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Baobab and Yggdrasil - our HPC clusters and their infrastructure

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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

[Glossary](#)

VDI - Interactive nodes

[hpc:interactivenodes#](#)

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