

High Performance Computing in a Nutshell

HPC Services, NHR@FAU

hpc-support@fau.de

<https://doc.nhr.fau.de>

Which application area do you come from?

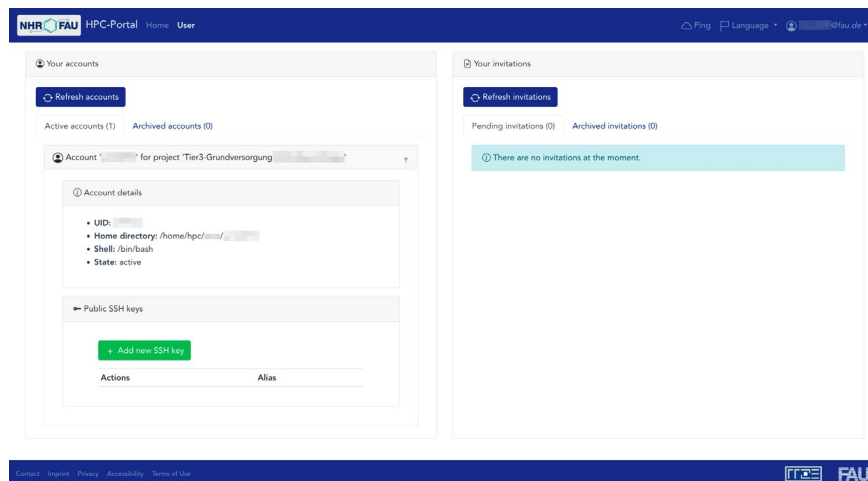


Getting an HPC account

<https://doc.nhr.fau.de/account/>

HPC account – HPC-portal

- Account via portal.hpc.fau.de
- Login to HPC portal with credentials of home institution via SSO
- Invitation has to be sent by project PI/technical contact/contact person at chair
- If you change your affiliation or project, you need a new HPC account. Data migration may be required



The screenshot displays the HPC-portal user interface. The top navigation bar includes the NHR and FAU logos, the text 'HPC-Portal Home User', and utility links for 'Ping', 'Language', and a user profile icon. The main content area is divided into two panels. The left panel, titled 'Your accounts', features a 'Refresh accounts' button and shows 'Active accounts (1)' and 'Archived accounts (0)'. A dropdown menu is open for the active account, showing details for a project 'Tier3-Grundversorgung'. The account details include: UID, Home directory (/home/hpc/...), Shell (/bin/bash), and State (active). Below this is a section for 'Public SSH keys' with an 'Add new SSH key' button and fields for 'Actions' and 'Alias'. The right panel, titled 'Your invitations', has a 'Refresh invitations' button and shows 'Pending invitations (0)' and 'Archived invitations (0)'. A message states 'There are no invitations at the moment.' The footer contains links for 'Contact', 'Help', 'Privacy', 'Accessibility', and 'Terms of Use', along with the NHR and FAU logos.

<https://doc.nhr.fau.de/hpc-portal/>

HPC account – HPC-portal

- No account passwords, cluster login only via SSH keys!
- SSH keys can be managed over HPC portal

The screenshot shows the HPC-Portal interface. At the top, there is a navigation bar with the NHR and FAU logos, the text 'HPC-Portal Home', and a 'User' dropdown menu. Below this, the 'Your accounts' section is visible, featuring a 'Refresh accounts' button and tabs for 'Active accounts (1)' and 'Archived accounts (0)'. A single account is listed, with its name and the project name 'Tier3-Grundversorgung' highlighted with red boxes. Below the account list, the 'Account details' section shows fields for UID, Home directory, Shell, and State. At the bottom of the account list, a '+ Add new SSH key' button is highlighted with a red box.

project is either:

- "Tier3-Grundversorgung"
- name of an NHR project

The screenshot shows the 'Public SSH keys' form. At the top, there are 'Back', 'Submit', and 'Reset' buttons. Below these is a section titled 'Add new SSH key'. It contains an 'Alias' input field with a placeholder text 'Please enter an alias for this SSH key.' and a 'Key Content' text area with a placeholder text 'Please enter the key content of this SSH key.' At the bottom of the form, there is a 'Hide advanced options' button.

How to create SSH keys:
<https://doc.nhr.fau.de/access/ssh-command-line/>

HPC systems at NHR@FAU

<https://doc.nhr.fau.de/clusters/overview/>

Which cluster should I use?

Does your application run on multiple nodes simultaneously?

Yes

(e.g. by using MPI)

Meggie

Fritz

(Tier3 after application)

Accessible for projects

- “Tier3-Grundversorgung”
- NHR

No

Only single-node or single-core work

Does your application use GPUs?

Yes

TinyGPU

Alex

(Tier3 after application)

No

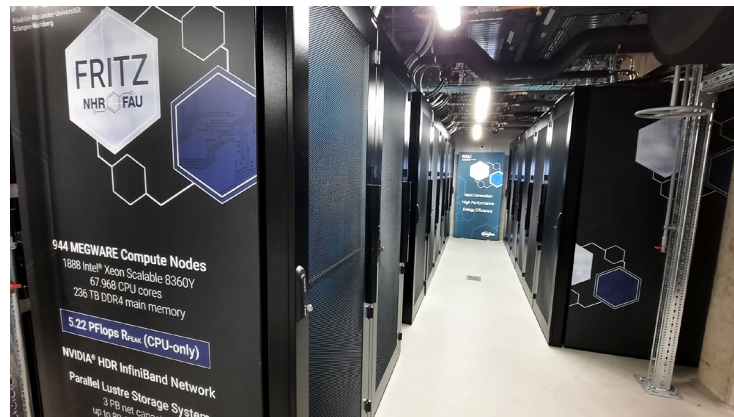
Woody

TinyFat

“Fritz” cluster

NHR parallel cluster, open for Tier3 users after application

- 992 compute nodes (71.424 cores)
 - 2 Intel Xeon Platinum 8360Y “Ice Lake”
2.4 GHz (36 cores)
 - 256 GB main memory per node
- 64 huge-memory nodes
 - 2 Intel Xeon Platinum 8470 “Sapphire Rapids” 2.0 GHz (52 cores)
 - 1 or 2 TB of main memory per node
- Blocking (1:4) HDR100 Infiniband network, up to 100 GBit/s
- Parallel file system with 3,5 PB capacity



“Meggie” cluster

cluster for parallel jobs, intended for highly parallel jobs (Tier3)

- 728 Compute nodes (14.560 cores)
 - 2 Intel Xeon E5-2630 v4 (Broadwell) 2.2 GHz (10 cores)
 - 20 cores/node
 - 64 GB main memory
- No local disks
- Intel OmniPath network: Up to 100 Gbit/s
- To be decommissioned “soon”



“Alex” cluster

NHR GPGPU cluster, open for Tier3 users after application

- 44 nodes with
 - 8x NVIDIA A100 (each 40 GB / 80GB HBM2)
 - 2x AMD EPYC 7713 “Milan” 2.0 GHz, 1024 GB / 2048 GB of main memory
 - 14TB local NVMe SSD
 - HDR200 Infiniband network
- 38 nodes with
 - 8x NVIDIA A40 (each with 48 GB DDR6)
 - 2x AMD EPYC 7713 “Milan” 2.0 GHz, 512 GB of main memory
 - 7 TB local NVMe SSD



“TinyGPU” cluster

for GPU workloads – not all nodes always generally available (Tier3)

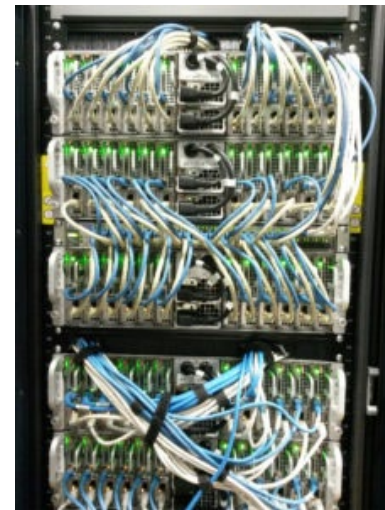
- 12 nodes with 2x “Skylake” @ 3.2 GHz, 96 GB RAM, 1.8 TB SSD, 4x RTX 2080Ti
- 4 nodes with 2x “Skylake” @3.2 GHz, 96 GB RAM, 2.9 TB SSD, 4x Tesla V100
- 7 nodes with 2x “Cascade Lake” @2.9 GHz, 384 GB RAM, 3.8 TB SSD, 8x RTX3080
- 8 nodes with 2x AMD Rome 7662 @2.0 GHz, 512 GB RAM, 5.8 TB SSD, 4x Volta A100



“Woody” cluster

Main workhorse for throughput and single-node jobs (Tier3)

- 176 nodes with 4 cores and high clock frequency (3.5/3.7 GHz) Intel Xeon E3-1240 v? processors
 - 64x Intel Skylake, 32 GB RAM
 - 112x Intel Kaby Lake, 32 GB RAM
- 70 nodes with 2x Intel Xeon Gold 6326 (32 cores total @2.9 GHz, 256 GB RAM)
- at least 960 GB local HDD/SSD
- Gbit network only



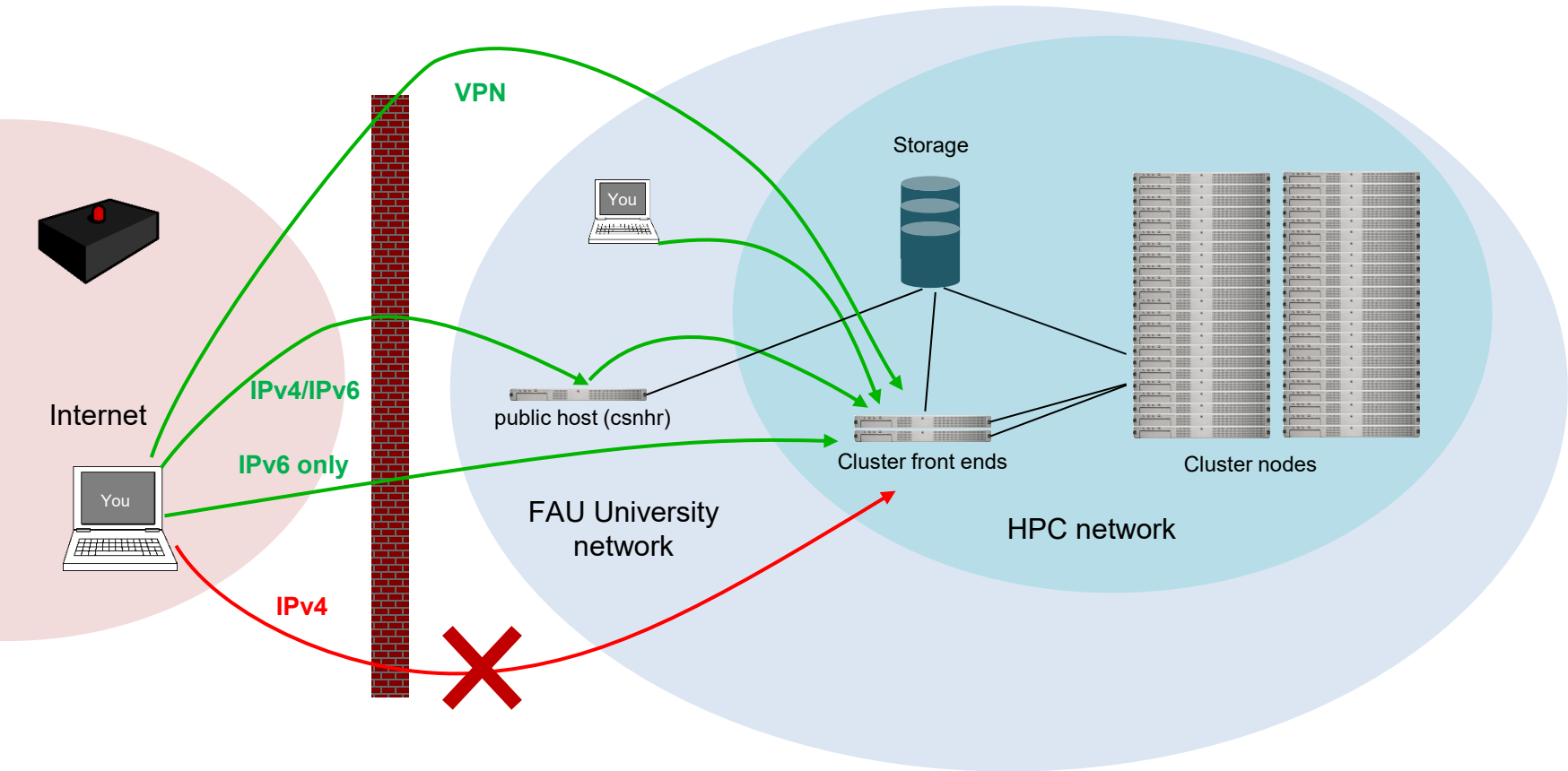
Which cluster(s) are you planning to use?



Accessing HPC systems

<https://doc.nhr.fau.de/access/overview/>

Cluster access



Cluster access

- Cluster frontends: only directly available from within FAU network or via IPv6
 - `meggie.rrze.fau.de`
 - `tinyx.nhr.fau.de` (for TinyGPU/TinyFat)
 - `woody.nhr.fau.de`
 - `alex.nhr.fau.de`
 - `fritz.nhr.fau.de`
- Access from outside FAU network via ProxyJump over dialog server
 - `csnhr.nhr.fau.de`

SSH – Secure Shell

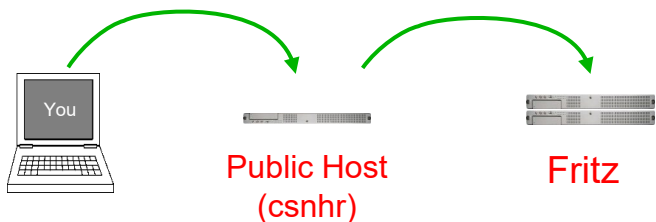
- No GUI is available on the HPC systems. Basic knowledge of file handling, scripting, editing, etc. under Linux is required.
- SSH usage:

```
ssh hpcaccount@csnhr.nhr.fau.de  
ssh hpcaccount@fritz.nhr.fau.de  
ssh hpcaccount@meggie.rrze.fau.de  
ssh hpcaccount@alex.nhr.fau.de
```

- Authentication only with SSH keys uploaded to HPC Portal, no passwords!

SSH – ProxyJump

- On your local machine, modify the file: `~/.ssh/config`
- Connect directly to Fritz using: **ssh fritz**
- General documentation on SSH, how to generate an SSH key and example ssh-config including ProxyJump:
<https://doc.nhr.fau.de/access/ssh-command-line>



```
Host public_host
HostName csnhr.nhr.fau.de
User hpc-account
IdentityFile ~/.ssh/key-file
IdentitiesOnly yes
PasswordAuthentication no
PreferredAuthentications publickey
```

```
Host fritz
HostName fritz.nhr.fau.de
User hpc-account
ProxyJump public_host
IdentityFile ~/.ssh/key-file
IdentitiesOnly yes
PasswordAuthentication no
PreferredAuthentications publickey
```

Secure Shell client programs

- Linux: OpenSSH available
- Mac: OpenSSH available
- Windows
 - MobaXterm (<https://doc.nhr.fau.de/access/ssh-mobaxterm/>)
 - OpenSSH via Command/PowerShell (since Windows 10 v1803)
 - Linux Subsystem for Windows

SSH – Troubleshooting

- Troubleshooting guide: <https://doc.nhr.fau.de/access/ssh-command-line/#troubleshooting>
- FAQs for most frequent SSH problems: <https://doc.nhr.fau.de/faq/#ssh>
- In case of problems with login, send output of the following command to hpc-support@fau.de: `ssh -vv hpcaccount@csnhr.nhr.fau.de`

Working with data

<https://doc.nhr.fau.de/data/filesystems/>

File systems overview

Available file systems differ in size, redundancy and how they should be used

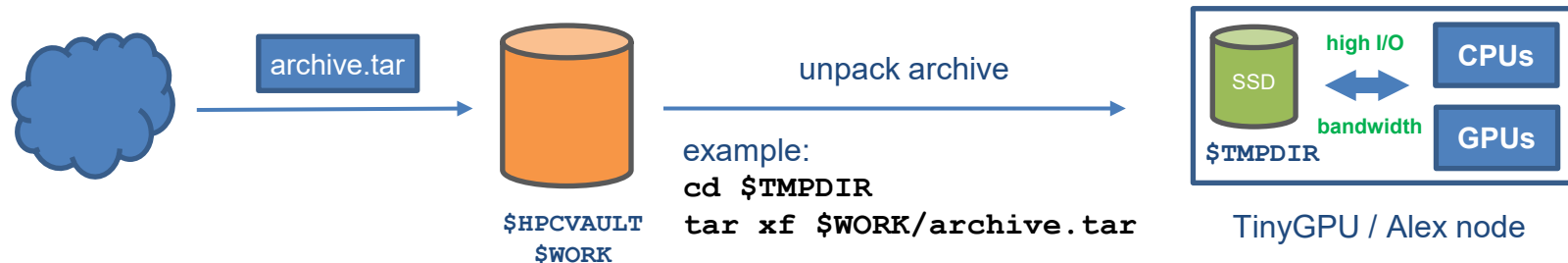
Mount point	Access	Purpose	Technology	Backup	Snapshots	Data lifetime	Quota
/home/hpc	\$HOME	Source, input, important results	NFS	YES	YES	Account lifetime	50 GB
/home/vault	\$HPCVAULT	Mid-/long-term storage	NFS	YES	YES	Account lifetime	500 GB
/home/{woody, saturn, titan, janus, atuin}	\$WORK	General-purpose, log files	NFS	NO	NO	Account lifetime	500 GB NHR project
/lxf /lustre	\$FASTTMP (fritz)	High performance parallel I/O	Lustre via InfiniBand	NO	NO	High watermark	Only inodes
/???	\$TMPDIR	Node-local job-specific dir	SSD/ ramdisk	NO	NO	Job runtime	NO

Working with large datasets containing small files

Best case: use a container file format (HDF5, Parquet, ...)

Alternative: pack small files into archive. Do not unpack archive to
`$HOME/$HPCVAULT/$WORK`

Unpack files to node-local SSDs only and use them from there



More details: <https://doc.nhr.fau.de/data/staging/>

File system quotas

- File system may impose quotas on data volume and/or number of files
- Quotas may be set per user or per group (or both)
- Soft quota
 - Can be exceeded temporarily (7 days)
 - Turns into hard quota at end of grace period
- Hard quota:
 - absolute upper limit, cannot be exceeded

```
$ quota -s           # generic command

$ shownicerquota.pl # only on RRZE systems
  Path                Used      SoftQ    HardQ    Gracetime  Filec    FileQ    FiHaQ    FileGrace
/home/hpc             5.7G    52.5G   104.9G   N/A        72K     500K    1,000K   N/A
/home/woody           112G    333.0G  499.5G   N/A        188K    500K    1,000K   N/A
```


Data transfer

- `$HOME`, `$HPCVAULT`, `$WORK` are mounted on all HPC systems
- `scp` / `rsync` is used to transfer files from and to the outside
<https://doc.nhr.fau.de/data/copying/>

```
scp [options] source destination
source/destination: local-path | username@host:remote-path
```

```
# local file to remote
# -r recurse into directories
scp -r code unrz55@csnhr.nhr.fau.de:/home/woody/unrz/unrz55
# remote file to local
scp unrz55@csnhr.nhr.fau.de:results/output.dat .
```

- Additionally on Windows: WinSCP, MobaXTerm
- Mount filesystems locally via `sshfs` or your Linux desktop
<https://doc.nhr.fau.de/data/mounting/>

Snapshots for \$HOME and \$HPCVAULT

- Files can be recovered, if they are included in a previous snapshot
- Snapshots are stored in the hidden directory *.snapshots*

```
cd .snapshots= #Snapshots Folder
```

- Display the list of snapshots

```
ls -l  
drwx----- 22 hpcxxx hpc 16384 Nov  5 08:25 @GMT-2024.11.08-03.00.00  
drwx----- 22 hpcxxx hpc  4096 Nov  8 13:16 @GMT-2024.11.11-08.00.00
```

- Restore a deleted file

```
cp '$HOME/PATH/.snapshots/@GMT-2019.03.05-03.00.00/myfile' '$HOME/PATH/myfile'
```

<https://doc.nhr.fau.de/data/filesystems/#snapshots-for-home-and-hpcvault>

Software

Environment modules: <https://doc.nhr.fau.de/environment/modules/>
Development and Tools: <https://doc.nhr.fau.de/sdt/overview/>
Applications: <https://doc.nhr.fau.de/apps/overview/>

What type of software are you using?



One thing up front...

- The clusters at the computing center are not like your own PC
 - **You are not root**, even if the “How-To” in the github repo you found assumes that
 - **Do not blindly copy&paste** commands you do not understand
 - **Your home directory is not a local hard disk** but a shared volume that is mounted over the network
- Things that do not work:
 - `sudo apt install python-3.9`
 - `make && sudo make install`
 - `sudo <anything>`
 - `pip install pandas`

Environment modules

- Linux **standard distro packages** are available on **frontends** and to some extent on compute nodes, but they might be outdated.
- **Additional software** is provided via **environment modules**
 - Compilers, libraries, commercial and open software
 - Installed on central server and available on all cluster nodes
- Environment modules are **managed through the `module` command**
- All **`module`** commands affect **the current shell only!**

The module command

Show all available modules: `module avail`

```
$ module avail
```

```
----- /apps/modules/data/applications -----  
amber/20p12-at21p11-impi-gnu                gromacs/2021.5-gcc11.2.0-impi-mkl  
amber/20p12-at21p11-impi-intel             gromacs/2022.1-gcc11.2.0-ompi-mkl  
amber/20p12-at21p11-openmpi-gnu-cuda11.5   gromacs/2022.1-gcc11.2.0-mkl-cuda  
----- /apps/modules/data/compiler -----  
gcc/10.3.0  gcc/11.2.0  gcc/12.1.0  intel/2021.4.0  intel/2022.1.0  nvhpc/22.1  nvhpc/22.2  
----- /apps/modules/data/development -----  
cuda/11.3.1                intelmpi/2021.4.0                openmpi/4.1.2-gcc11.2.0-cuda  
cuda/11.4.2                intelmpi/2021.6.0                openmpi/4.1.2-intel2021.4.0-cuda  
cuda/11.5.0                openmpi/4.1.2-gcc10.3.0-cuda     openmpi/4.1.2-oneapi2021.4.0-cuda
```

The module command

Load a module: `module load <modulename>`

```
$ module load intel/2021.4.0
$ icc -V
Intel(R) C Intel(R) 64 Compiler Classic for applications running on Intel(R) 64, Version 2021.4.0 Build
20210910_000000
Copyright (C) 1985-2021 Intel Corporation. All rights reserved.
```

Display loaded modules: `module list`

```
$ module load openmpi/4.1.2-intel2021.4.0
$ module list
Currently Loaded Modulefiles:
1) intel/2021.4.0 <aL> 2) openmpi/4.1.2-intel2021.4.0
```


Module command summary

Command	What it does
<code>module avail</code>	List available modules
<code>module whatis</code>	Shows verbose listing of all modules
<code>module list</code>	Shows which modules are currently loaded
<code>module load</code> <code><pkg>/<version></code>	Loads specific version of module package, i.e. adjusts environment
<code>module unload <pkg></code>	Undoes what the load command did
<code>module help <pkg></code>	Shows a detailed description of package
<code>module show <pkg></code>	Shows which environment variables are modified and how

<https://doc.nhr.fau.de/environment/modules/>

Using Python

- Use anaconda modules instead of system installation

```
$ module avail python
----- /apps/modules/modulefiles/tools -----
python/3.6-anaconda  python/3.7-anaconda (default)  python/3.8-anaconda
```

- Install packages via conda/pip with `--user` option
- Change default package installation path from `$HOME` to `$WORK`
- It might be necessary to configure a proxy to access external repositories
- Build packages in an interactive job on the target cluster (especially for GPUs)

- More details:
 - <https://doc.nhr.fau.de/sdt/python/>
 - <https://doc.nhr.fau.de/environment/python-env/>

- More info on using python modules with AI-based workflows in the AI Nutshell Intro (tomorrow)

Running jobs

https://doc.nhr.fau.de/batch-processing/batch_system_slurm/

Interactive work on the front-ends

- The cluster **frontends** are for **interactive work**
 - Editing, compiling, preparing input,...
 - Front-ends are shared among all users, so **be considerate!**
 - Amount of compute time per binary is limited by system limits
 - E.g., after 1 hour of CPU time your process will be killed
 - **MPI jobs are not allowed on front ends**
- **Submit** computational **intensive work** to the **batch system** to be run on the compute nodes!
- Use interactive batch jobs for debugging and testing.

Batch System

- Users can interact with the resources of the cluster via the “Batch system”
- “Batch jobs” encapsulate:
 - Resource requirements (number of nodes, number of GPUs, ...)
 - Job runtime (usually max. 24 hours)
 - Setup of runtime environment
 - Commands for application run
- Batch system will handle queuing of jobs, resource distribution and allocation
- Job will run when resources become available



Example: Batch script for Fritz

```
#!/bin/bash -l
#SBATCH --nodes=4
#SBATCH --ntasks-per-node=72
#SBATCH --time=06:00:00
#SBATCH --job-name=testjob_cpu
#SBATCH --export=NONE

unset SLURM_EXPORT_ENV

module load openmpi

srun ${HOME}/bin/a.out -i inp
```

Resource requirements

Max. runtime

Other job options (name, notifications,...)

Prevent export of environment to job

Set up job environment

Actual run of your binary

Example: Batch script for Alex

```
#!/bin/bash -l
```

```
#SBATCH --gres=gpu:a40:1
```

Resource requirements

```
#SBATCH --time=06:00:00
```

Max. runtime

```
#SBATCH --job-name=testjob_gpu
```

```
#SBATCH --export=NONE
```

Other job options (name, notifications,...)

```
unset SLURM_EXPORT_ENV
```

Prevent export of environment to job

```
module load python
```

```
conda activate test-environment
```

Set up job environment

```
python train.py
```

Actual run of your binary

Example: Batch script for Alex

```
#!/bin/bash -l
```

```
#SBATCH --gres=gpu:a40:1
```

Resource requirements

```
#SBATCH --time=06:00:00
```

Max. runtime

```
#SBATCH --job-name=testjob_gpu
```

```
#SBATCH --export=NONE
```

Other job options (name, notifications,...)

```
unset SLURM_EXPORT_ENV
```

Prevent export of environment to job

```
module load python
```

```
conda activate test-environment
```

```
cd $TMPDIR
```

Set up job environment

```
tar xzf $WORK/large-archive-with-conda-environment.tar.gz
```

```
python train.py
```

Actual run of your binary

Slurm batch job submission

```
hpcuser@fritz1$ sbatch script.sh
Submitted batch job 675329
```

```
hpcuser@fritz1:~ $ squeue -l
```

JOBID	PARTITION	NAME	USER	STATE	TIME	TIME_LIMI	NODES	NODELIST (REASON)
675329	multinode	testjob_cpu	hpcuser	RUNNING	0:06	06:00:00	4	f[0116,0120,0159,0264]

Job stdout/stderr will be stored in files in the submit directory

- Use `--output=<outfile>` and `--error=<errfile>` options to change that

Specific for TinyFat/TinyGPU:

- All jobs are submitted from the frontend `tinym.nhr.fau.de`
- Wrapper scripts have to be used for all Slurm commands (e.g. `sbatch.tinygpu`, `sbatch.tinyfat`, `squeue.tinygpu`, ...)

GPU Jobs on TinyGPU / Alex

- Nodes are shared, GPUs are always exclusive
- Granularity is one GPU with a corresponding portion of CPU and main memory
- Request GPUs with **sbatch** option e.g.
 - `--gres=gpu:rtx3080:1` (to request a specific type)
 - `--gres=gpu:a100:1 --partition=a100` (necessary for V100 and A100 GPUs on TinyGPU)
- More details and examples:
<https://doc.nhr.fau.de/clusters/alex/>
<https://doc.nhr.fau.de/clusters/tinygpu/>

Interactive batch job with Slurm

- TinyGPU / Alex

```
iww042@tinysx$ salloc.tinygpu --gres=gpu:1 --time=01:00:00
```

```
iww042@alex1$ salloc --gres=gpu:a40:1 --time=01:00:00
```

- Meggie / Fritz:

```
iww042@meggie1$ salloc --nodes=1 --time=01:00:00
```

- Woody / TinyFat

```
iww042@woody$ salloc --ntasks=1 --time=01:00:00
```

```
iww042@tinysx$ salloc.tinyfat --cpus-per-task=10 --time=01:00:00
```

Slurm documentation

- NHR@FAU
 - General: https://doc.nhr.fau.de/batch-processing/batch_system_slurm/
 - Cluster-specific: <https://doc.nhr.fau.de/clusters/overview/>
 - HPC Café on “Slurm - basics, best practices and advanced usage”:
<https://hpc.fau.de/files/2022/04/2022-04-12-hpc-cafe-slurm.pdf>,
<https://www.fau.tv/clip/id/41306>
- Official Slurm documentation
 - Separate documentation for every command and the available options:
https://slurm.schedmd.com/man_index.html
 - Slurm commands and their counterparts in different batch systems:
<https://slurm.schedmd.com/rosetta.pdf>
 - Slurm tutorials: <https://slurm.schedmd.com/tutorials.html>

Some Dos and don'ts

Good practices

- **Be considerate.** Clusters are **valuable shared resources** that have been paid by the **taxpayer**.
- Use the **appropriate** amount of **parallelism**
 - Most workloads are not highly scalable
 - Best to run scaling experiments to figure out “sweet spot”
- Use the **appropriate file system(s)**
 - #1 mistake: Overload file servers by doing tiny-size, high-frequency I/O to FS
 - Delete obsolete data

Good practices

- **Check your jobs** regularly
 - Are the results OK?
 - Does the job actually use the allocated nodes in the intended way? Does it run with the expected performance?
 - Check if your job makes use of the GPUs
 - **Attach to a running job** (https://doc.nhr.fau.de/batch-processing/batch_system_slurm/#attach-to-a-running-job)
 - Use e.g. nvidia-smi to check GPU utilization
- **Job Monitoring**
 - How to use it and what to look out for: <https://doc.nhr.fau.de/job-monitoring-with-clustercockpit/>

Good practices

- **Talk to co-workers** who are more experienced cluster users; let them educate you
- **Do not re-use** other people's job scripts **if you don't understand** them completely
- Look at tips and tricks for various applications (e.g. example batch scripts):
<https://doc.nhr.fau.de/apps/overview/>
- Have a look at **HPC Café** talks from past events:
<https://hpc.fau.de/systems-services/support/hpc-cafe/>

Good practices

When reporting a problem to NHR@FAU:

- Mail to hpc-support@fau.de – this will immediately open a helpdesk ticket
- **Provide as much detail as possible** so we know where to look
 - “My jobs always crash” will not do
 - Cluster, JobID, file system, time of event, ...
 - Batch script, output files, ...
 - SSH problems: `ssh -vv`



THANK YOU.

NHR@FAU

<https://doc.nhr.fau.de>

hpc-support@fau.de