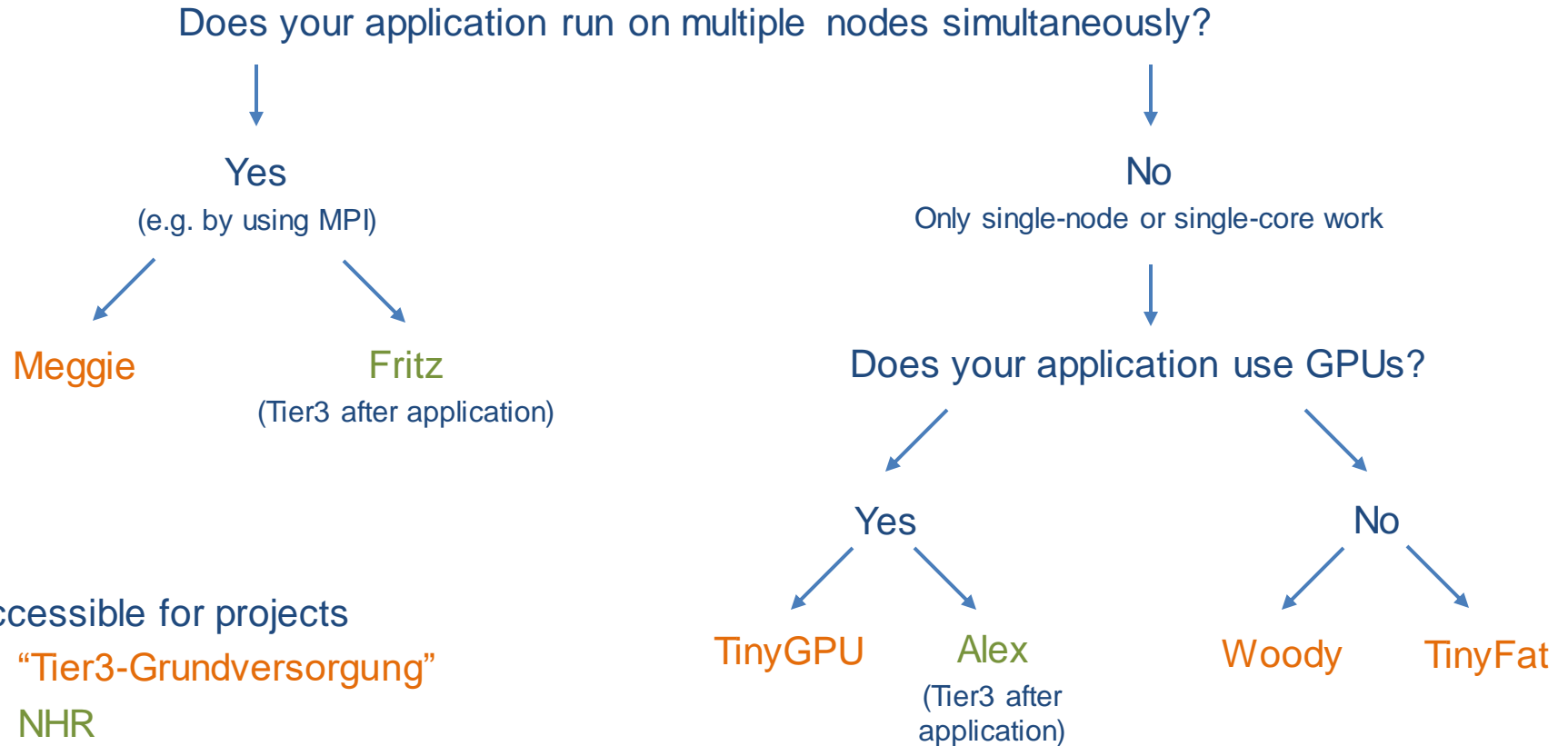


HPC systems at NHR@FAU

<https://hpc.fau.de/systems-services/documentation-instructions/>

Which cluster should I use?



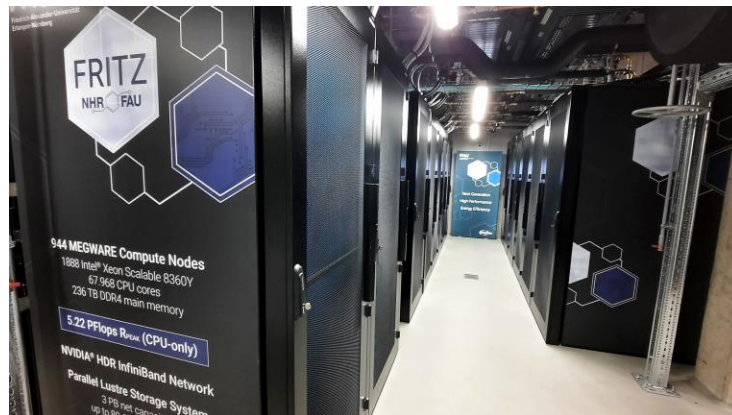
Accessible for projects

- “Tier3-Grundversorgung”
- NHR

“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

current main 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



“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



File Systems

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 (Tier3) NHR project quota
/lxf /lustre	\$FASTTMP (fritz+alex)	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

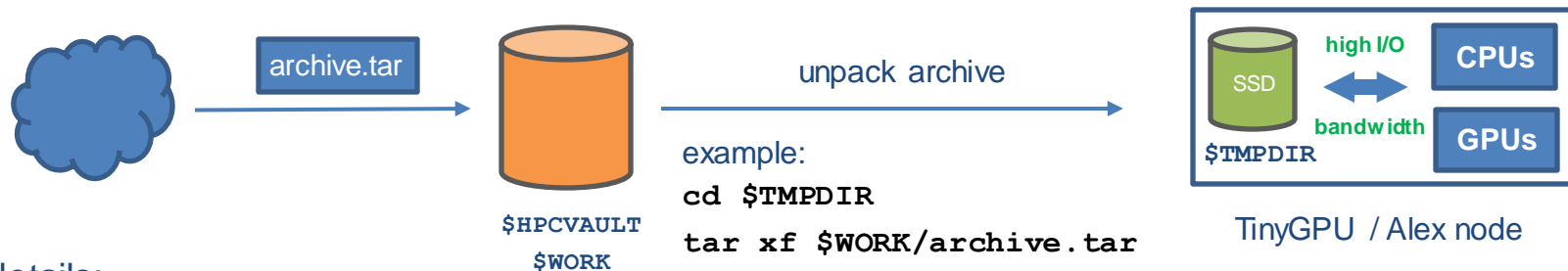
Working with large datasets containing small files

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

- if necessary, copy to node-local SSD

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://hpc.fau.de/files/2022/01/2022-01-11-hpc-cafe-file-systems.pdf>

<https://www.fau.tv/clip/id/40199>

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
```

Data transfer

- `$HOME`, `$HPCVAULT`, `$WORK` are mounted on all HPC systems
- `scp` / `rsync` is used to transfer files from and to the outside

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

```
# local file to remote  
# -r recurse into directories  
scp -r code user@cshpc.rrze.fau.de:/home/woody/group/user  
# remote file to local  
scp user@cshpc.rrze.fau.de:results/output.dat .
```

- Additionally on Windows: WinSCP, MobaXTerm