Karlsruher Institut für Technologie

Institut für Experimentelle Teilchenphysik

Use of GPU resources for the Training of Neural Networks

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Karlsruher Institut für Technologie (KIT) - Institut für experimentelle Teilchenphysik (ETP)

Will a GPU speed up your Machine Learning application?

It's complicated

- GPU speed up training immensely by parallelizing demanding tasks
- Some overhead is necessary to transfer data
- Individual computations are also a bit slower
- Usually a GPU replaces multiple CPU cores

➤ **Hard to determine if an ML application will be sped up**

Rule of thumb: GPUs help most for

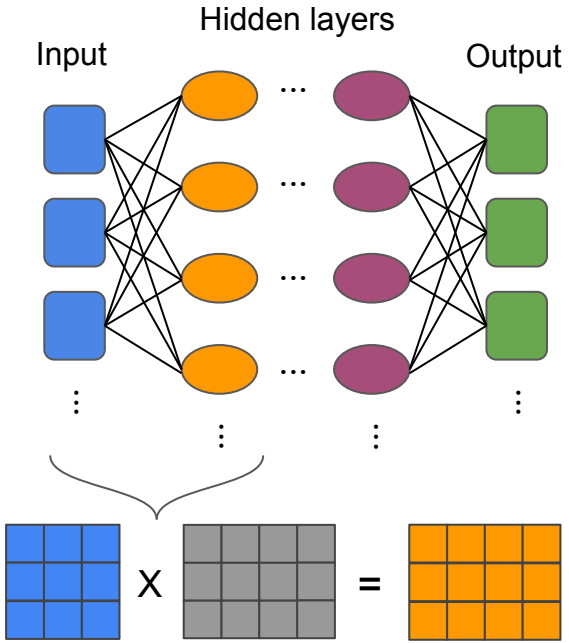
- Bigger networks
- Less complex networks

There are many hyperparameters to tune

The only sure way to know, is to try it out

Example: Event Discrimination via NN

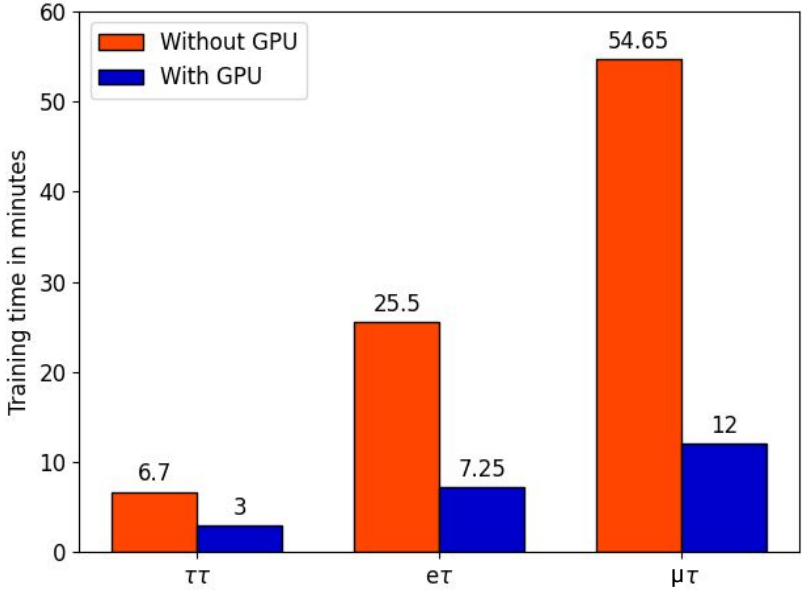
- **To differentiate between signal and background, Neural Networks are trained**
  - **22** to **28** physical variables are used as inputs
  - **5** classes are used as outputs
    - **4** are composed of various backgrounds
    - The signal for a specific group of mass hypotheses
  - The network is comparably simple
    - Feed forward fully connected network
    - **3** hidden layers with **512** nodes each
  - ➤ Around **45,000** parameters



InceptionResnetV2 has around **56,000,000** Parameters

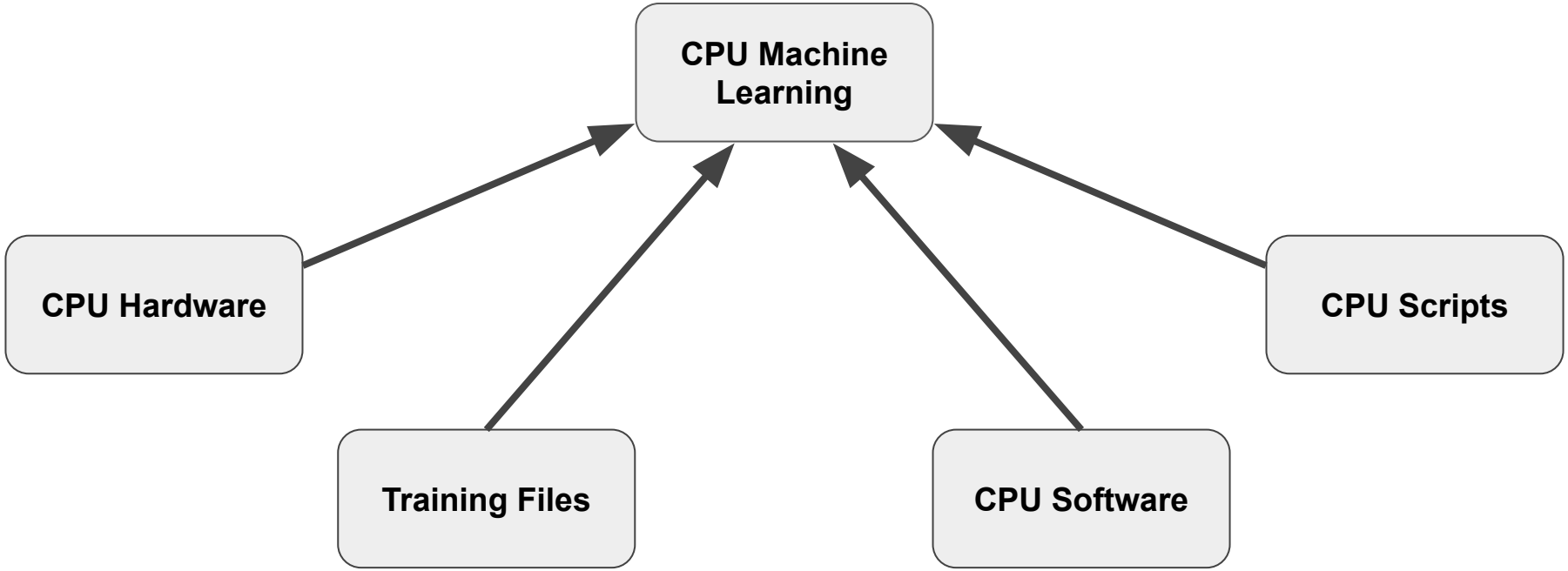
Example: CPU vs GPU

- **Part of Master thesis:**
  - Adapt training for GPU
  - Find ideal Hyperparameters
  - Compare with CPU
- **CPU only**
  - 12 CPU cores
  - Average runtime: 29 minutes
- **CPU + GPU**
  - 2 CPU cores + A100 GPU
  - Average runtime: 7.5 Minutes



➤ **Inclusion of GPU leads to a significant speedup while using fewer CPU resources**

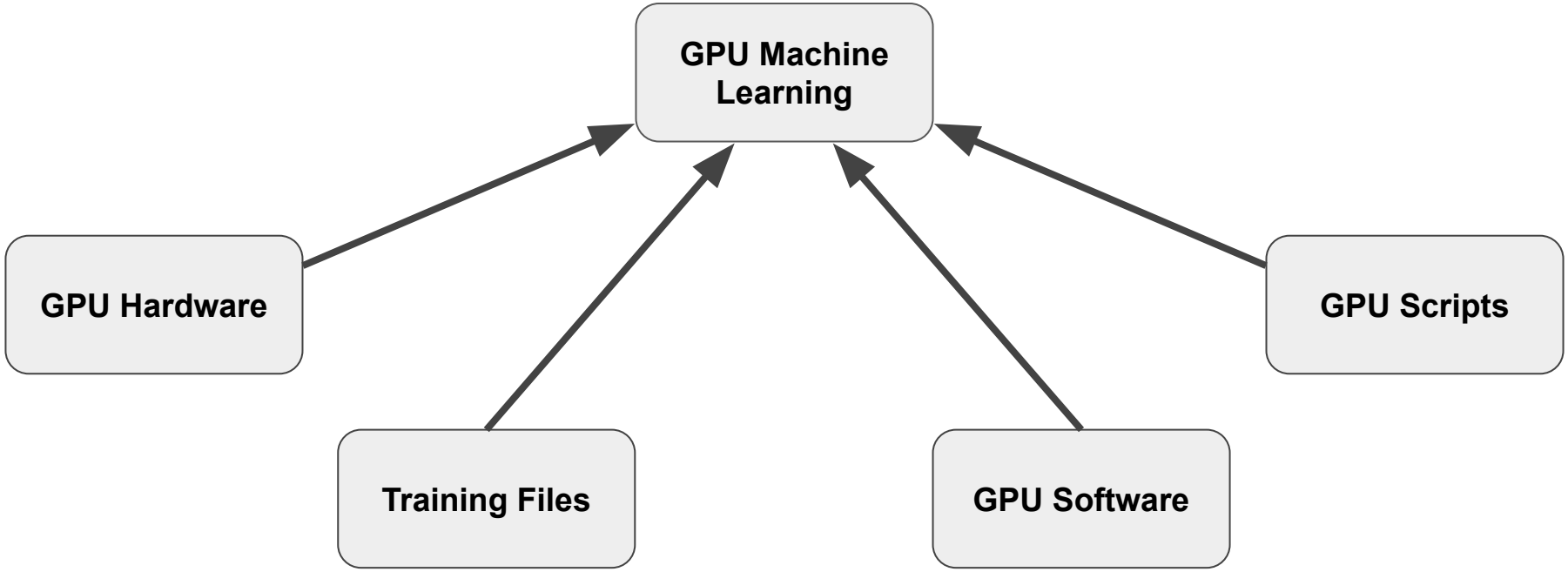
What so we need for CPU training



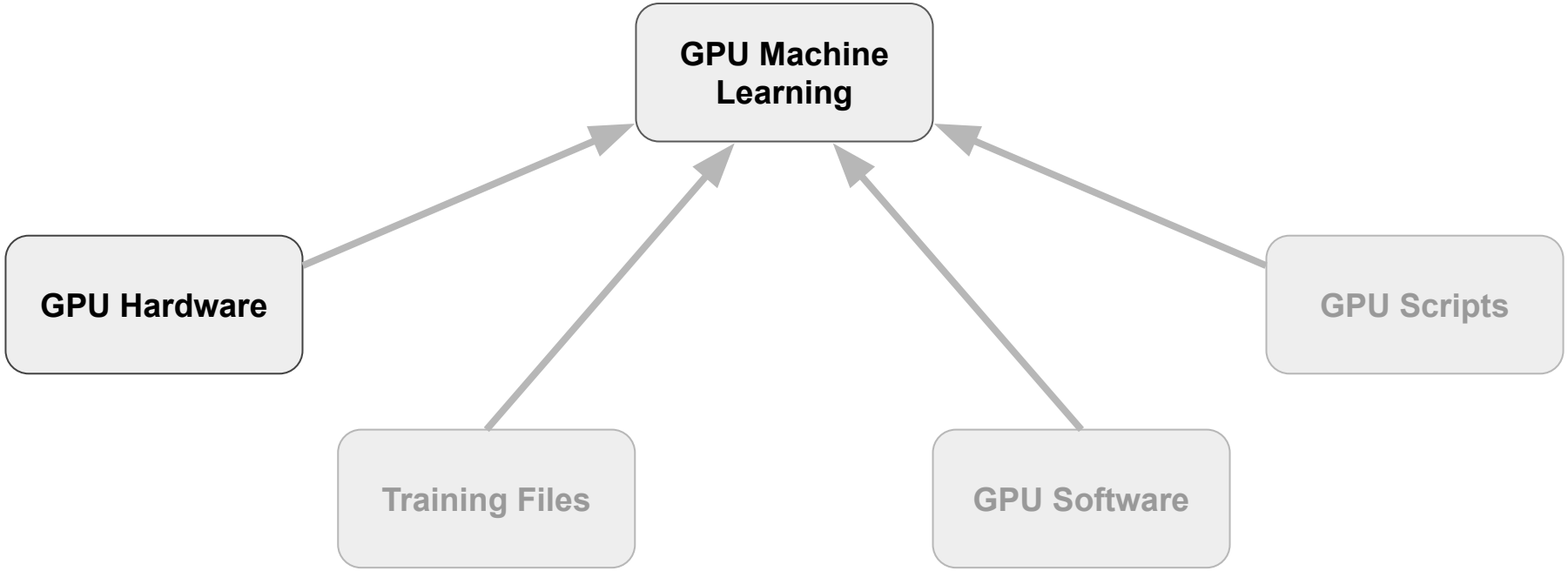
How a training on local CPU might look like (executable.sh)

```
#/bin/bash

# Source all necessary software

source /work/name/some/local/environment/setup.sh


# Run the training

python3 /work/name/some/local/files/mnist_training.py
    --files /ceph/name/some/local/files/training_data
```

What so we need for GPU training



What so we need for GPU training



What GPUs can you use?

The “Deepthought” machine

- Local development machine
- Ubuntu 18.04
- 4 GTX TITAN X

The TOpAS cluster

- Remotely usable through the ETP batch system
- CentOS7
- Multiple machines with
  - V100, V100S, A100
- 56 GPUs in total

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What is in the Jobfile for a CPU job

```
# The Executable that is run in the Job

Executable = ./executable.sh

...

# The hardware requirements

RequestCPUs = 1         # 1 CPU core

RequestMemory = 2000      # 2 GB of memory

request_disk = 2000000   # 2 GB of disk space

...
```

HTCondor Talk by Matthias Schnepf

Corresponding GitLab repo

What is in the Jobfile for a GPU job on TOpAS

```
...
## Additional Arguments in submission.jdl
# Request GPU resources
# Can also be >1 to request more GPUs
request_GPUs = 1
# Mark as remote job
+RemoteJob = True
```

What is in the Jobfile for a GPU job on TOpAS

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What is a Remote Job?

Remote jobs do not have access to `/ceph`, `/work` and `/home`

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Neither

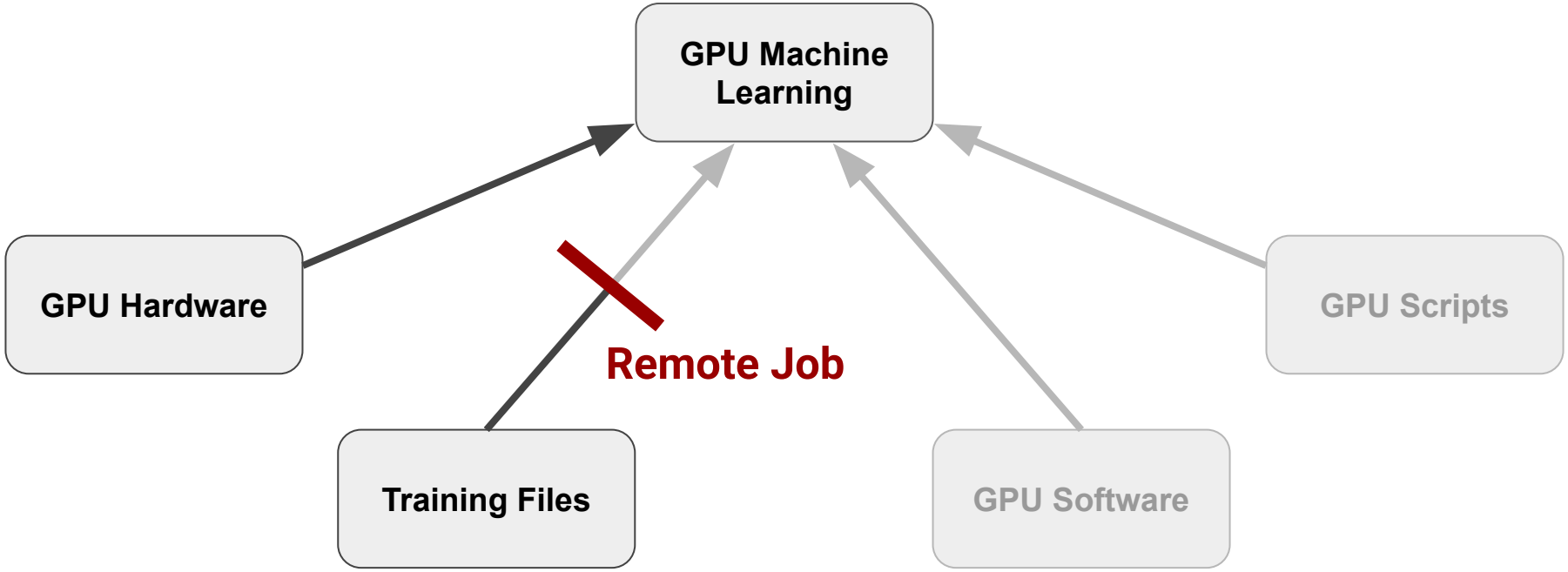
```
source /work/name/some/local/environment/setup.sh
```

nor

```
python3 /work/name/some/local/files/mnist_training.py
    --files /ceph/name/some/local/files/training_data
```

will work!

What so we need for GPU training on TOpAS



How to transfer Files to Remote Batch Jobs

Small files (Together < 1 GB):

- Through HTCondor internal transfer

Shown in GitLab examples

How to transfer small files

```
...
## Additional Arguments in submission.jdl
# List of files to transfer into job
transfer_input_files = mnist_training.py
# List of files to transfer out of job
transfer_output_files = trained_model.pt
# Paths can be adjusted with transfer_output_remaps
```

How to transfer Files to Remote Batch Jobs

Small files (Together < 1 GB):

- Through HTCondor internal transfer

Shown in GitLab examples

Big Files:

- Transfer with Grid protocols (SRM, XRootD, etc.)
  - Directly from `/ceph` via `/ceph/srv`
    - Can be slow
  - Through intermediate Grid storage
    - Often requires VOMS proxy

Shown in GitLab examples

How to transfer big files

1. **Place files on accessible storage before the job starts**
   a. `/ceph/srv` works for ETP and TOpAS
   b. Remote storage like NRG

How to transfer big files

1. **Place files on accessible storage before the job starts**
   a. `/ceph/srv` works for ETP and TOpAS
   b. Remote storage like NRG
2. **Copy files into the job with Grid Protocols at runtime** (like `xrdcp`)

Files on
`/ceph/srv/name/path/to/dataset`
can be found as
`root://ceph-node-a.etp.kit.edu://name/path/to/dataset`

Documentation of XRootD

How to transfer Files to Remote Batch Jobs

Small files (Together < 1 GB):

- Through HTCondor internal transfer

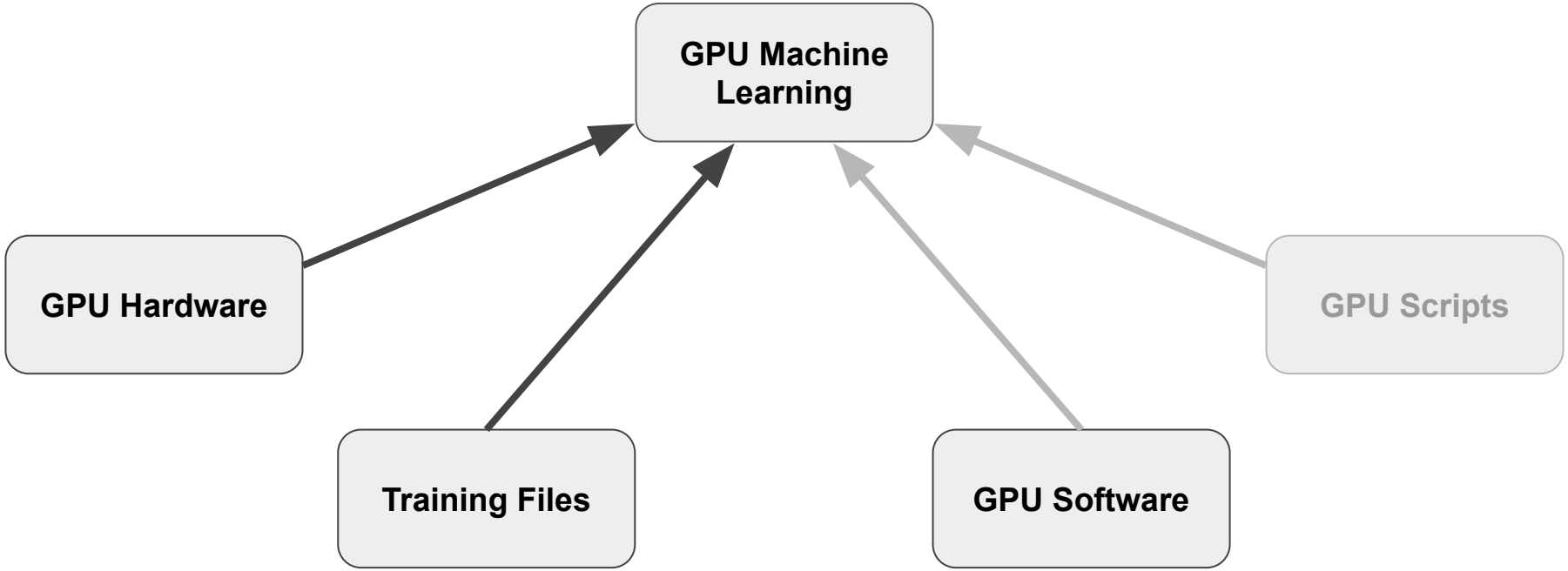
Shown in GitLab examples

Big Files:

- Transfer with Grid protocols (SRM, XRootD, etc.)
  - Directly from `/ceph` via `/ceph/srv`
    - Can be slow
  - Through intermediate Grid storage
    - Often requires VOMS proxy
- Some data types can be streamed
- Subject to caching on TOpAS

Shown in GitLab examples

What so we need for GPU training on TOpAS



Requirements for your GPU Environment

Set-up has to be:

- **GPU capable**

CUDA + **cuDNN** + **GPU versions of software**

- **Portable**

Send with job | **Get from CVMFS** | **Get from Web**

GPU Environment Examples: LCG Stack

```
source /cvmfs/.../LCG_101cuda/.../setup.sh
HOME=$_CONDOR_JOB_IWD
python3 -m venv venv
source venv/bin/activate
python3 -m pip install pip --upgrade
python3 -m pip install torch==1.9.0+cu111
    torchvision==0.10.0+cu111 torchaudio==0.9.0
    -f https://download.pytorch.org/whl/torch_stable.html
```

List of available LCG stacks

Source base environment from CUDA LCG stacks

GPU Environment Examples: LCG Stack

```
source /cvmfs/.../LCG_101cuda/.../setup.sh
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List of available LCG stacks

Set `$HOME` to writable directory. `$_CONDOR_JOB_IWD` is the job start directory

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List of available LCG stacks

Set up local `venv` to install missing modules

GPU Environment Examples: LCG Stack

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    -f https://download.pytorch.org/whl/torch_stable.html
```

List of available LCG stacks

Install modules compatible with GPU Hardware and LCG stack libraries

GPU Environment Examples: LCG Stack

```
source /cvmfs/.../LCG_101cuda/.../setup.sh
HOME=$_CONDOR_JOB_IWD
python3 -m venv venv
source venv/bin/activate
python3 -m p
python3 -m p
    torchvision==0.10.0+cu111 torchaudio==0.9.0
    -f https://download.pytorch.org/whl/torch_stable.html
```

List of available LCG stacks

Newest available CUDA version is 11.2

Install modules compatible with GPU Hardware and LCG stack libraries

GPU Environment Examples: Anaconda

```
HOME=$_CONDOR_JOB_IWD
wget https://repo.anaconda.com/miniconda/
    Miniconda3-latest-Linux-x86_64.sh
chmod +x Miniconda3-latest-Linux-x86_64.sh
./Miniconda3-latest-Linux-x86_64.sh -b -p $(pwd)/miniconda
source miniconda/bin/activate
conda install pytorch torchvision torchaudio
    cudatoolkit=11.3 -c pytorch -y
```

Set `$HOME` to writable directory. `$_CONDOR_JOB_IWD` is the job start directory

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Download an Anaconda installer

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```

Set up Anaconda environment

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Install software compatible with GPU Hardware

GPU Environment Examples: Anaconda

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./Miniconda3                                    /miniconda
source minic
conda install pytorch torchvision torchaudio
    cudatoolkit=11.3 -c pytorch -y
```

Newest available CUDA version is 11.3

Install software compatible with GPU Hardware

GPU Environment Examples: Docker

Batch jobs at ETP are usually set up to run in a docker container

```
...
Universe = docker
## Docker image used by the job
# Default container
docker_image = mschnepf/slc7-condocker
# Container with CUDA + cuDNN libraries preinstalled
docker_image =
    tvoigtlaender/slc7-condocker-cuda-11.6-cudnn8-devel:base
```

GPU Environment Examples: Docker

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docker_image =
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```

GPU Environment Examples: Docker

```
# CUDA and cuDNN are already installed from the start
HOME=$_CONDOR_JOB_IWD
python3 -m venv venv
source venv/bin/activate
python3 -m pip install pip --upgrade
python3 -m pip install torch==1.9.0+cu111
    torchvision==0.10.0+cu111 torchaudio==0.9.0
    -f https://download.pytorch.org/whl/torch_stable.html
```

Set `$HOME` to writable directory. `$_CONDOR_JOB_IWD` is the job start directory

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```

Install modules compatible with GPU Hardware and preinstalled libraries

GPU Environment Examples: Docker

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HOME=$_CONDOR_JOB_IWD
python3 -m venv venv
source venv/bin/activate
python3 -m p
python3 -m p
    torchvision==0.10.0+cu111 torchaudio==0.9.0
    -f https://download.pytorch.org/whl/torch_stable.html
```

Newest available CUDA version is 11.6

Install modules compatible with GPU Hardware and preinstalled libraries

GPU Environment Examples: `/cvmfs/etp.kit.edu`

If you have a stable environment setup, it can be put on

`/cvmfs/etp.kit.edu`

Files there can be **read** from inside the batch job

CVMFS Documentation

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If you have a stable environment setup, it can be put on

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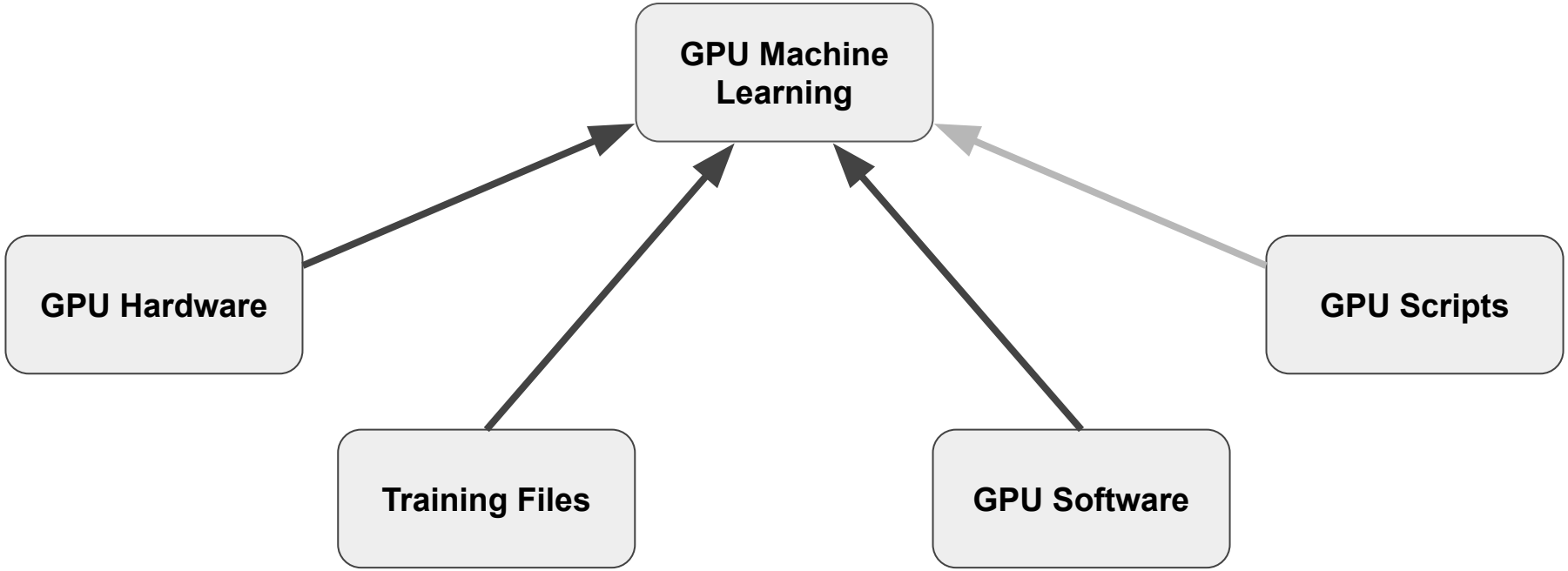
Files there can be **read** from inside the batch job

CVMFS Documentation

The **Anaconda** environment setup placed on **`/cvmfs/etp.kit.edu`** :

```
source
    /cvmfs/etp.kit.edu/GPU_examples/miniconda/bin/activate
    GPU_ML
```

What so we need for GPU training on TOpAS



How to train on GPU: Some Notes

- The example is a shortened version of the GitLab example (Link)
- Everything was tested on fairly new versions (PyTorch **1.9**, Tensorflow **2.4**)
  - Significantly older versions (especially Tensorflow 1) will deviate
  - GPU training with Tensorflow 1 is still possible but requires more work
- Ideally, analyses should not run on old software
- I can provide examples for older versions if necessary

The Training on CPU (`mnist_training.py`)

```
# Define NN model
class Net(torch.nn.Module):
    < Definition of model >
model = Net()



# Other setups
optimizer, scheduler,
train_loader, validation_loader
```

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```
# Run training loop
for epoch in range(1, epochs + 1):
    train(model, ...)
    validation(model, ...)
    scheduler.step()


# Export trained model
torch.save(model.state_dict(), out_dir)
```

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The Training on CPU (mnist_training.py)

```
# The training step
def train(model, train_loader, optimizer):
    model.train()
    for data, target in train_loader:

        optimizer.zero_grad()
        output = model(data)
        loss = LossFunctional(output, target)
        loss.backward()
        optimizer.step()
```

The Training on CPU (mnist_training.py)

```
# The validation step
def validation(model, validation_loader):
    model.eval()
    loss = 0
    with torch.no_grad():
        for data, target in validation_loader:

            output = model(data)
            loss += LossFunctional(output, target)
```

How to train on GPU with PyTorch

1. **Detect the GPU**
2. Place model on GPU
3. Place data on GPU

Article on GPU usage in PyTorch

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2. Place model on GPU
3. Place data on GPU

Article on GPU usage in PyTorch

→ PyTorch commands utilize the GPU

How to detect the GPU

```
# Detect if GPU are usable
GPU_check = torch.cuda.is_available()

# Detect how many GPUs are usable
num_GPUs = torch.cuda.device_count()

# Set which device to use
device = torch.device("cuda" if GPU_check
   else "cpu")
```

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The Training on GPU (`mnist_training.py`)

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# Define NN model
class Net(torch.nn.Module):
    < Definition of model >
model = Net()
model = model.to(device)

# Other setups
optimizer, scheduler,
train_loader, validation_loader
```

- On CPU
- On Device

The Training on CPU (`mnist_training.py`)

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# Run training loop
for epoch in range(1, epochs + 1):
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- On Device

The Training on CPU (mnist_training.py)

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    model.train()
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```

The Training on GPU (`mnist_training.py`)

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        data, target = data.to(device), target.to(device)
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- On CPU
- On Device

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- On CPU
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How to train on GPU with TensorFlow

➔ **TensorFlow commands utilize the GPU by default**

Guide to GPU usage with TensorFlow

How to train on GPU with TensorFlow

➔ **TensorFlow commands utilize the GPU by default**

- **GPUs can still be managed manually**

[Guide to GPU usage with TensorFlow]

```
# Detect which GPUs are available
GPU_list = tensorflow.config.list_physical_devices('GPU')


# Run code on specific device
with tensorflow.device(GPU_list[0]):
    < Some calculation >
```

How to train on GPU with TensorFlow

➔ **TensorFlow commands utilize the GPU by default**

- **GPUs can still be managed manually**

Guide to GPU usage with TensorFlow

```
# Detect which GPUs are available
GPU_list = tensorflow.config.list_physical_devices('GPU')


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GPU training on TOpAS: Putting it all together

Submit remote GPU job via `condor_submit submit.jdl`

GPU training on TOpAS: Putting it all together

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What should happen in the Executable of the job:

1. Set up GPU capable environment

GPU training on TOpAS: Putting it all together

Submit remote GPU job via `condor_submit submit.jdl`

What should happen in the Executable of the job:

1. Set up GPU capable environment
2. Copy training data into job

GPU training on TOpAS: Putting it all together

Submit remote GPU job via `condor_submit submit.jdl`

What should happen in the Executable of the job:

1. Set up GPU capable environment
2. Copy training data into job
3. Run GPU adapted NN training

GPU training on TOpAS: Putting it all together

Submit remote GPU job via `condor_submit submit.jdl`

What should happen in the Executable of the job:

1. Set up GPU capable environment
2. Copy training data into job
3. Run GPU adapted NN training
4. Return trained model from job

Related Topics

- Partial- and Multi GPU usage
- (GPU)-Job management
- GPU related Hyperparameter tuning
- Framework specific performance optimization
- More about Hardware related improvements for ML
- ML Profiling with Tensorboard

Let us know if you are interested in any of these topics

Collection of Links

- GitLab repo with examples for this talk
- Indico of Matthias Schnepfs HTCondor talk
  - Corresponding GitLab repo
- Documentation of XRootD
- List of available LCG stacks
- CVMFS Documentation
- Article on GPU usage in PyTorch
- Guide to GPU usage with TensorFlow
- TOpAS monitoring

Thank you for your attention