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HPC start

- HPC User Documentation
- HPC clusters at UNIGE
    - Use the HPC resources
- RoadMap
    - Other resources
- Support - get help

How to use Linux

- Linux on HPC clusters
- External resources

Baobab and Yggdrasil - our HPC clusters and their infrastructure

- How our clusters work
- The clusters : Baobab, Yggdrasil and Bamboo
- How do our clusters work ?
    - Overview
- Purchase: Hardware Pricing
    - AMD CPU
    - GPU H100 with AMD
    - GPU RTX4090 with AMD
- Use Baobab for teaching
- How do I use your clusters ?
- For advanced users
    - Infrastructure schema
    - Compute nodes
        - CPUs models available
        - GPUs models available
        - Bamboo
            - CPU MODELS — bamboo
            - GPUs on Bamboo
        - Baobab
            - CPU MODELS — baobab
            - GPUs on Baobab

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

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
            - SSH Host Keys Verification
                - Current fingerprints
                - Important
                - How to compute fingerprints (for administrators)
                - X2Go / alternative fingerprint (SHA1)
                - Notes
            - 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

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

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
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- Sharing files with other users
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        - Check disk usage on NASAC
    - File transfer (between nodes)
- Backup
- Archive
- Access external storage
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            - 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

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
  - Slurm Quota
  - 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

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

Glossary

- Glossary

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

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