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Baobab and Yggdrasil - our HPC clusters and their infrastructure

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- CPU MODELS — baobab
- CPU MODELS — baobab
 - GPUs on Baobab
- Yggdrasil
 - CPU MODELS — yggdrasil
 - GPUs on Yggdrasil
- Monitoring performance

How to use the HPC clusters

- [hpc:how_to_use_the_hpc_clusters#](#)

Access : SSH, X2GO

- Access the clusters
 - Account
 - Standard Account
 - External Account
 - Outsider Account
 - Inactivity Notice and Account Deletion Policy
 - Cluster connection
 - login nodes
 - Connect using SSH
 - ssh PublicKey
 - multiple ssh key
 - From Linux and Mac OS
 - From Windows
 - Access to the compute nodes
 - GUI access / Desktop with X2Go
 - File transfer
 - From Linux
 - From Windows
 - SSH tunnel and socks proxy
 - Alternative to using ProxyJump

Best practices and smart use of the HPC resources

- Introduction
- First steps
- Rules and etiquette
- Think green
- Stop wasting resources!

- Which resources ?
- Single thread vs multi thread vs distributed jobs
- Bad CPU usage
- Bad memory usage
- Bad time estimation
- Conclusion
- How to write a good Slurm sbatch script
- Transfer data from one cluster to another
 - Rsync
- SWITCHfilesender from the cluster
 - Configuring the CLI tools
 - Transferring files
- HPC cluster user departure procedure

FAQ

- FAQ: Frequently Asked Question
 - General
 - Cost
 - Account
 - Connection to Cluster
 - X2GO-Desktop
 - Storage
 - Applications
 - Slurm: job scheduler
 - Issues
 - Switch edu-ID Login Issues
 - HPC community forum

Slurm and job management

- Slurm and job management
- What is Slurm ?
- Resources
 - Partitions
 - What is a partition ?
 - Which partition for my job ?
 - Partitions lists
 - Clusters partitions
 - Private partitions
 - Wall time
 - Memory
 - GPU

- CPU
- CPU types
- Single thread vs multi thread vs distributed jobs
- Submitting jobs
 - Batch mode (sbatch)
 - Monothreaded jobs
 - Multithreaded jobs
 - Distributed jobs
 - GPGPU jobs
 - Interactive jobs
 - Job array
 - Advanced usage
 - Job dependency
 - Master/Slave
 - Checkpoint
- Reservation
- Job monitoring
 - Email notification of job events
 - Memory and CPU usage
 - Energy usage
 - CPUs
 - GPUs
 - Other tools
 - spart
 - pestat
 - seff
 - HDF5 profiling plugin
- Cancel jobs
- Job priorities
 - How is the priority of a job determined ?
 - Priority vs. waiting time
 - Backfill mechanism

Storage

- Storage
- Cluster storage
 - Home directory
 - Quota
 - Scratch Directory
 - Quota
 - Data Retention Policy
 - Fast directory
 - Quota

- Local storage
 - Scratch directory (local on each node)
 - Temporary private space
 - Temporary shared space
- Sharing files with other users
- Best practices
 - I/O performance
 - Check disk usage on the clusters
 - Check disk usage on home and scratch
 - Check disk usage on NASAC
 - File transfer (between nodes)
- Backup
- Archive
- Access external storage
 - NASAC
 - Troubleshooting
 - Where does gio mounts my data?
 - List the user DBUS process
 - Sometimes mount is not available but you can browse/copy/interract with gio commands
 - CVMFS
 - EOS
- Robinhood
 - Policies
 - Report

Applications and libraries

- Applications on the clusters
 - Module - lmod
 - How to use 'module'
 - What do I do when an application is not available via 'module' ?
 - Detailed example of using 'module'
 - Loading 'R'
 - Choosing the compiler toolchain
 - FOSS toolchain
 - Intel toolchain
 - Intel compiler licenses
 - fosscuda toolchain
- Examples for selected applications
 - OpenMPI
 - Specify MCA parameters through "srun"
 - Conda
 - How to Create a Conda Environment in a Container

- Benefits
- Limitations
- Step 1 – Define the Conda Environment
- Step 2 – Build the Container
- Step 3 – Use the Container
- Conda environment management
- Package management
- ADF
- Gaussian
- Git
- NVIDIA HPC SDK Installation in Home Directory on a Heterogeneous Cluster
 - Prerequisites
 - Installation Steps
 - Verify Installation
- Gurobi
- Jupyter notebook and Jupyter lab
- Mathematica
- Matlab
 - Parallel with Matlab
 - Pass sbatch arguments to Matlab
 - Compile your Matlab code
 - Matlab PATH
 - Matlab java.opts
 - CHROMIUM mailbox/texture errors
 - Wavelab
- OpenCL
- Distant Paraview
- Python
 - Custom Python lib
 - Pip install from source
- R project and RStudio
 - RStudio
 - R packages
- Variant Effect Predictor (VEP)
 - Install species
- Apptainer (was Singularity)
 - Intro
 - Pull an existing image
 - Convert a Docker image
 - Run a container
 - Modify the image (not persistent)
 - Modify the image (persistent)
 - References
- Stata
- TensorFlow

- [Compile and install a software in your /home](#)

Glossary

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From:

<https://doc.ererearch.unige.ch/> - **eResearch Doc**

Permanent link:

<https://doc.ererearch.unige.ch/hpc/toc?rev=1602166222>

Last update: **2025/06/11 12:27**

