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Friedrich-Alexander-Universität Erlangen-Nürnberg

AI on High Performance Computing in a Nutshell

HPC Services, NHR@FAU

hpc-support@fau.de

https://doc.nhr.fau.de

High Performance Computing

Agenda

This presentation is a follow-up to **"HPC in a Nutshell"** and assumes familiarity with foundational HPC concepts discussed there. It is highly recommended to review the **HPC in a Nutshell** presentation before proceeding with this material.

1. **Introduction**
   - Why efficient data formats matter in HPC.
   - Challenges with many small files.
2. **Common Dataset Formats**
   - Overview of formats like HDF5, NetCDF, Parquet, webdatasets
3. **When to Use Python venvs, Conda, or Containers**
   - Guidelines for choosing the right tool for environment management.
4. **Benefits of These Formats and Tools**
   - Parallel I/O, metadata efficiency, compression, and scalability.
5. **Conclusion and Best Practices**
   - Recap of efficient data handling on HPC systems.

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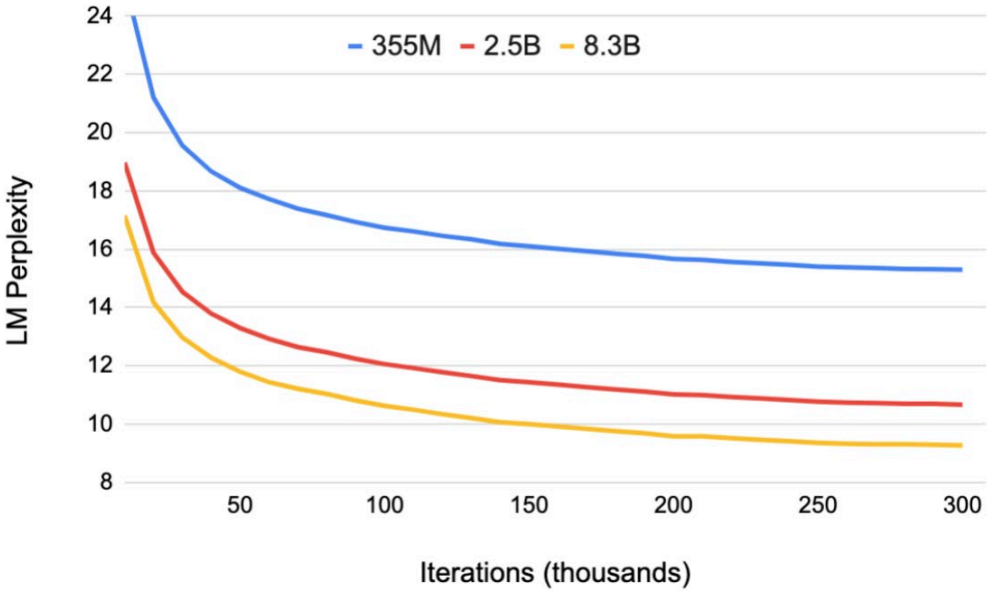
Introduction to AI and HPC

Why is HPC essential for AI workloads?

- AI scales with massive parallel processing
- GPUs can handle thousands of operations in parallel, greatly speeding up tasks like matrix multiplication in neural networks
- HPC GPU Clusters are needed to scale AI-Models and reduce training time

Why is scaling AI important?

- “As the model size increases, the validation perpelixity decreases and reaches a validation perplexity of 9.27 for the 8.3B model”
- “We observe the trend that increasing model size also leads to lower perplexity on WikiText103 and higher cloze accuracy on LAMBADA”



* Megatron-LM: Training Multi-Billion Parameter Language Models Using Model Parallelism https://arxiv.org/pdf/1909.08053

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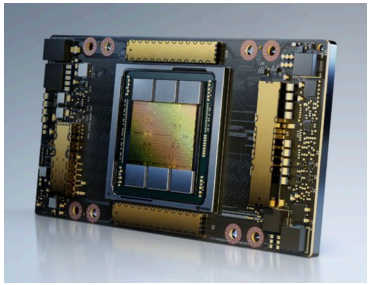
HPC systems at NHR@FAU

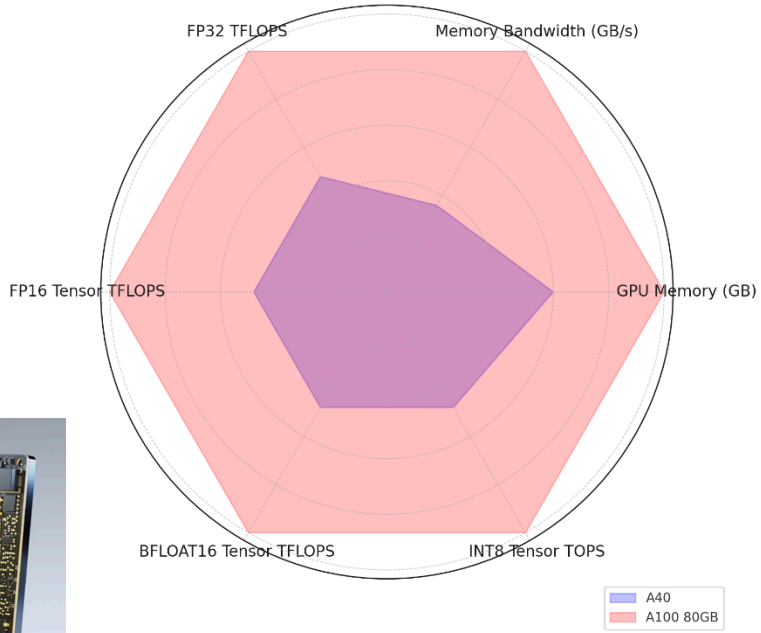
https://doc.nhr.fau.de/clusters/overview/

“Alex” cluster

NHR GPGPU cluster, open for Tier3 users after application
Application through PI

- 44 nodes with
  - 8x **NVIDIA A100** (each 40 GB / 80GB HBM2)
  - 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)
  - 512 GB of main memory
  - 7 TB local NVMe SSD

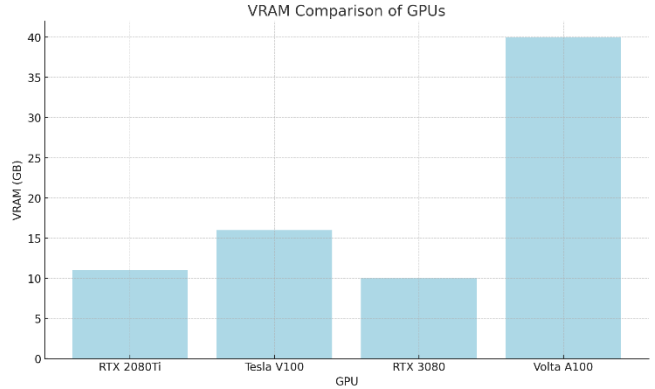


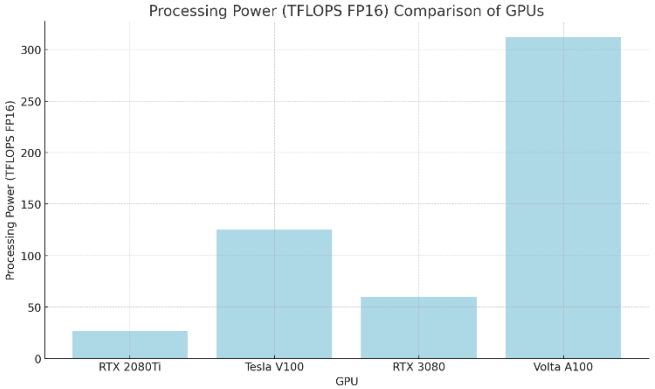


“TinyGPU” cluster

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

- 12 nodes with 4x RTX 2080Ti
- 4 nodes with 4x Tesla V100
- 7 nodes with 8x RTX3080
- 8 nodes with 4x Volta A100





Which GPUs should I use?

Does your training need multiple GPUs and your code is supporting it?

Yes
(e.g. by using fsdp or deepspeed)

Does your Model fit into the VRAM?
(for example Large Scale AI Models)

Yes

Look at A100 40GB or A40

No

Add GPUs or choose A100 80GB

Accessible for projects

- “Tier3-Grundversorgung”
- NHR

No
Only a single GPU

Do you need very large amounts of VRAM

Yes

A100 80GB

No

Is your GPU fully utilized and the training still too slow?

No

A40, TinyGPU

Yes

A100 40GB

Survey

Which cluster(s) are you planning to use?

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Accessing HPC systems

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

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`

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Working with data for AI

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	Snap-shots	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
/???	$TMPDIR	Node-local job-specific dir	SSD/ ramdisk	NO	NO	Job runtime	NO
/anvme/???	$ws_find <name>)	General-purpose	anvme	NO	NO	Upto 90 days, extendable 10x	-

Working with workspaces on ALEX

Store large models and datasets on workspaces and safe time while loading the model/data

- Create workspace with name <name> for the duration of <days> days:
  - After <days> the workspace will be deleted.
  - <days> must be in the range of 1 to 90 days.
  - If <days> is omitted, duration is 1 day.
  - Duration can be changed and extended multiple times later

- `ws_allocate <name> [<days>]`
- `ws_find <name>`

More details: https://doc.nhr.fau.de/data/workspaces/

Datasets Preprocessing

Use non GPU-Machines if you don‘t need GPU-acceleration for preprocessing

- Use standard dataset file formats and integrations (for example parquet)
- Preprocess the Dataset separately before the training and not during the training

- Example of CPU only machines for preprocessing:
  - Memoryhog
  - TinyFat

More details: https://doc.nhr.fau.de/clusters

Working with large datasets containing small files

- In a job, avoid *accessing* large numbers of files
  `$HOME, $HPCVAULT, $WORK, $SATURNHOME`
- Expensive operations on NFS (and also parallel file systems):
  - Access file stats like creation/modification time, permissions…
  - Opening/closing files
- These cause high load on servers
  - This slows down your job and impacts all other users
- Use instead
  - if supported by application: HDF5, file-based databases
  - pack files into an archive (e.g. tar + optional compression) and use node-local SSDs
    (huge amounts of file opens are no problem there)

Efficient Dataset Formats for HPC Clusters

- HPC systems handle large-scale data efficiently.
- Avoid many small files: reduces metadata overhead and optimizes I/O.
- Use formats designed for parallel processing and scalability.
- Example for formats:
  - **HDF5:** Hierarchical data, parallel I/O, compression.
  - **NetCDF:** Multidimensional scientific data, metadata-rich.
  - **Parquet:** Columnar storage, efficient for analytics.

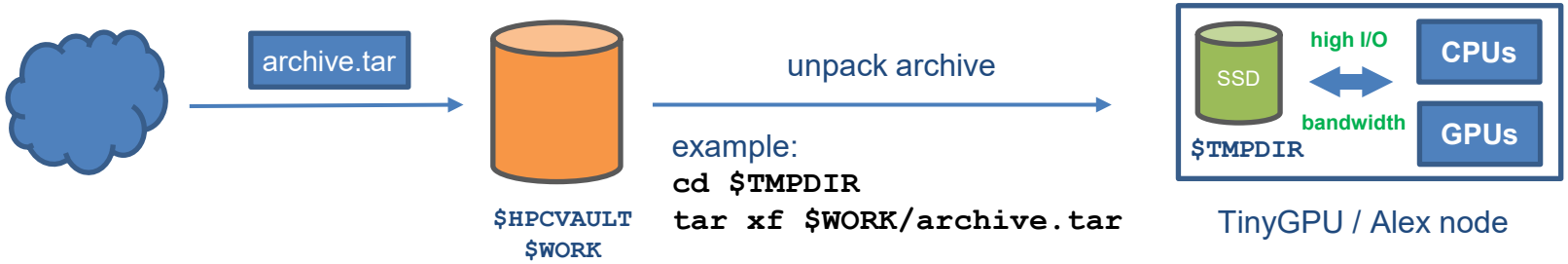
Efficient Dataset Formats for HPC Clusters

- Webdatasets https://huggingface.co/docs/hub/datasets-webdataset
- **Overview:** Efficient data pipeline for large-scale datasets.
- **Storage:** Dataset stored as sharded TAR archives.
- **Benefits:**
  - Reduces I/O overhead with fewer file operations.
  - Optimized for streaming and parallel loading.
- **Use Case:** Ideal for training ML models on distributed systems.
- **Integration:** Compatible with Hugging Face and PyTorch DataLoaders.

Working with large datasets containing small files

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

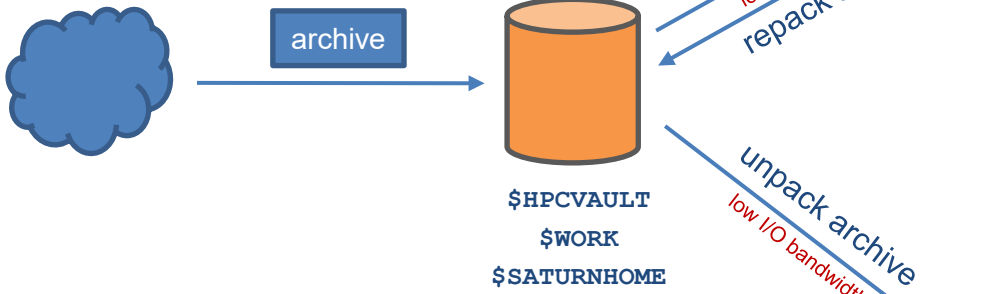
Alternative: pack small files into archive. Do not unpack archive to `$HOME/$HPCVAULT/$WORK`
Unpack files to node-local SSDs only and use them from there



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

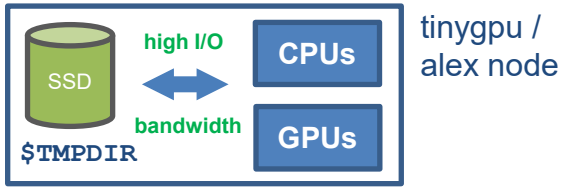
Working with large datasets containing small files

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



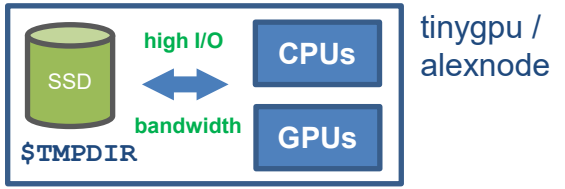
Optionally: if original archive must be altered

- unpack it to node local SSD (interactive job)
- optionally change files
- repack files and copy back to NFS



For simulation, training, …

- unpack archive to node local SSD
- perform simulation/training
- see later slides for details



Environments

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/

Survey

What type of frameworks are you using?

One thing up front…

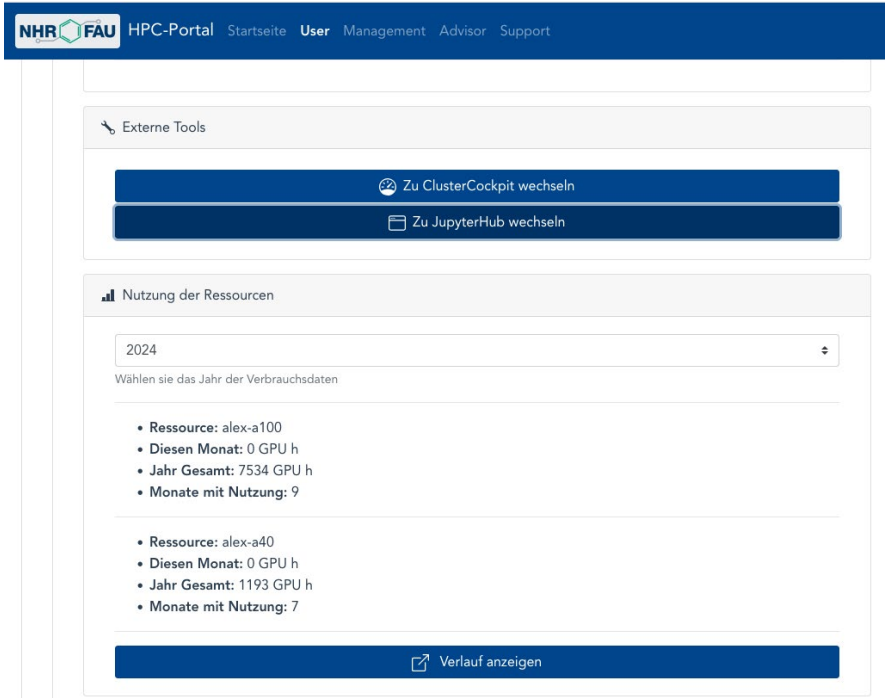
- The clusters at the computing center are not like your own PC
  - You are not root, even if the “How-To” in the github repo you found assumes that
  - Do not blindly copy&paste commands you do not understand
  - Your home directory is not a local hard disk but a shared volume that is mounted over the network

- Things that do not work:
  - `sudo apt install python-3.9`
  - `yum install`
  - `make && sudo make install`
  - `sudo <anything>`
  - `pip install pandas`

JupyterNotebook

- Start your Jupyternotebook from https://portal.hpc.fau.de

1. Login at the HPC Portal.
2. Go to the **User** page.
3. Under **Your accounts**, select the **Account** you want to use for JupyterHub. You might have more than one account.
4. Click on the button **Go to JupyterHub**.
5. A new window opens where you have to accept our Terms of Service and then get redirected to the actual JupyterHub.

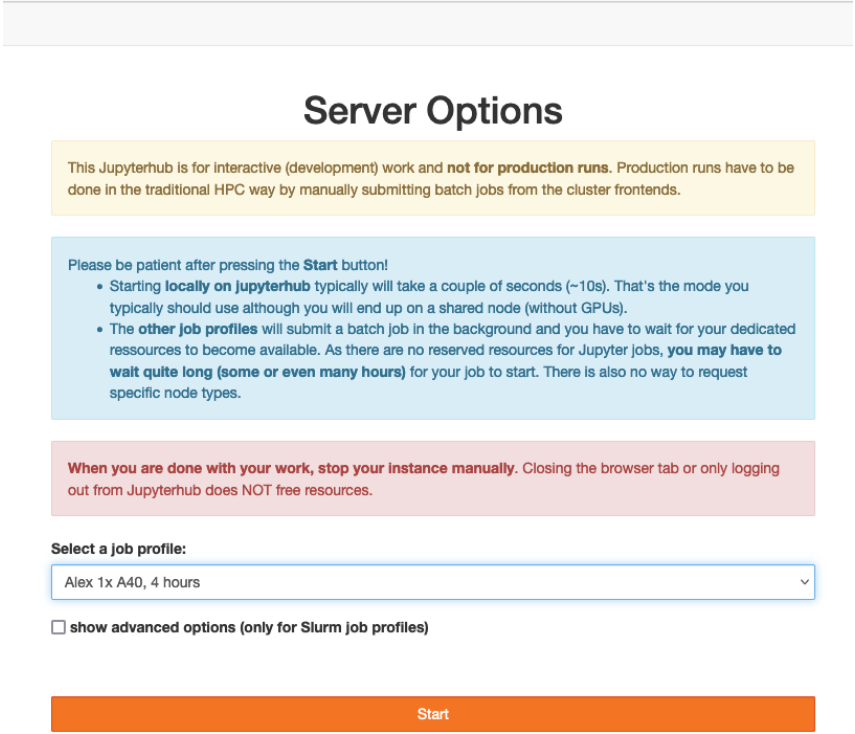


- Available ressources NHR:

JupyterNotebook

- Available resources NHR:
  - 2 cores/4GB on a shared node,
  - one A40 or A100 GPU in Alex,
  - one node of Fritz
- Available resources Tier-3:
  - 2 cores/4GB on a shared node
  - 1 – 4 dedicated GTX1080Ti GPUs
  - 1 – 4 cores and 8 – 32 GB on TinyFat

When you are done with your work, **stop** your jupyter instance manually. Closing the browser tab or only logging out from Jupyterhub does NOT free resources.



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
```

Load a module: `module load <modulename>`

Display loaded modules: `module list`

Module command summary

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

Setting up a python environment

1. If not already exists, create the file ~/.bash_profile (located in your $HOME) with the following content:
   ```
   if [ -f ~/.bashrc ]; then . ~/.bashrc; fi
   ```
2. Ensure you have a Python module loaded:
   ```
   module list
   # output should contain a Python module:
   # Currently Loaded Modulefiles:
   # 1) python/3.9-conda
   ```
3. Store newly installed conda packages and conda environments under $WORK to save space in $HOME by executing:
   ```
   conda config --add pkgs_dirs $WORK/software/private/conda/pkgs
   conda config --add envs_dirs $WORK/software/private/conda/envs
   ```
4. Check the configuration is used, note that the variable $WORK will be expanded to the real path:
   ```
   conda info
   # output should contain:
   # package cache : /apps/python/...
   # <real path of $WORK>/software/private/conda/pkgs
   # envs directories : /apps/python/...
   # <real path of $WORK>/software/private/conda/envs
   ```

Setting up a python environment

- Not all compute nodes have direct internet access. Configure a proxy to enable access, either in the shell:

```
export http_proxy=http://proxy:80
export https_proxy=http://proxy:80
```

- `conda create -n <env. name> python=<py. version>`
  - This creates a conda environment named <env. name>
  - The new environment uses Python of the specified version <py. version>
- `conda activate <env. name>`

Source: https://doc.nhr.fau.de/environment/python-env/

Installing LitGPT example

- Claim GPU:

```
srun --gres=gpu:1 --partition=a40 -t 0-2 --pty /bin/bash -l
```

- Load Module

```
module avail ..
module load git/2.X.X
module load python/3.X-anaconda
```

- Get internet connection

```
export http_proxy=http://proxy:80
export https_proxy=http://proxy:80
```

- Create and activate Conda Environment

```
conda create -n litgpt python=3.10
conda activate litgpt
```

- Create or use workspace

```
ws_allocate litgpt 90
ws_find <name>
```

Installing LitGPT example

- Clone litgpt into workspace directory:

```
cd /anvme/workspace...
git clone https://github.com/Lightning-AI/litgpt
cd litgpt
pip install -e '.[all]'
```

Example conda module installation

- [93m [WARNING] [0m async_io: please install the libaio-devel package with yum
- Package is not available and we have no rights to do yum install

```
conda config --add channels conda-forge
conda config --set channel_priority strict
conda install libaio
```

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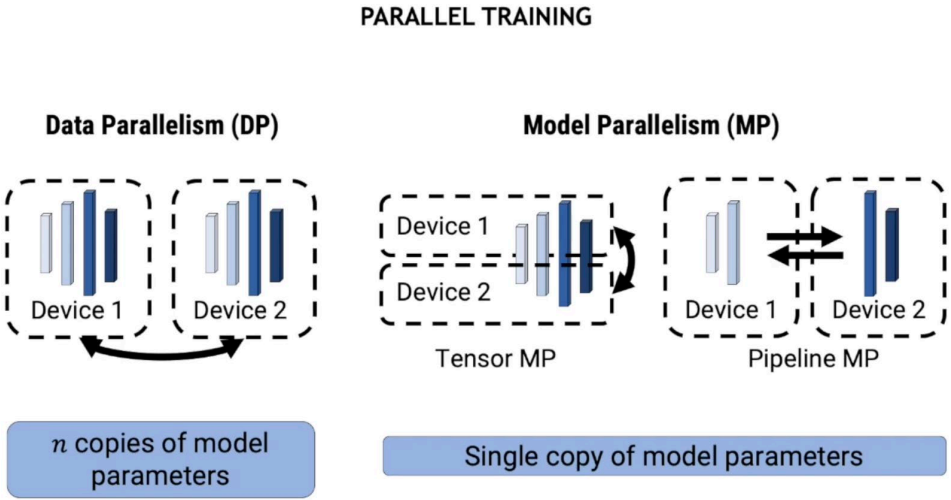
Scaling AI

Parallel Training



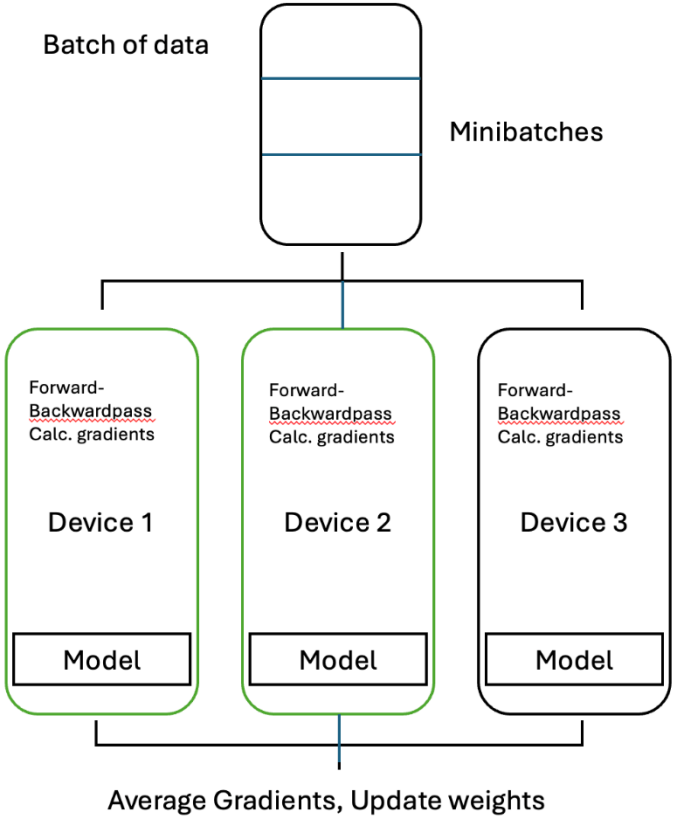
- Trainings will not automatically scale across GPUs
- The right techniques have to be chosen for your model and data
- Trainingframeworks are useful as they often propose best practices

Data Parallelism

- Batch gets split up between models
- Weight updates combined by Allreduce

- Shortcomings:
  - Cannot scale infinitively like 3000 gpu -> Batchsize has to be big enough for example
  - Large models don't fit on a single device

➔ That's why we need Model Level Parallelism
  - ➔ Splits up the layer of a model and calculates only a part of the input
  - ➔ That's Tensor level Parallelism



Implementations

- Frameworks should be used instead of coding parallelization strategies from scratch
- Compatibility with model requirements: Ensure the framework supports the model's architecture, size, and resource needs (e.g., sharding, pipeline parallelism)

Pytorch:

- FSDP (Fully Sharded Data Parallel) enables memory-efficient large model training

Deepspeed:

- Efficient memory use with ZeRO, supports trillion-parameter models
- Mixed precision and pipeline parallelism for faster training

Tensorflow:

- tf.distribute.Strategy for scalable multi-GPU/TPU training

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Running jobs

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

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

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/

Example: Batch script for Alex

```
#!/bin/bash -l
#SBATCH --gres=gpu:a40:1
#SBATCH --time=06:00:00
#SBATCH --job-name=testjob_gpu
#SBATCH --export=NONE

unset SLURM_EXPORT_ENV

module load python
conda activate test-environment

python train.py
```

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
#SBATCH --time=06:00:00
#SBATCH --job-name=testjob_gpu
#SBATCH --export=NONE

unset SLURM_EXPORT_ENV

module load python
conda activate test-environment

cd $TMPDIR
tar xzf $WORK/large-archive-with-small-files.tar.gz

python train.py
```

Resource requirements

Max. runtime

Other job options (name, notifications,…)

Prevent export of environment to job

Set up job environment

Actual run of your binary

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

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Containers

https://doc.nhr.fau.de/environment/apptainer

Using Containers

- Use pre-built containers or build them yourself.
- Building containers from scratch (interactively or via definition file) requires root access, so build them on your local machine.
- Run/shell/import of a (pre-built) container in a production environment is possible as a normal user.
- Generally: you are the same user inside the container than outside!
- Container images are build immutable to preserve reproducibility.

Using Containers

At NHR@FAU, Apptainer (formerly known as Singularity) is the standard container solution. It is specifically designed for HPC systems and causes no performance penalties.

1. Using existing containers:
   - Download / pull a container from a container repository (DockerHub) and it will be automatically converted into the Apptainer (.sif) format: `apptainer pull docker://<repository>`
   - Enter container with a shell: `apptainer shell <container_name>`
   - Execute commands inside a container: `apptainer exec <container_name> <command>`
   - Run pre-defined runscript of container: `apptainer run <container_name> or ./<container name>`

2. Building your own containers:
   - Containers can be build on the cluster frontend nodes. They can be build interactively via a sandbox or using a definition file (similar to a Dockerfile)

More details:

- https://doc.nhr.fau.de/environment/apptainer

Using containers

Hints:
export https_proxy="http://proxy.rrze.uni-erlangen.de:80"
export https_proxy="http://proxy.rrze.uni-erlangen.de:80"

If disk out of space:
export APPTAINER_CACHEDIR=$TMPDIR or $WORK
export APPTAINER_TMPDIR=$TMPDIR or $WORK

Nvidia:

```
apptainer remote login --username \$oauthtoken docker://nvcr.io
docker login nvcr.io

Username: $oauthtoken
Password: <token>

apptainer instance list
apptainer pull docker://nvcr.io/nvidia/nemo:24.09
```

Docker:

```
apptainer pull docker://lmsysorg/sglang:v0.4.0.post1-cu124-srt
```

- .sif containers will be saved to the current path of the terminal

When to Use Python venvs, Conda, or Containers

- **Python venvs:**
  - Lightweight environment management.
  - Suitable for simple Python dependencies.
  - Limited control over non-Python libraries.

- **Conda:**
  - Manages Python and non-Python dependencies.
  - Supports complex workflows.
  - Ideal for multi-language (e.g., Python + C/C++) requirements.

- **Containers (Apptainer):**
  - Portable, reproducible environments.
  - Encapsulate entire software stack.
  - Ideal for cross-platform compatibility and complex applications.

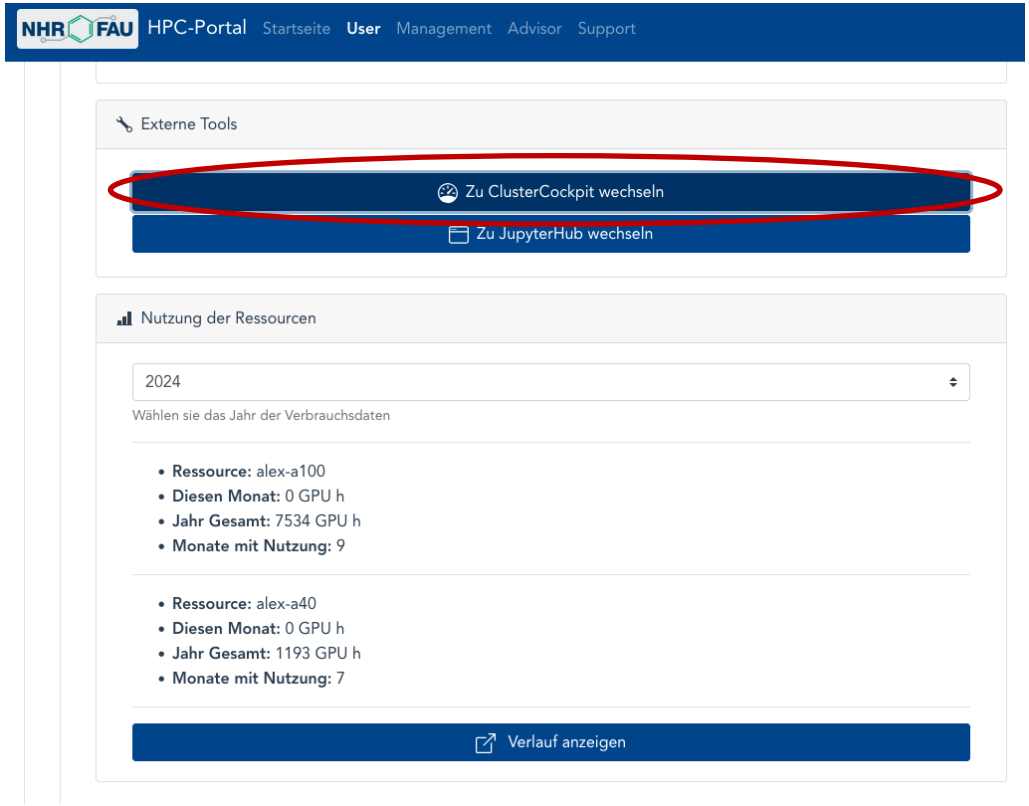
Some troubleshooting

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

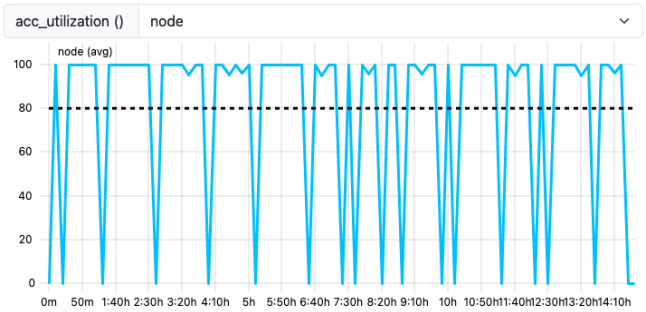
- Job Monitoring
  - How to use it and what to look out for: https://doc.nhr.fau.de/job-monitoring-with-clustercockpit/

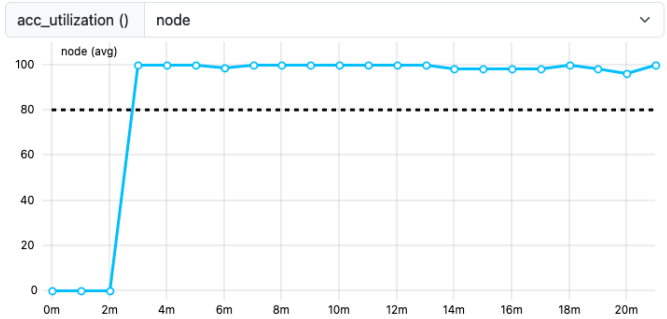
ClusterCockpit



Resource underutilization

- Inefficient usage of allocated resources, like training on a single GPU instead of all available GPUs, often occurs due to improper configuration or unoptimized code
- This results in wasted resources and longer training times
- To address this, ensure the training script explicitly supports multi-GPU setups, and verify GPU utilization across all devices
- Claim the appropriate GPUs for you (not always highend GPU)





Clustercockpit

The GPU out of memory problem

```
[rank7]:     return Variable._execution_engine.run_backward(  # Calls into the C++ engine to run the backward pass
[rank7]: torch.cuda.OutOfMemoryError: CUDA out of memory. Tried to allocate 1.53 GiB. GPU  has a total capacity of 79.26 GiB of which 1.28 GiB is free.
a0931:247812:247812 [7] NCCL INFO cudaDriverVersion 12050
```

- **Start Small**: Use low batch size, minimum model, monitor memory
- **Optimize Inputs/Model**: Resize inputs, adapt architecture, mixed precision
- **Consider Larger GPUs**: Use high-VRAM GPUs
- **Utilize Multi-GPU**: Distribute load with data/model parallelism
- **Consider CPU offloading:** Only for short finetunings

Data bottlenecks

- Low data loading and transfer rates, especially when handling large datasets, can create I/O bottlenecks, reducing GPU utilization
- Monitor your job on ClusterCockpit
  - More details: https://hpc.fau.de/systems-services/documentation-instructions/job-monitoring-with-clustercockpit/
- GPU Utilization should be close to 100% for optimized trainings

NHR FAU

FAU Friedrich-Alexander-Universität Erlangen-Nürnberg

THANK YOU.

NHR@FAU
https://doc.nhr.fau.de
hpc-support@fau.de

HPC High Performance Computing