Introduction to HPC Cluster Use

How to transform Sněhurka into Chimera

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GOALS FOR TODAY

By the end of this session, you should be able to:
- ▶ Log into a Chimera cluster
- ▶ Navigate storage (home, scratch, project) and move data in/out
- ▶ Run software with environment modules
- ▶ Submit and manage batch jobs (Slurm examples)

- ▶ Typical components as represented on Sněhurka:
- ▶ **Login nodes** `r3d3.karlin.mff.cuni.cz` (interactive: edit code, prepare jobs, file/data management)
- ▶ **Compute nodes** `r41, r42, ...` (where your jobs run)
- ▶ **Shared storage** (`/home` , `/work` , `/scratch`)
- ▶ **Scheduler** Slurm (allocates resources and queues work to partitions `express` , `long`)

SOME DEFINITIONS....

Sněhurka (Snow White and the Seven Dwarfs)

Oxford Learner's Dictionaries: a traditional children's story. Snow White is a beautiful princess. Her stepmother is jealous of her beauty and orders a man to kill her. He feels pity for her and leaves her alive in a forest, where she lives happily with seven dwarfs.

Chimera (Χίμαιρα)

Oxford Learner's Dictionaries: a **chimera** is
- a fire-breathing female monster with a lion's head, a goat's body, and a snake's tail
- something that is hoped for but is impossible to achieve.

Merriam-Webster Dictionary: a **chimera** is
- a mythical fire-breathing monster made of parts of different animals
- something made up of very different parts (or an unrealizable illusion).

BASIC COMPARISON

Sněhurka

- about 1024 cores (intel, amd)
- internal net 100 GB/s InfiniBand
- Ubuntu 22.04 LTS

login node: `r3d3.karlin.mff.cuni.cz`
compute nodes: `r30, r31, ..., r50`
home path: `/usr/users/<login>`
work path: `/usr/work/<login>`
local temp path: node local `/tmp`
shared temp path: none

Chimera

- about 3064 cores (intel, amd)
- internal net 200 GB/s InfiniBand
- Rocky Linux 9 OS (EL9 Linux)

login node: `hpc.troja.mff.cuni.cz`
compute nodes: various names + (`r42`)
home path: `/home/<login>`
work path: `/work/<login>` (on request)
local temp path: memory mapped `/tmp`
shared temp path: `/scratch`

Chimera: Information resources

Our info page monitoring the transition:
  - **o** https://cluster.karlin.mff.cuni.cz/relocation/

Main MFF HPC info page:
  - **1** https://www.mff.cuni.cz/en/hpc-cluster/general-information
  - **▶** https://www.mff.cuni.cz/en/hpc-cluster/jupyter-hub

Faculty gitlab service:
  - **2** https://gitlab.mff.cuni.cz/mff/hpc/clusters#mff-hpc-metacenter
  - **3** https://gitlab.mff.cuni.cz/mff/hpc/clusters/-/issues

Existing tutorials from other departments:
ucjf https://ipnp.cz/?page_id=8244

Chimera: Initial steps to create your account

1. Initialize your gitlab account at https://gitlab.mff.cuni.cz
   (Note: Karlin local gitlab is separate service https://gitlab.karlin.mff.cuni.cz)

2. Create your account on Mattermost ☑.

   This is useful to get notifications from admins about planned outages and report possible issues with Chimera and/or JupyterHub.

3. Initialize your Chimera account by loging to JupyterHub service at https://hpc.troja.mff.cuni.cz:8000

   See https://www.mff.cuni.cz/en/hpc-cluster/jupyter-hub for detailed guide.

Credentials

All credentials are your SIS login name and password.

LOGGING IN (SSH)

- From macOS/Linux/WSL (or Windows with an SSH client): use terminal with `ssh` client
- Windows - MobaXterm (`https://mobaxterm.mobatek.net/`), Bitvise ssh (`https://bitvise.com/`)
- Windows VisualCode - caution!

CHIMERA: SSH ACCESS

Once you have you account activated:

```
# 1) Connect to a headnode
ssh <CASname>@hpc.troja.mff.cuni.cz

# 2) Then access the cluster environment
[<CASname>@hpc-head ~]$ pwd
/home/<CASname>
[<CASname>@hpc-head ~]$ ~hron/bin/freenodes
```

Credentials

All credentials are your SIS login name and password.

CHIMERA: SLURM PARTITIONS (QUEUES)

Chimera uses Slurm (`https://slurm.schedmd.com/documentation.html`).
The cluster is divided into several partitions (≈ queues)

- "free-for-all": `ffa` (1h-12h), `ffa-short` (30min-2h), `ffa-preempt`, `ffa-checkpoint`, `gpu-ffa`
- matematicka sekce: `express` (6h-12h), associated only with our nodes
- Education: `edu` (2h-4h)

Always request the **smallest** resources/time that fit your job to start sooner.

CHIMERA: SLURM QUICK COMMANDS

```
# Partitions and node state
sinfo

# Your jobs
squeue -u $USER

# Interactive allocation (example)
salloc -p ffa -n 4 --mem=8G --time 02:00:00

# Batch submission (example)
sbatch -p express job.sbatch
```

Chimera provides:

- ▶ **Environment modules**
- ▶ **Apptainer/Singularity** containers (reproducible environments)
- ▶ **Charliecloud** based on a user-defined software stack (UDSS)

Common storage areas:

- ▶ `/home/<name>` (backed up, smaller quota): suitable for configs, scripts, source code.
- ▶ `/work/<name>` (optional, medium/large): Bigger datasets, computed results.
- ▶ `/scratch/` (fast, temporary): job I/O, checkpoints, intermediates.
- ▶ `/archive/` (slow, permanent :): Archive for bigger data not need imediately

```
df -h

# lfs quota -h /home/<name>
# du -sh /home/<name>/folder
```

Typical options:

- ▶ **scp** (simple copies)
- ▶ **rsync** (fast incremental sync)

```
# Copy a file from local machine to the cluster
scp local.dat <name>@hpc.troja.mff.cuni.cz:/path/to/

# Sync a directory (recommended for repeated transfers)
rsync -avzP ./results/ <name>@hpc.troja.mff.cuni.cz:/path/to/results/
```

SOFTWARE ENVIRONMENTS: MODULES

Many clusters use **environment modules** to manage compilers and applications.

- ▶ You typically start with a clean environment and load what you need.
- ▶ Modules ensure consistent versions across users.

```
module avail
module spider gcc
module load gcc/12.2.0
module list
module purge
```