Scaling AI training to multiple GPUs

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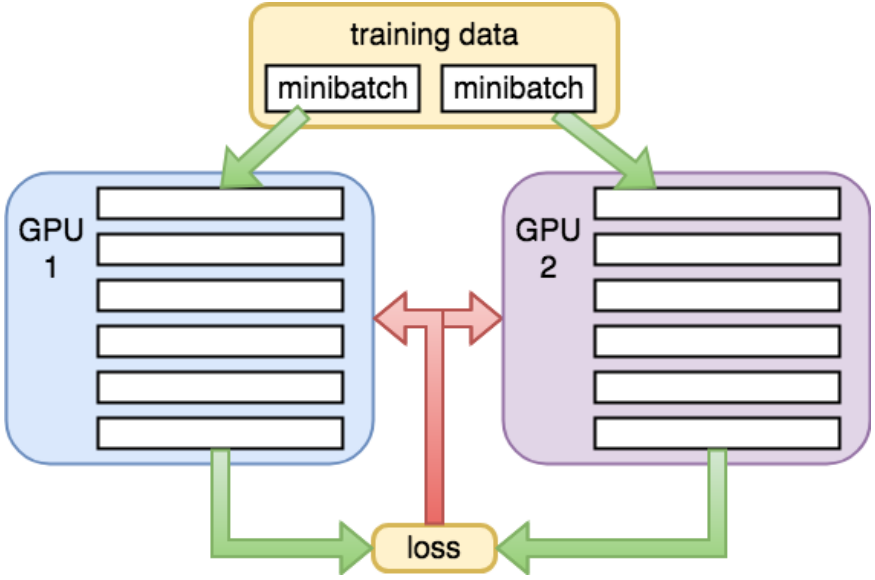
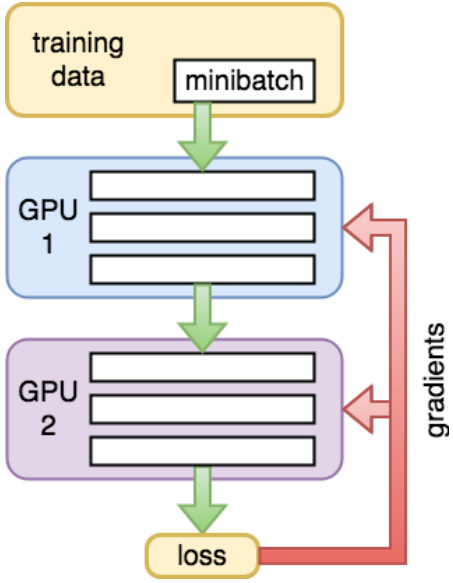
Reasons to use multiple GPUs

Training takes a long time and I have a lot of data
→ **data parallelism**



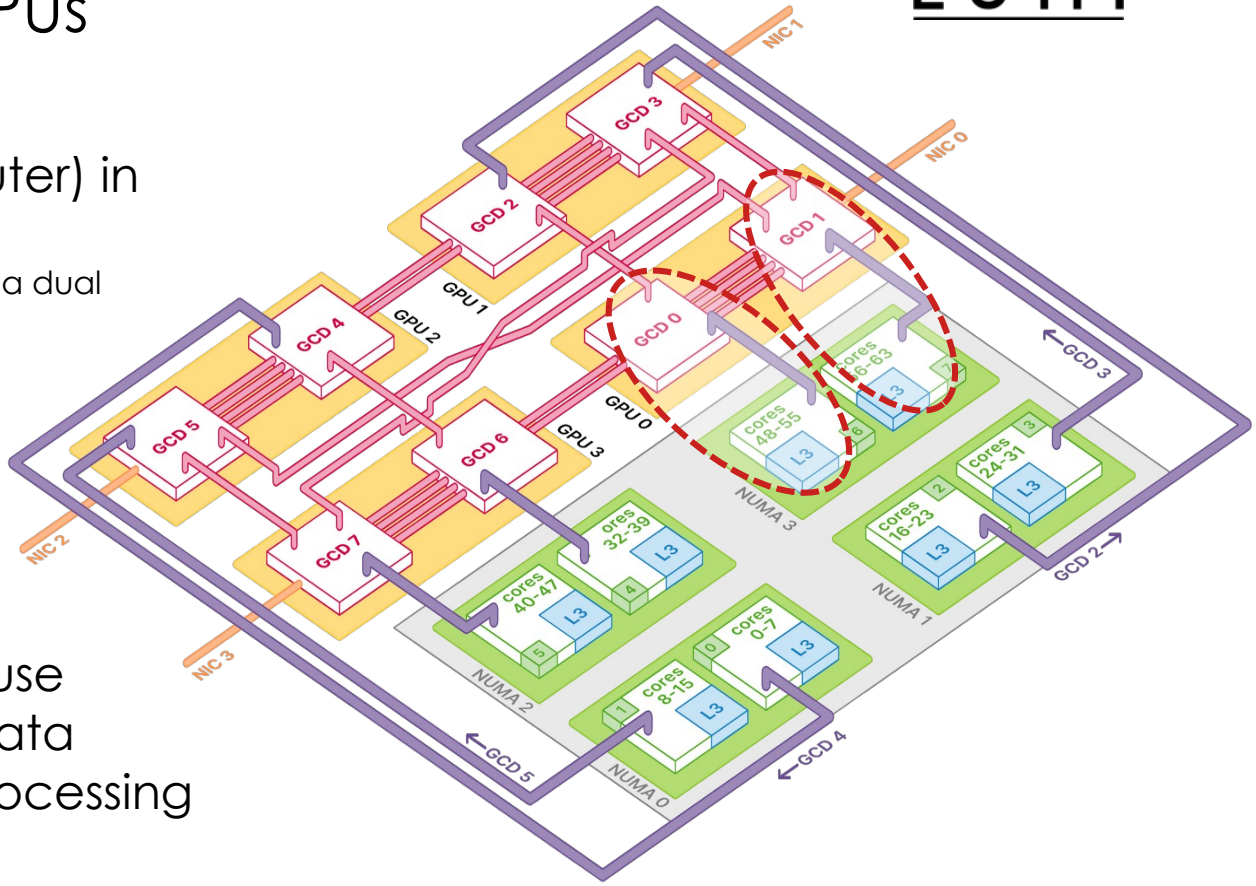
My model is too big to fit into one GPU
→ **model parallelism**



Using multiple GPUs

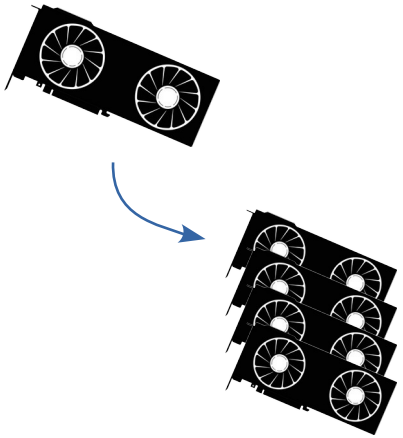
- Each node (computer) in LUMI has 8 GPUs
  (Actually 4 x MI250x, which is a dual chip card = 8 GCDs)

- For each GPU you use 1-7 CPU cores for data loading and pre-processing



Using multiple GPUs

- Not automatic: **your code needs to support multiple GPUs**
- Frameworks like Hugging Face, Lightning or Accelerate *may* auto-detect multiple GPUs (with the right options)
- For pure PyTorch code, there are many options depending on the scenario:
  - DistributedDataParallel (DDP)
  - Hybrid approaches for models too big for a single GPU:
    - Fully-sharded Data Parallel (FSDP)
    - DeepSpeed



Multi-GPU resource allocation on LUMI

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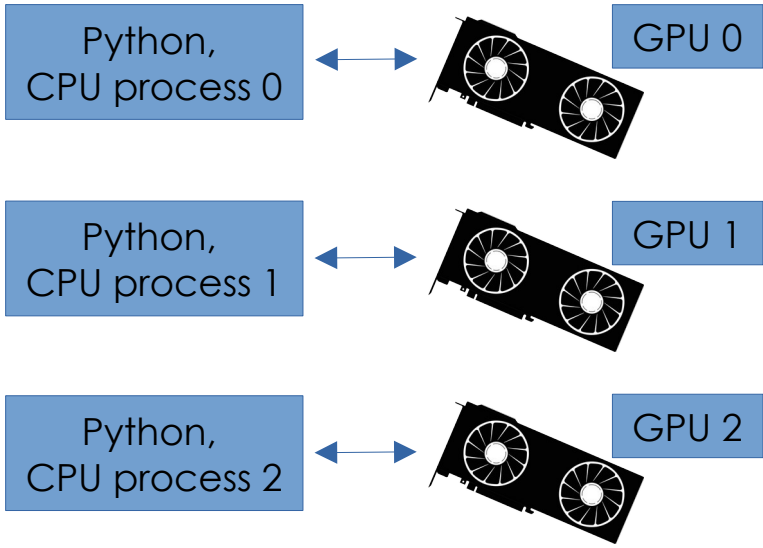
- Use **`--gpus-per-node=N`** where `N=2,…,8`
  (`--gpus-per-task` option not currently recommended due to bug in Slurm)
- Allocate a maximum of **1/8 of resources per GPU**:
  - 60 GB **CPU memory** and 7 CPU cores per GPU
  - Full node: 480 GB and 56 cores
    (leaving some "slack" for the system)
  - Note: you **always get the full GPU memory** of 64 GB per GCD
    (no need to allocate that with Slurm options)
  - Resources billed in GPUh according to 1/8 slice

One Python CPU control process per GPU

- Torchrun can handle launching the processes. Launch single torchrun: `--tasks-per-node=1`
- Without torchrun, use Slurm tasks: `--tasks-per-node=8`
- Each process should know which GPU to use, e.g.

```
gpu_id = int(os.environ["LOCAL_RANK"])
device = torch.device("cuda", gpu_id)
```

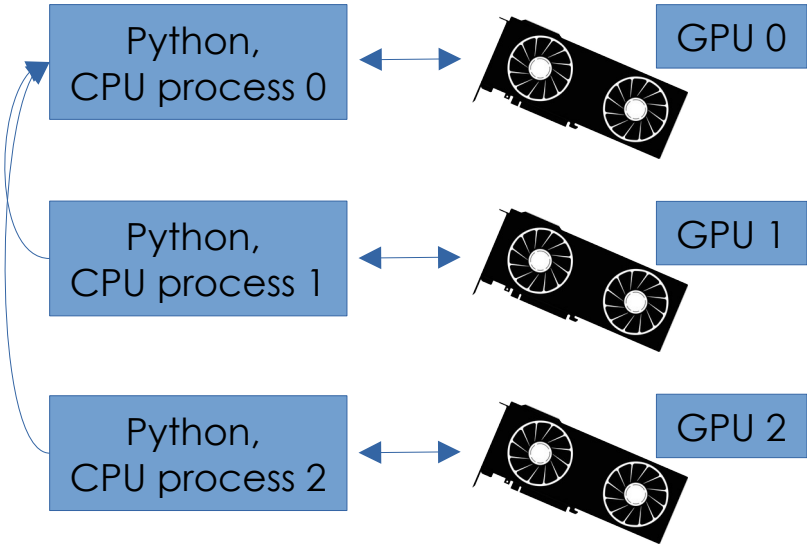


Set up communication between processes

- First process is the "master" and the others connect back to it
- Torchrun can handle this automatically:
  `torchrun --standalone ...`
- Without torchrun you need to set up environment variables:

```
MASTER_ADDR=$(hostname)
MASTER_PORT=25900
WORLD_SIZE=$SLURM_NPROCS
RANK=$SLURM_PROCID
```

  - Note: rank needs to be set differently for each process, see exercise for example



Example: 2 GPUs with torchrun

```
#!/bin/bash
#SBATCH --account=project_465001707
#SBATCH --partition=small-g
#SBATCH --gpus-per-node=2
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=14
#SBATCH --mem=120G
#SBATCH --time=1:00:00
## < module loading part as before – removed for readability>

srun singularity exec $CONTAINER \
    torchrun --standalone \
             --nnodes=1 \
             --nproc-per-node=${SLURM_GPUS_PER_NODE} \
             my_python_script.py
```

Remember rule-of-thumb:

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

torchrun will take care of launching one process per GPU

Example: 8 GPUs with torchrun

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```
#!/bin/bash
#SBATCH --account=project_465001707
#SBATCH --partition=standard-g
#SBATCH --gpus-per-node=8
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=56
#SBATCH --mem=480G
#SBATCH --time=1:00:00
## < module loading part as before – removed for readability>

srun singularity exec $CONTAINER \
    torchrun --standalone \
             --nnodes=1 \
             --nproc-per-node=${SLURM_GPUS_PER_NODE} \
             my_python_script.py
```

Full node = we can also use standard-g

Example: 8 GPUs *without* torchrun

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```
#!/bin/bash
#SBATCH --account=project_465001707
#SBATCH --partition=standard-g
#SBATCH --gpus-per-node=8
#SBATCH --ntasks-per-node=8
#SBATCH --cpus-per-task=7
#SBATCH --mem=480G
#SBATCH --time=1:00:00
## < module loading part as before – removed for readability>

export MASTER_ADDR=$(hostname)
export MASTER_PORT=24500
export WORLD_SIZE=$SLURM_NPROCS

srun bash -c "RANK=\$SLURM_PROCID LOCAL_RANK=\$SLURM_LOCALID singularity exec ... "
```

We use Slurm tasks to launch 8 Python processes

Where to connect to?

How many processes are there?

Which process am I?

Do we need to change the Python code?

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- For plain PyTorch: **yes, use DistributedDataParallel (DDP)**
- For higher level frameworks, **mostly no:**
  - `transformers.Trainer` is automatically set up for distributed training when `WORLD_SIZE & RANK` environment variables are set
  - Similar for other high-level frameworks like PyTorch Lightning or Accelerate
- BUT: Pay attention to **global batch size vs per device batch size**!
  - Example: global batch size = 32 for one GPU, split over 8 GPUs, per-device batch size is 4
- Cosmetic: You might want to print some things only on rank 0

PyTorch DistributedDataParallel (DDP)

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1) Initialize PyTorch distributed:

```
torch.distributed.init_process_group(backend='nccl')
```

2) Wrap your model:

```
model = torch.nn.parallel.DistributedDataParallel(model, …)
```

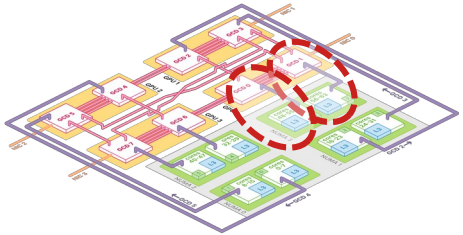
3) Use the distributed sampler:

```
train_dataset =  ...
train_sampler = DistributedSampler(train_dataset)
train_loader  = DataLoader(dataset=train_dataset,
                           shuffle=False,
                           sampler=train_sampler)
```

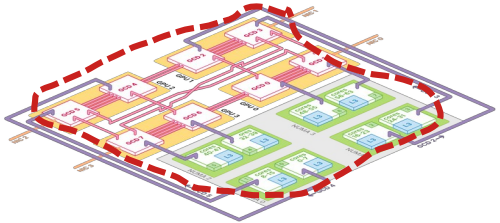
Check that you are actually using all GPUs!

Check GPU utilization

```
$ srun --interactive --pty --jobid=123456 watch rocm-smi
```



- Utilization should be > 0% for all requested GPUs
- Note: showing high utilization is a **necessary, but not sufficient** condition for it actually doing something useful!
  - Refer back to lecture 4 yesterday *Understanding GPU activity & checking jobs*
  - Check GPU power and use profiling



Multi-GPU tips & tricks

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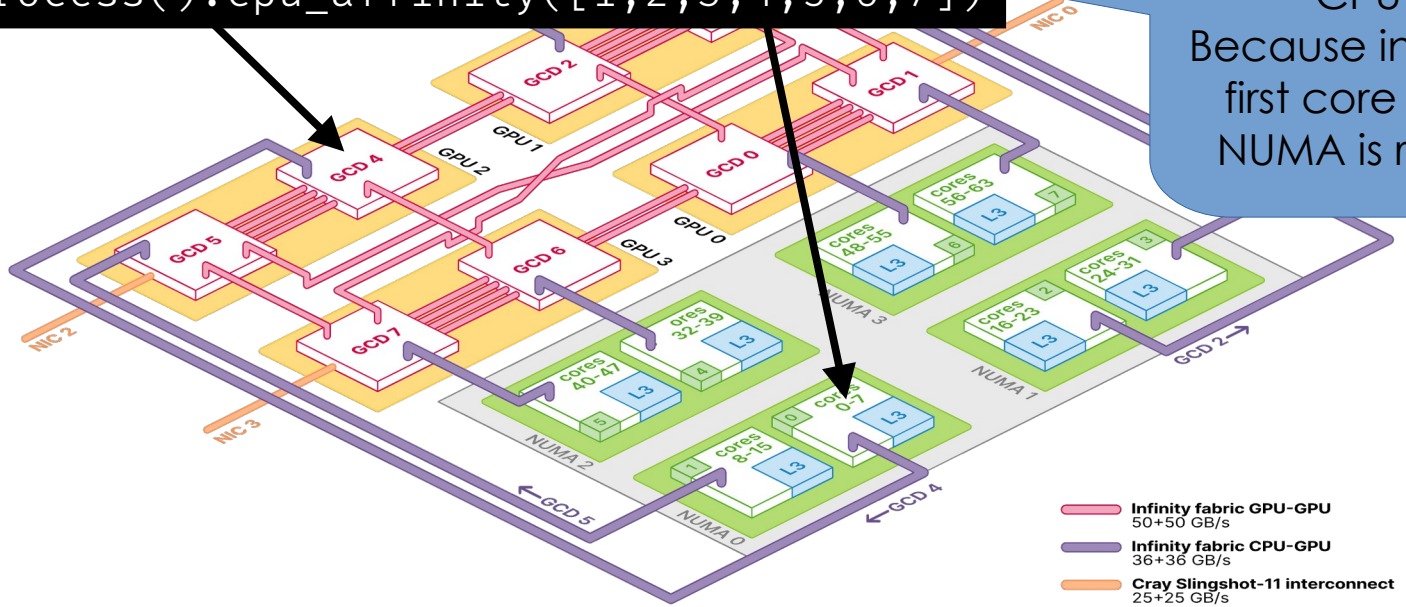
- Use RCCL and libfabric for efficient communication
  - AWS OFI RCCL plugin for containers: https://github.com/ROCm/aws-ofi-rccl
- Add fault tolerance when possible, especially for huge jobs
  - Checkpointing!
- (Optionally) bind the processes to optimal CPU cores
  - Improves CPU-GPU I/O, might speed up cases with high I/O
- Issues with multi-worker data loaders segfaulting:

```
if __name__ == __main__:
  multiprocessing.set_start_method("spawn")
```

GPU and CPU Bindings

Example: GCD 4:
`psutil.Process().cpu_affinity([1,2,3,4,5,6,7])`

Why do we skip CPU 0?
Because in LUMI the first core in each NUMA is reserved



https://docs.lumi-supercomputer.eu/runjobs/scheduled-jobs/distribution-binding/#gpu-binding