First AI training job on LUMI

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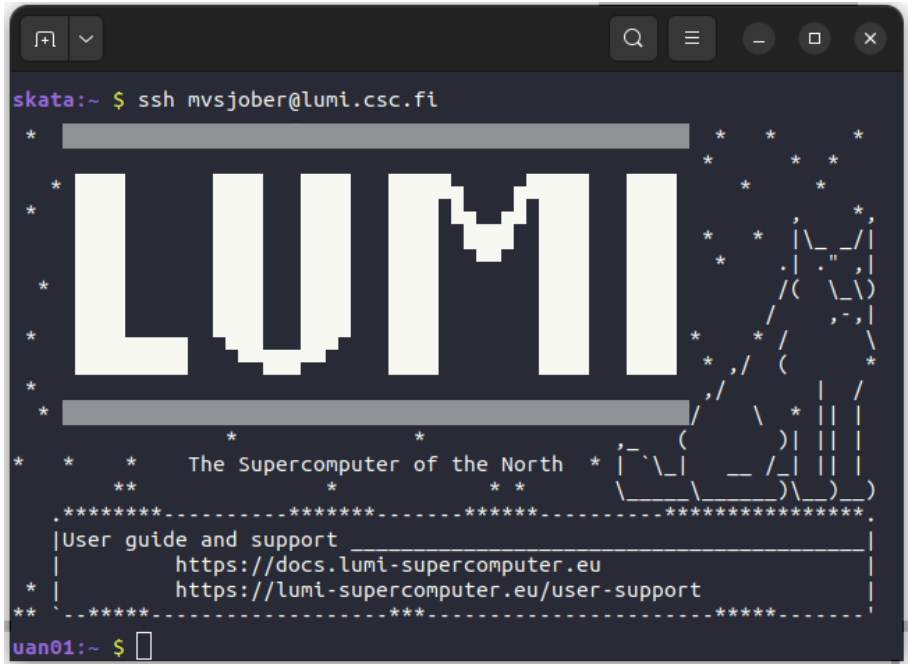
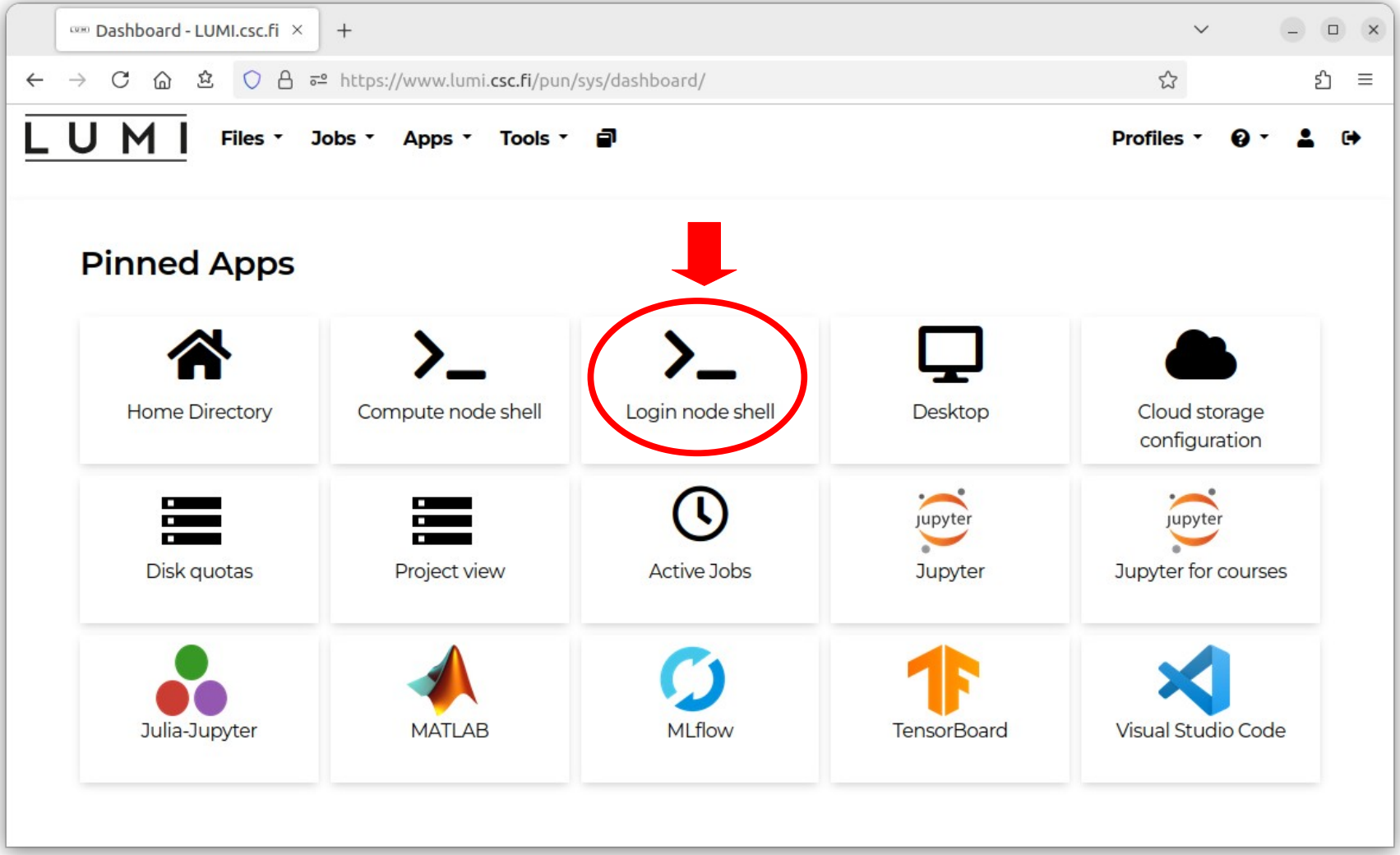
Accessing LUMI via SSH

- No passwords
  → SSH key pair **required**
- register your public key in your MyAccessID user profile
  - Finnish users with MyCSC linked account should use MyCSC for SSH keys!

```
ssh -i <path-to-private-key> \
       <username>@lumi.csc.fi
```

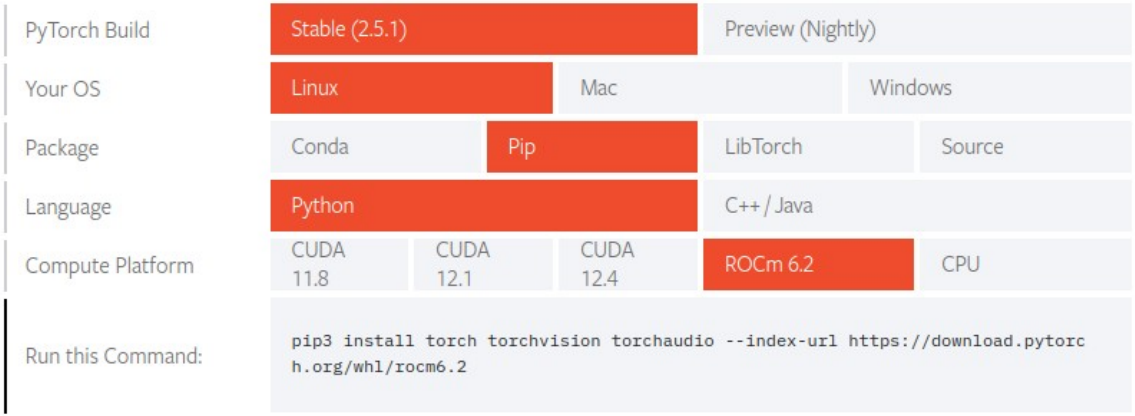
https://docs.lumi-supercomputer.eu/firststeps/




Dashboard - LUMI.csc.fi
https://www.lumi.csc.fi/pun/sys/dashboard/
LUMI
Files
Jobs
Apps
Tools
Profiles
Pinned Apps
Home Directory
Compute node shell
Login node shell
Desktop
Cloud storage configuration
Disk quotas
Project view
Active Jobs
Jupyter
Jupyter for courses
Julia-Jupyter
MATLAB
MLflow
TensorBoard
Visual Studio Code

Setting up the Software Environment

https://pytorch.org/



! environment-minimal.yml

```yaml
channels:
  - pytorch
  - conda-forge
  - defaults
dependencies:
  - accelerate=0.29.1
  - datasets=2.18.0
  - python=3.10.14
  - pytorch=2.2.2
  - transformers=4.39.3
```

~47k files

↓

bad for the shared network filesystem

Container icon: Iconjam @ flaticon.com

https://docs.lumi-supercomputer.eu/software/

Setting up the Software Environment

LUMI

- Singularity/Apptainer containers recommended for ML applications on LUMI
- Similar to Docker, better suited for multi-user supercomputers
  - Isolated environment
  - Easier to manage complex software dependencies
- For now we'll provide a pre-installed container
  - Later lectures will discuss how to create your own containers

`python`  `singularity exec $CONTAINER python`

Setting up the Software Environment

Set up the software environment

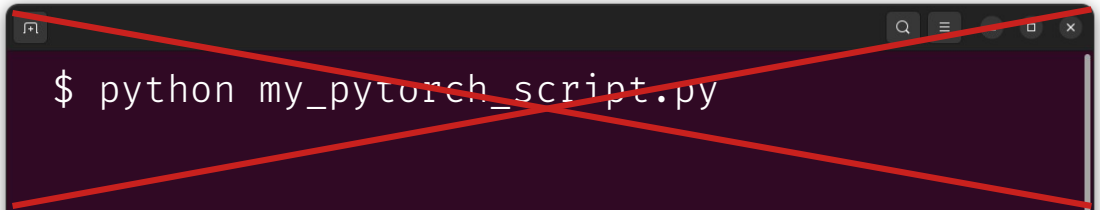
```
$ module purge
$ module use /appl/local/training/modules/AI-20250204/
$ module load singularity-userfilesystems singularity-CPEbits
```

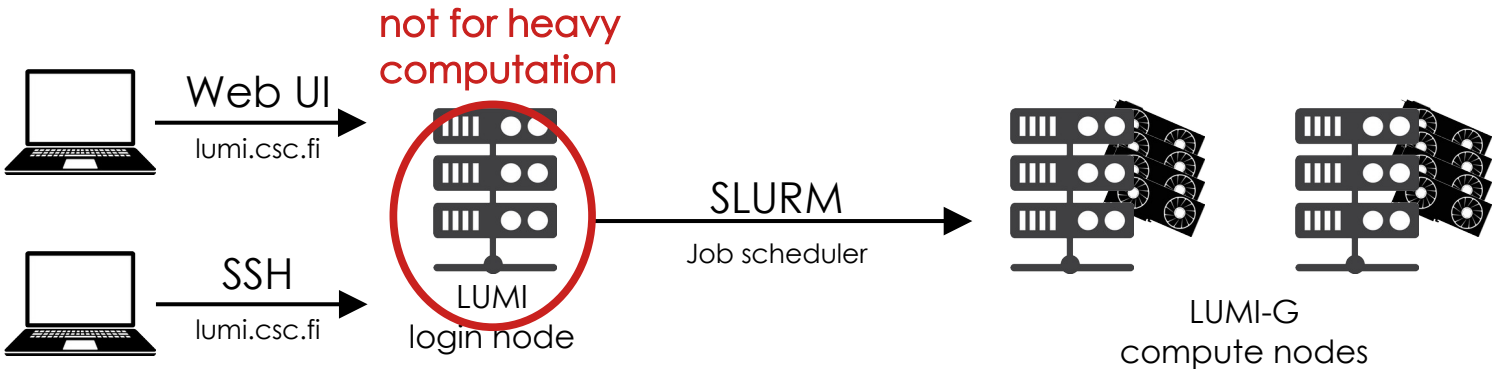
Launch the PyTorch container

```
$ CONTAINER=/project/project_465001707/containers/pytorch_transformers.sif
$ singularity exec $CONTAINER python
```

https://docs.lumi-supercomputer.eu/software/
https://docs.lumi-supercomputer.eu/runjobs/lumi_env/Lmod_modules/

Don't run computation on the login node – use the Slurm job scheduler!

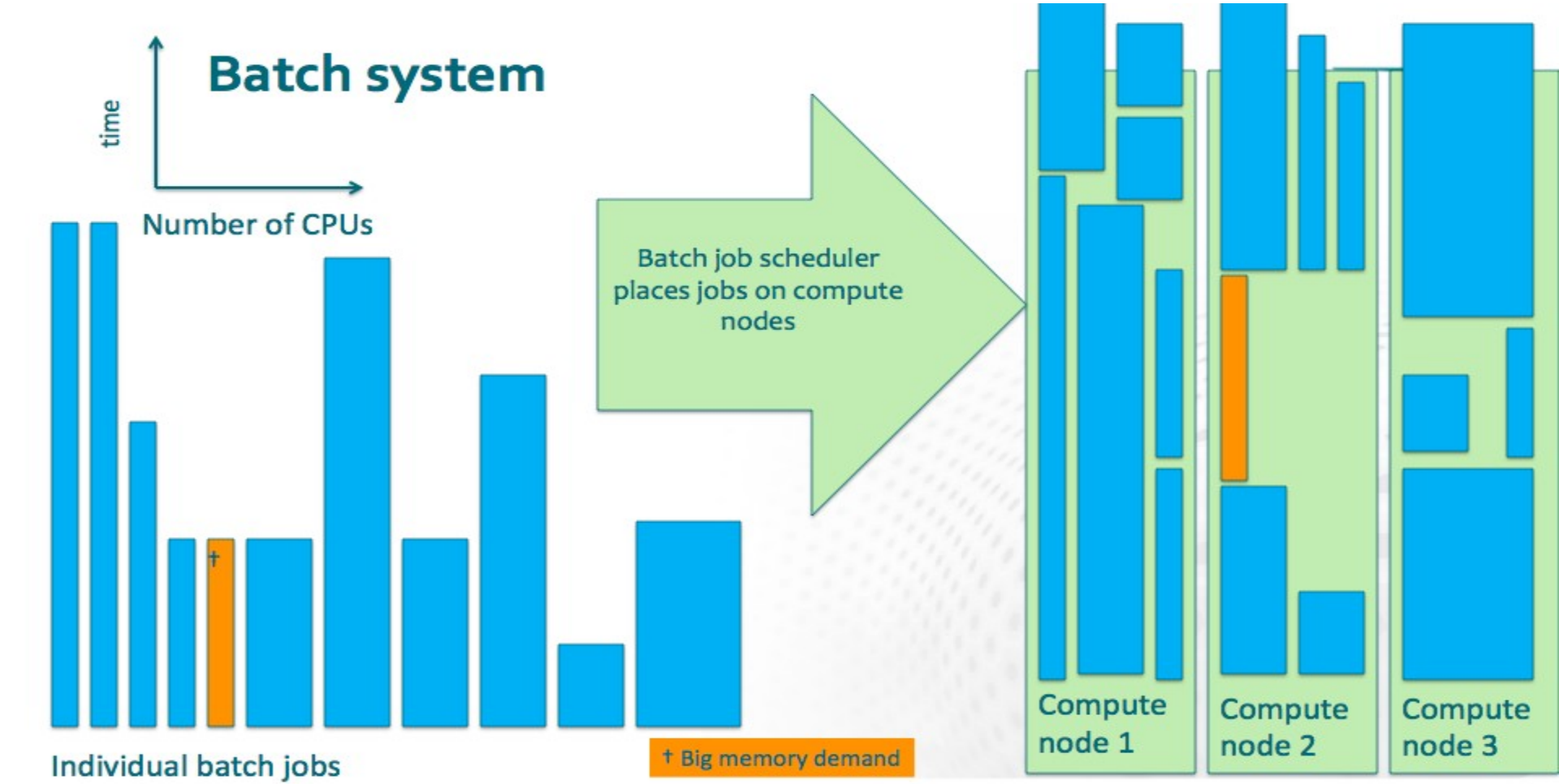




SLURM is used to reserve resources and submit scripts for running on the compute nodes

Icons: vecteezy.com

https://docs.lumi-supercomputer.eu/runjobs/


Batch system
time
Number of CPUs
†
Individual batch jobs
Batch job scheduler places jobs on compute nodes
† Big memory demand
Compute node 1
Compute node 2
Compute node 3

Training on a single Graphics Compute Die

SLURM batch script (run.sh)

```
#!/bin/bash
#SBATCH --account=project_465001707
#SBATCH --partition=small-g
#SBATCH --gpus-per-node=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=7
#SBATCH --mem-per-gpu=60G
#SBATCH --time=1:00:00

module purge
module use /appl/local/training/modules/AI-20250204/
module load singularity-userfilesystems singularity-CPEbits
CONTAINER=/project/project_465001707/containers/pytorch_transformers.sif

srun singularity exec $CONTAINER python my_pytorch_script.py
```

What resources requested?

What software to load?

- 1 GPU = 1/8 of node
- Use also ≤ 1/8 of CPU cores and memory

Available GPU partitions

- **standard-g**
  ≤ 48h, whole nodes only, max 1024 nodes/job
- **small-g**
  ≤ 72h, individual GCDs, max 4 nodes/job
- **dev-g**
  ≤ 3h, individual GCDs, max 32 nodes/job, *max 2 jobs running*

https://docs.lumi-supercomputer.eu/runjobs/scheduled-jobs/partitions/

Useful SLURM commands

Submit the SLURM batch script

```
$ sbatch run.sh
Submitted batch job 987654
```

Check the SLURM queue

```
$ squeue --me
JOBID   PARTITION NAME   ST TIME  NODES NODELIST
987654  small-g   run.sh R  0:18      1 compute_node
```

Cancel a job

```
$ scancel 987654
```

Useful SLURM commands

Read job outputs

```
$ tail -f slurm-987654.out
```

Access compute node for diagnostics

```
$ srun --interactive --pty --jobid=987654 bash
[compute_node] $ rocm-smi
```

Useful SLURM commands for monitoring job progress

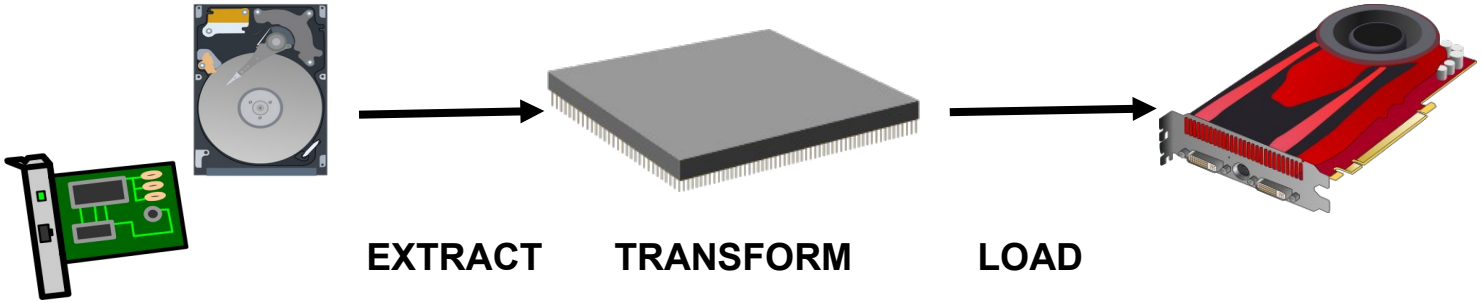
LUMI

Check the status of partitions

A = allocated
I = idle
O = other states
T = total

```
$ sinfo -s
PARTITION   AVAIL  TIMELIMIT   NODES(A/I/O/T) N                    
debug          up      30:00          8/0/0/8 nid[                002595-002597]
interactive    up    8:00:00          4/0/0/4 nid[002502,002507,002594,002599]
q_fiqci     inact      15:00          0/1/0/1 nid002598
q_industry     up      15:00          0/1/0/1 nid002598
q_nordiq       up      15:00          0/1/0/1 nid002503
small          up 3-00:00:00     280/6/20/306 nid[002280-002499,002508-002593]
standard       up 2-00:00:00 1493/111/124/172 nid[001000-002279,002600-003047]
dev-g          up    3:00:00       30/17/1/48 nid[005002-005025,007954-007977]
small-g        up 3-00:00:00      193/2/3/198 nid[005026-005123,007852-007951]
standard-g     up 2-00:00:00 2555/23/150/2728 nid[005124-007851]
largemem       up 1-00:00:00          1/5/0/6 nid[000101-000106]
lumid          up    4:00:00          1/6/1/8 nid[000016-000023]
```

Using multiple CPUs for ETL



- Reserve enough CPU cores per GPU, 7 cores/GPU on LUMI

```
#SBATCH --cpus-per-task=7
```

- Use multiple workers (processes) in PyTorch DataLoader:

```
train_loader = torch.utils.data.DataLoader( ... ,
  num_workers=N)
```

Use checkpointing!

Checkpointing = save the model weights every now and then

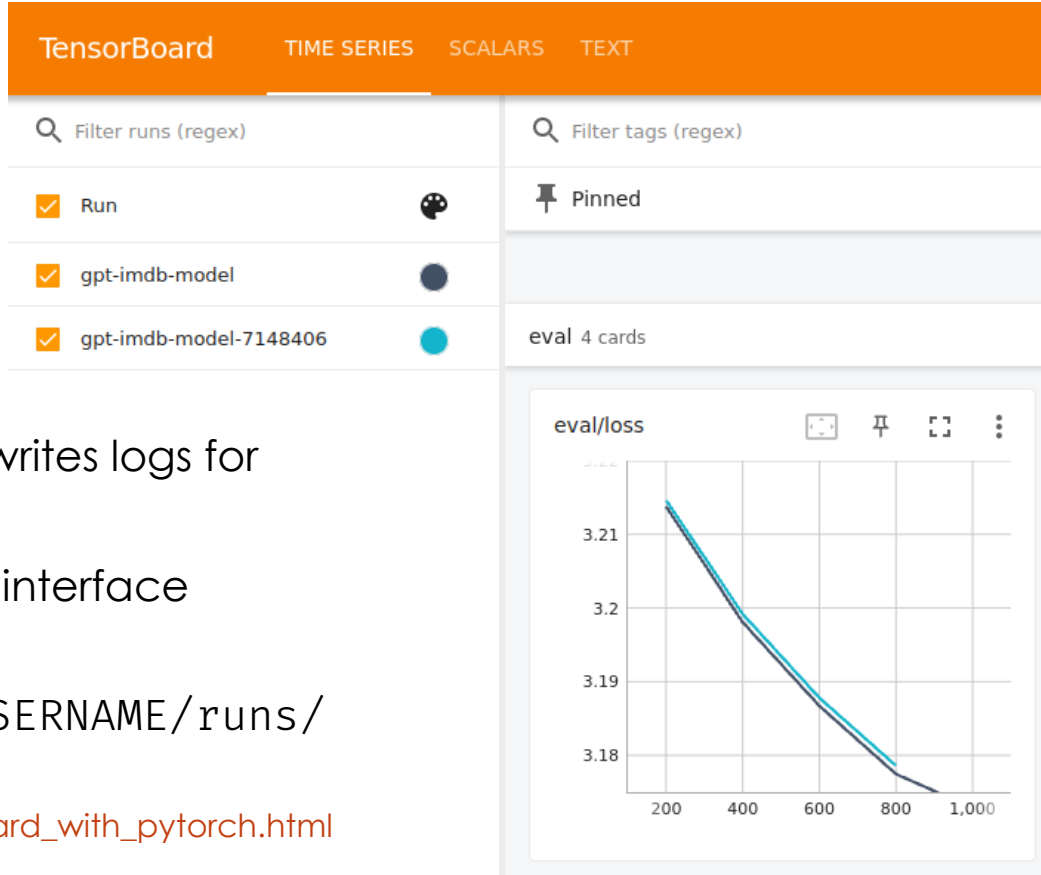
- E.g. after each epoch, or every N batches
- If your run crashes, simply restart from the latest checkpoint
- Train for longer than the “short” 2-3 days limit on LUMI partitions
- Exploit scheduling “backfilling”

HuggingFace Trainer example

```
training_args =
  TrainingArguments(
    ... ,
    overwrite_output_dir=False,
    ...
  )

trainer = Trainer( ... )
trainer.train(
  resume_from_checkpoint=True
)
```

Monitoring Progress with TensorBoard



- HuggingFace trainer automatically writes logs for TensorBoard
- You can start the UI in the LUMI web interface
- For the exercises use path: `/scratch/project_465001707/USERNAME/runs/`

https://pytorch.org/tutorials/recipes/recipes/tensorboard_with_pytorch.html