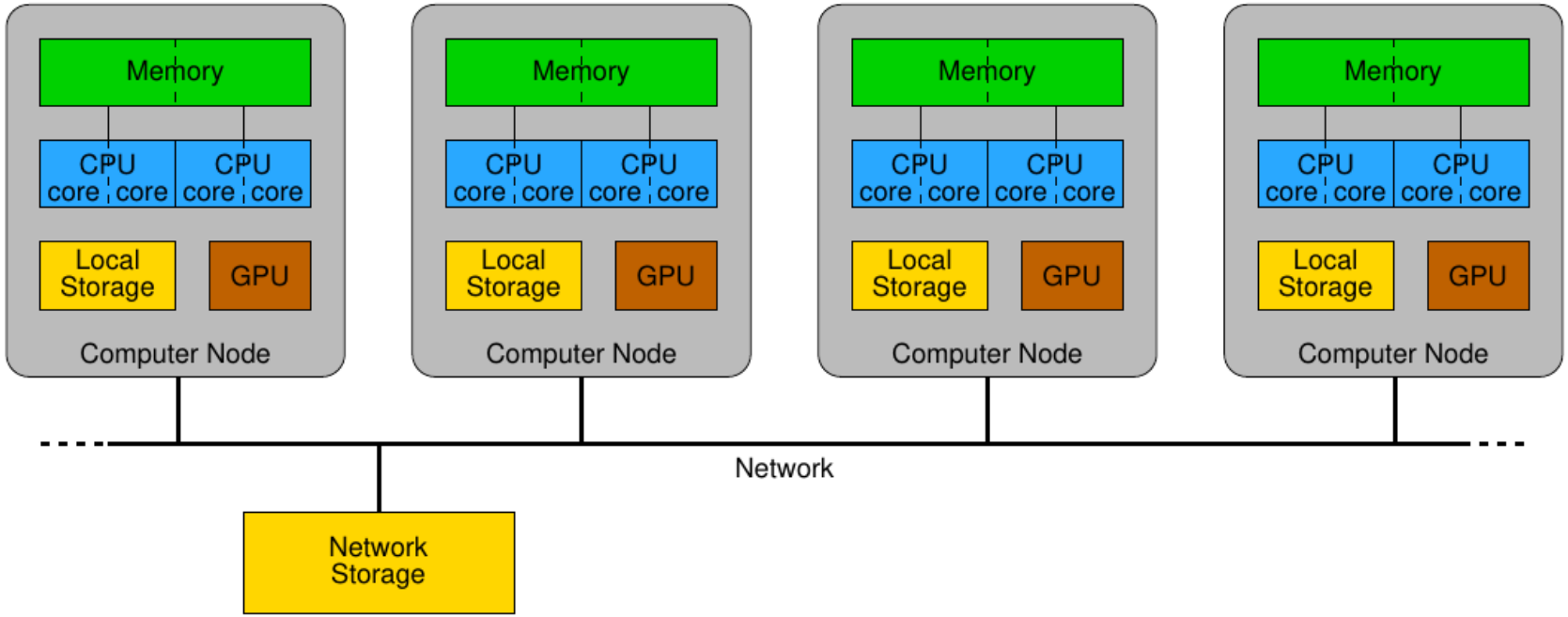
Photos: Garry McLeod/LLNL



El Capitan, Lawrence Livermore National Laboratory, USA

MeluXina, LuxProvide,

HPC platform: Hardware View



Different components or type of **resources**:

- Processors, GPU/Accelerators, Memory, Storage, Network, ...

HPC platform: Software View

Operating System

- Manage hardware resources
- Interface between userspace and hardware

HPC Tools

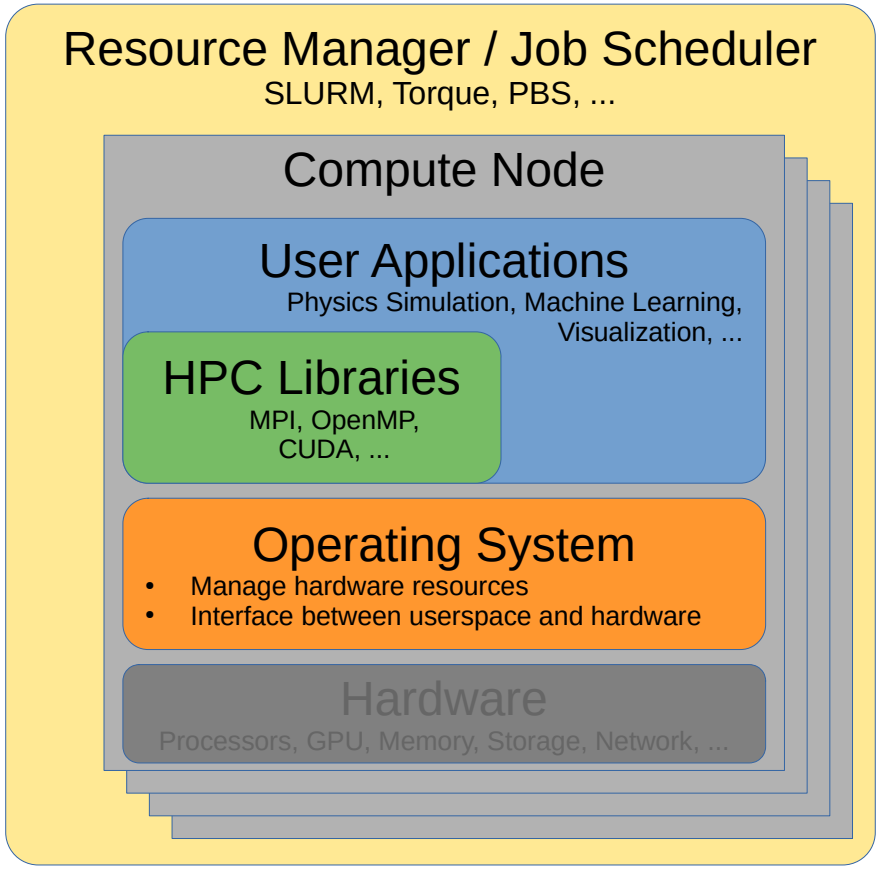
- Libraries, compilers and tools for developing and running parallel programs
- MPI, OpenMP, CUDA, TensorFlow, ...

User Applications

- Scientific, engineering, and commercial
- Simulation, Machine Learning, Visualization, ...

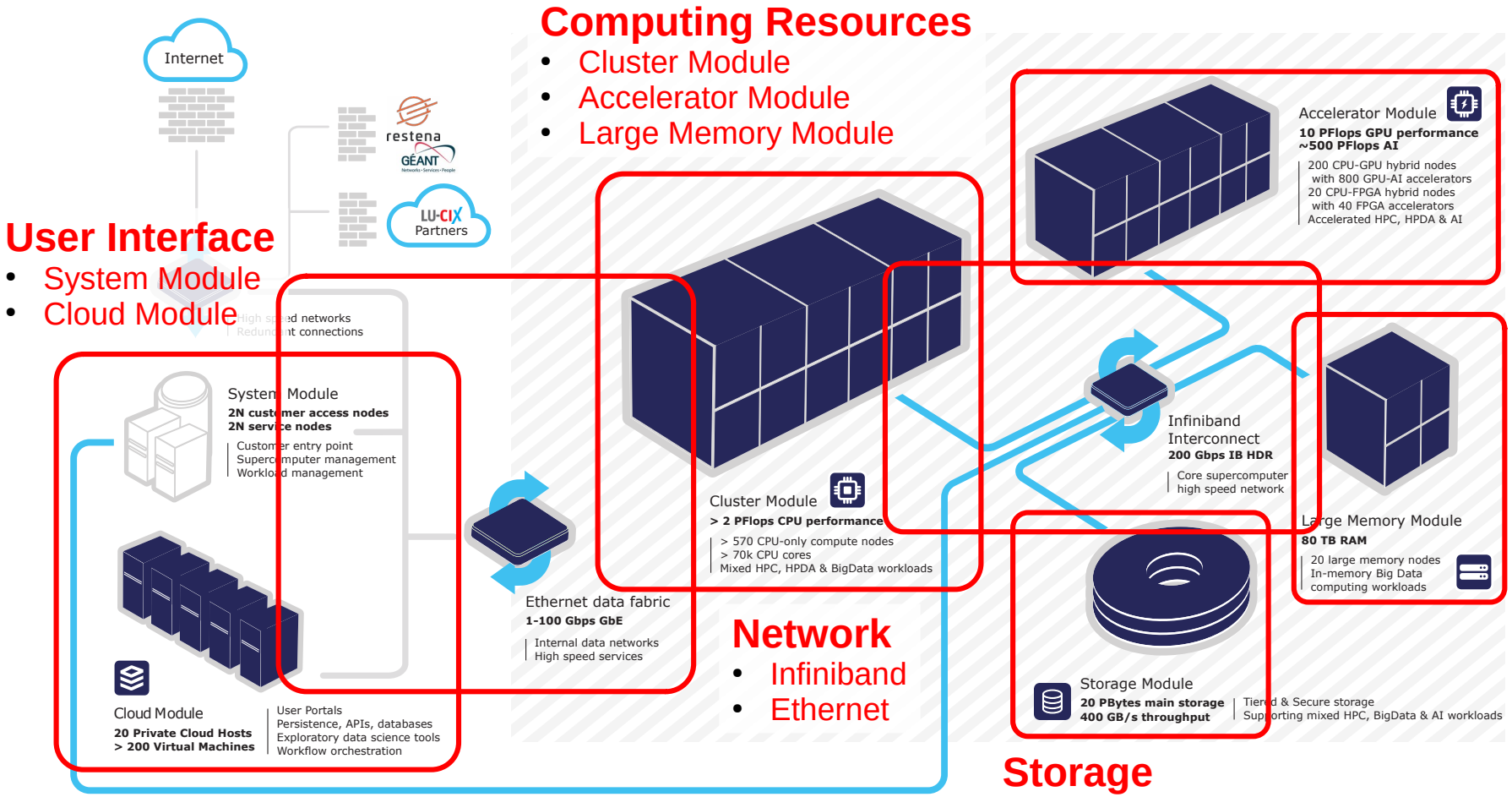
Resource Manager / Job Scheduler

- Allocate resources and schedule user jobs
- Ensure efficient and fair resource sharing



Example: MeluXina Supercomputer

Source: https://docs.lxp.lu/system/overview/



Using an HPC Platform

HPC from the user point of view

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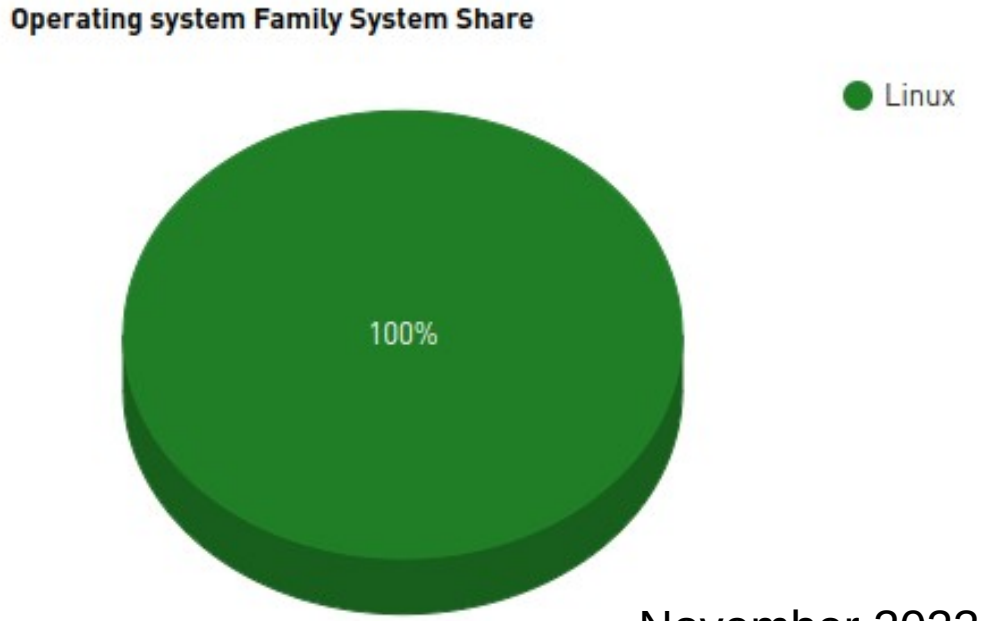
Quiz!

What is the Operating System used on the Top500 supercomputers?



November 2023

Source: https://www.top500.org/statistics/list/

User Interfaces for HPC

Command Line Interface (CLI)

- By far the most common

Advantages

- Simple (always works)
- Easy to program/automatize
- Fast and low bandwidth requirements

Disadvantages

- Not user friendly
- Requires knowledge and memorizing

Alternatives to CLI

Web portal

- Dedicated to some specific tasks

Remote connection

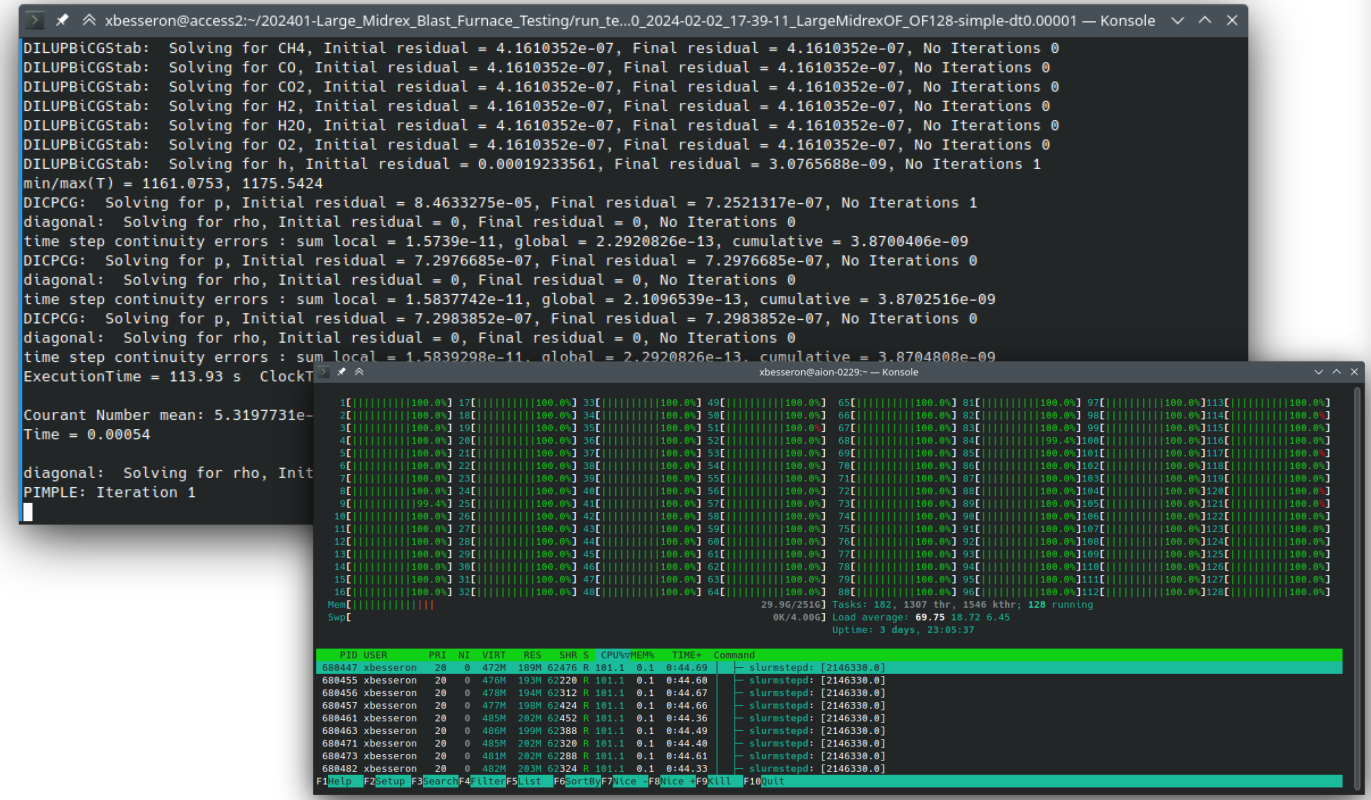
- Client GUI and remote server for dedicated applications

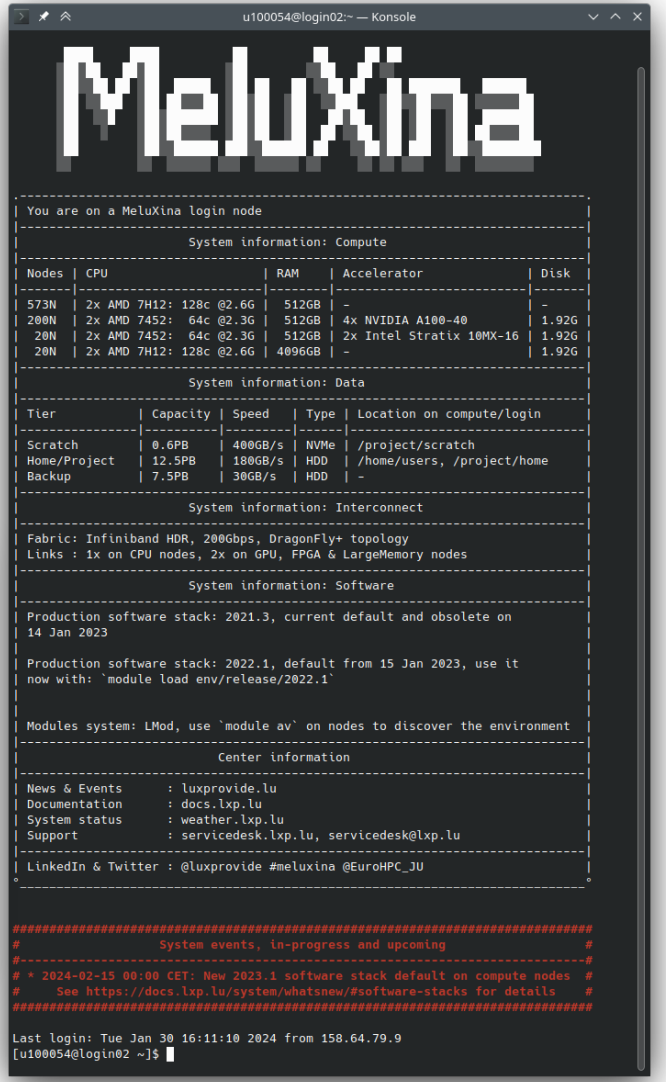
API for remote execution

GUI for dedicated tasks

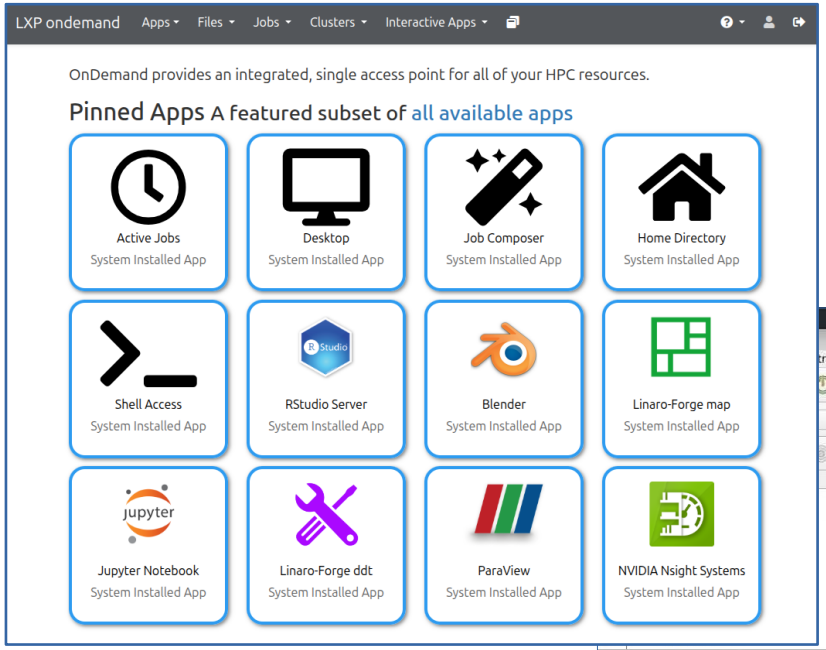
- For example, file transfer

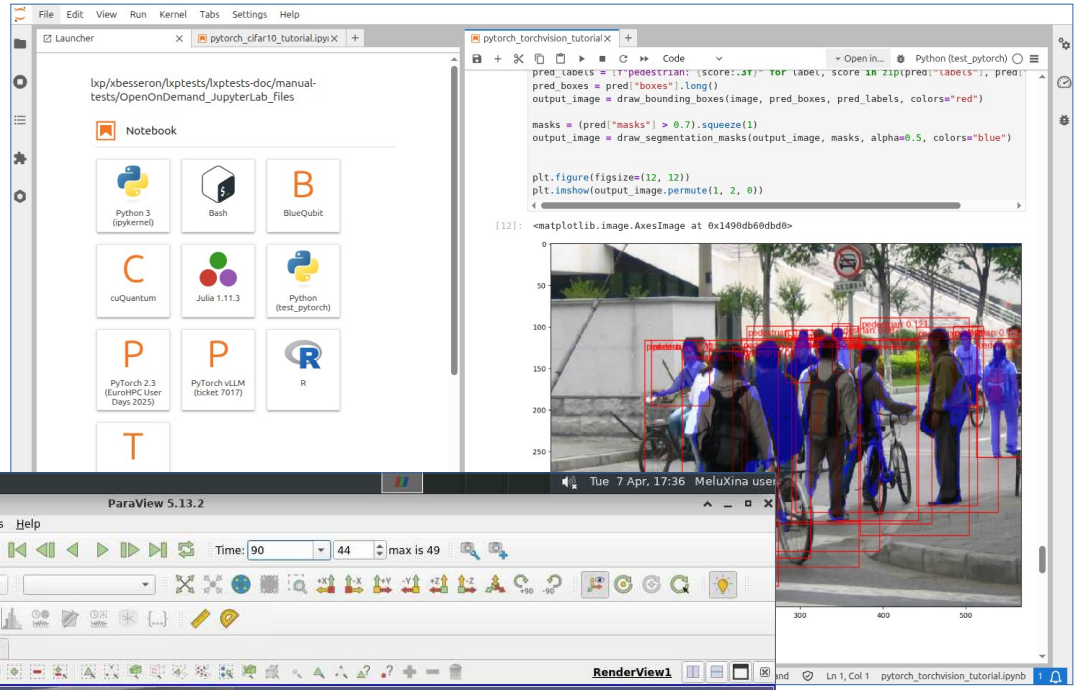
Command Line Interface





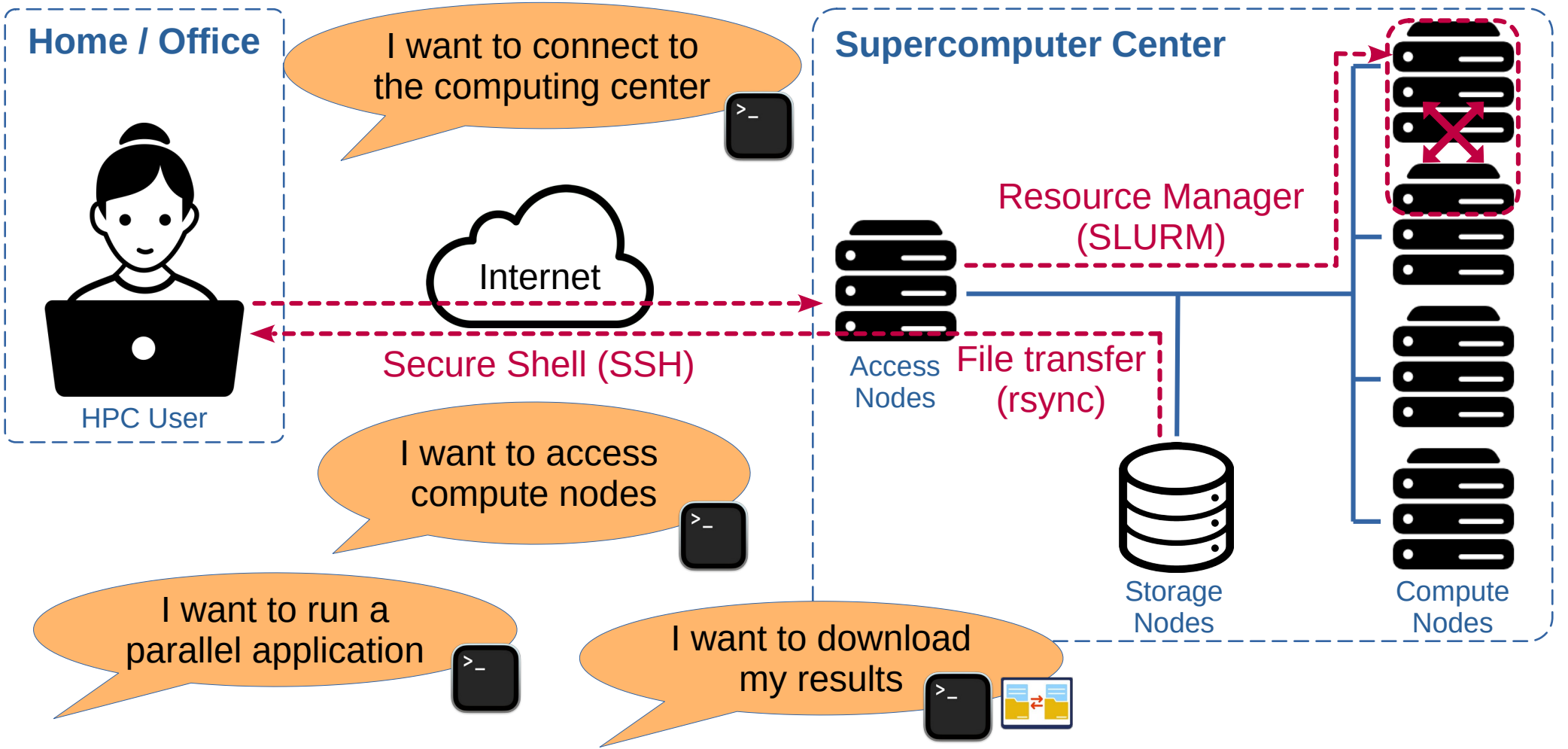
Web-portal Interface





HPC platform: User point of view

Parallel Computing library (MPI, PyTorch)



HPC usage: **Interactive** vs **Batch**

Interactive jobs

- ***Immediate*** access to compute resources
- Commands are run manually (e.g. via an interactive shell, Jupyter notebook, ...)
- Used for debugging, development, testing, or small exploratory runs
- Usually limited to small number of resources and a short time

Batch jobs (non-interactive)

- Execution is **deferred** until resources become available
- No user interaction during runtime
- Used for production workloads, long simulations, large parameter sweeps, ...
- Can use large number of nodes and long execution time
- → This is the most standard usage

- In both cases, resource requests (or jobs) are submitted to the **resource manager**
  - Traditionally, HPC do offer infinite jobs or services

SLURM: Simple Linux Utility for Resource Management

What is SLURM?

- Open-source, highly configurable, and fault-tolerant workload manager for Linux clusters
- Widely used in HPC to manage and schedule large-scale computational jobs, including on MeluXina

Main functions

- **Resource allocation**: It allocates resources like CPUs, memory, and storage to submitted jobs based on their requirements and configured policies.
- **Job scheduling**: It queues and prioritizes jobs, ensuring fair access and efficient utilization of resources.

Main concepts of SLURM

Partitions

- Group of **nodes with similar characteristics** (CPU type, memory capacity, available software)
- Users submit jobs to specific partitions based on their resource requirements

QoS (Quality of Service)

- QoS defines **scheduling policies** for jobs within a partition, influencing priority and resource allocation
- For example, limits on job wait time and duration, pre-emption rules

Jobs

- Jobs are the **units of work** that are submitted to SLURM.
- Each job has a specific resource requirement, such as number of CPUs, memory, and disk space.
- Jobs are submitted within specific partitions and QoS levels.

Queue

- **Holding area** for submitted jobs within a partition and QoS
- Jobs are added to the queue according to arrival time and priority rules defined by the QoS
- Jobs can be PENDING, RUNNING, COMPLETED (and many more)

Job Scheduling
Simple Example

QoS:

`default`	`long`
- max 100 jobs - max 2 days - priority: normal	- max 1 job - max 6 days - priority: low

Queues:

Pending:	Job 1 PENDING **priority: 1**	Job 2 PENDING **priority: 99**	Job 3 PENDING **priority: 10**
Running:	Job 1 RUNNING	Job 3 RUNNING	Job 2 RUNNING
Completed:	Job 1 COMPLETED	Job 3 COMPLETED	Job 2 COMPLETED

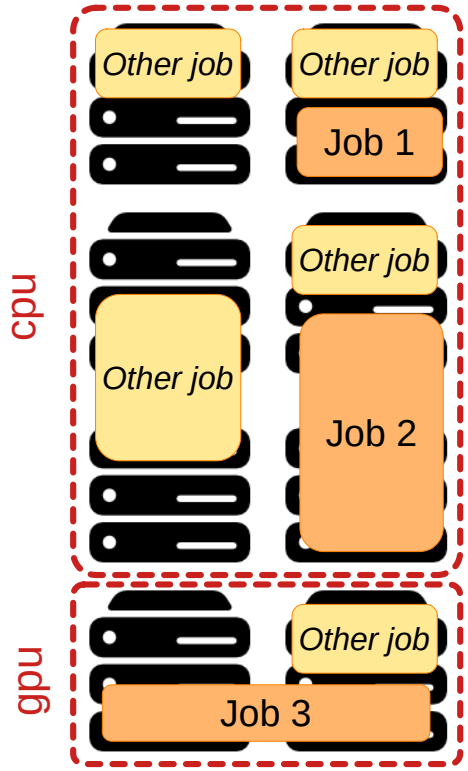
HPC User
submits jobs

```
salloc -A p20XXXX -N 1 -t 2:00 -p cpu -q default
```
→ *Job 1 for 1 CPU node for 2 hours*

```
salloc -A p20XXXX -N 4 -t 6-0  -p cpu -q long
```
→ *Job 2 for 4 CPU nodes for 6 days*

```
salloc -A p20XXXX -N 2 -t 8:00 -p gpu -q default
```
→ *Job 3 for 2 GPU nodes for 8 hours*

Partitions



Compute Nodes

Find and Using Software on HPC with Lmod

Software Modules on HPC

- Manage **user environment** using Environment Modules
- Search and make software available to users
- Using `PATH`, `LD_LIBRARY_PATH` and other environment variables
- Various implementations: **Lmod**, C and Tcl Environment Modules

```
[         @mel0319 ~]$ module avail GROMACS

-------- /apps/USE/easybuild/release/2025.1/modules/all --------
   GROMACS/2025.2-foss-2025a-CUDA-12.8.0
   GROMACS/2025.2-foss-2025a             (D)

  Where:
   D:  Default Module
```

`module avail`: Lists all available modules

`module list`: Shows the loaded modules

`module load <module_name>`: Loads a module to make the software accessible

`module unload <module_name>`: Removes a module from your environment

Other useful commands: `overview`, `spider`, `swap`, `help`, `purge`, `keyword`, …

➔ https://docs.lxp.lu/first-steps/module_system/

MeluXina in practice

What you need to know to use MeluXina

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MeluXina user and project accounts

User account: `u10XXXX`

It identifies a **person** (you)

- First and last name
- Email

It serves for authentication with

- Password
- One-Time Password (OTP)
- Authorized SSH keys

Datapath:

`/home/users/u10XXXX`

Project account: `p20YYYY`

It identifies a **project** (that you can be part of)

- Group of users
- Start and end time

It tracks the resources

- **Computing resources**: `cpu`, `gpu`, `fpga`, `largemem`
- **Storage resources**: `scratch` (Tier1) and `project` (Tier2)

Datapath:

`/project/home/p20YYYY`

`/project/scratch/p20YYYY`

MeluXina shared data storage

Shared storage accessible from any compute node

- Tier1: fast but small → temporary storage
- Tier2: slower but larger → permanent storage

User storage → personal and limited

`/home/users/u10XXXX` → located on Tier2

Project storage → shared with project members, size specific to each project

`/project/home/p20YYYY` → located on Tier2

Preferred location for your work files

`/project/scratch/p20YYYY` → located on Tier1

For multi-user projects → create personal directory within project directory

`/project/home/p20YYYY/u10XXXX`

`/project/home/p201259/workspaces/u10XXXX`

SCynergy 2026 trainings

Tracking your resource usage → myquota

COMPUTE ALLOCATIONS FOR CURRENT MONTH
COMPUTE USAGE FROM 2026-04-01 to NOW

Project	CPU node-hours Used	CPU Max	CPU %used	GPU node-hours Used	GPU Max	GPU %used	FPGA node-hours Used	FPGA Max	FPGA %used
p20[redacted]	0			0			0		
p20[redacted]	0	328	0.0%	0	65	0.0%	0		
p20[redacted]	0			8	130	6.2%	0		

Compute

DATA ALLOCATIONS

Datapath	Data GiB Used	Data GiB Max	Data GiB Use%	No. Files Used	No. Files Max	No. Files Use%
/home/users/[redacted]	90	100	90%	94566	100000	94%
/project/home/p20[redacted]	0	1000	0%	142	1000000	0%
/project/home/p20[redacted]	2428	20000	12%	850390	2000000	42%
/project/scratch/p20[redacted]	0	1024	0%	1	1000000	0%
/project/home/p20[redacted]	0	10240	0%	1467	1000000	0%

Data

Authentication & Access to MeluXina

SSH Key

- Fast, lightweight, and secure
- Allows password-less access
- Most common on HPC platforms
- Requires an advanced configuration

Public SSH key to be upload via the service desk

Used for frequent and password-less operations

- **Shell access** via native terminal applications
- File transfer and synchronization

Username + Password (+ OTP)

- Beginner friendly, easier to setup
- Similar to usual online web-service
- Manual authentication process

Username: **`u10xxxx`**
Password: defined at service desk setup
OTP: defined at first use

Used for interactive and graphical accesses

- **Web-portal access**
  (also includes a shell access)
- Simple file transfer only

Shell Access via SSH

Configuration

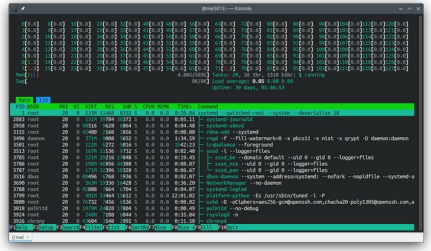
- Public SSH key to be added via service desk
- Configuration file `~/.ssh/config`

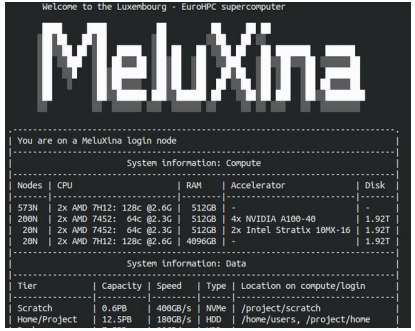
Access

```
ssh meluxina
```

Documentation

- Generating an SSH key
- Uploading your public SSH key
- Connect to MeluXina





Web-portal Access

Configuration

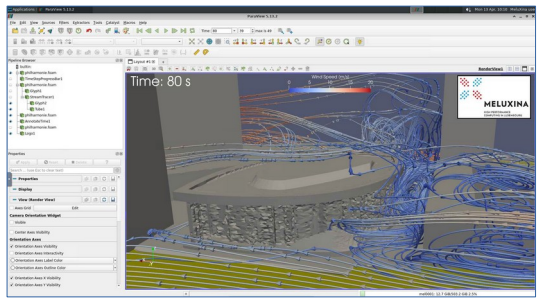
- Password setup in service desk
- One-Time Password (OTP) setup at first access

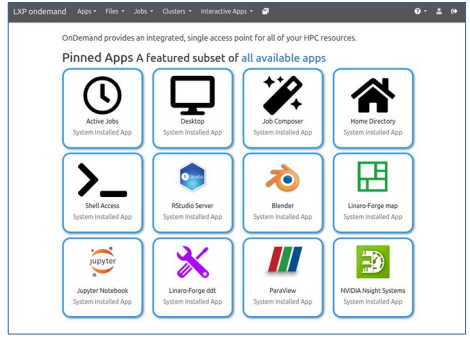
Access

https://portal.lxp.lu/

Documentation

- How to connect to Open Ondemand
- Multi-factor authentication setup





Hands-on!

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- Connecting the MeluXina
- HPC workflow: Urban wind simulation
- AI workflow: Deep learning with PyTorch

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