Scaling AI training to multiple GPUs

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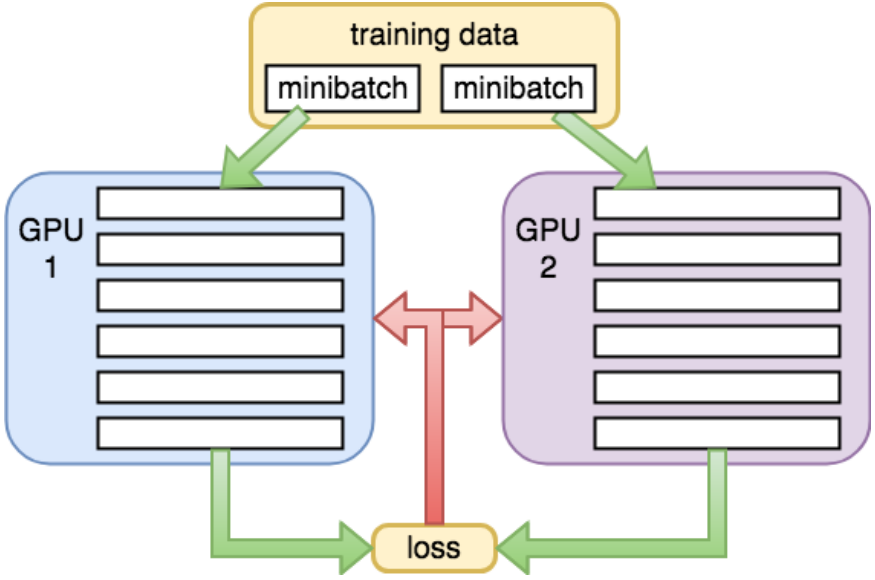
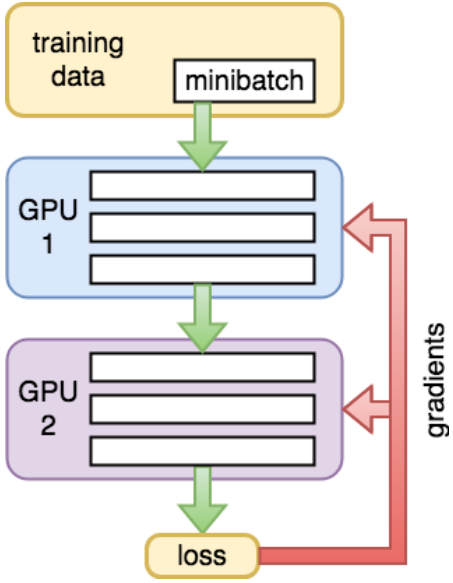
Reasons to use multiple GPUs

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



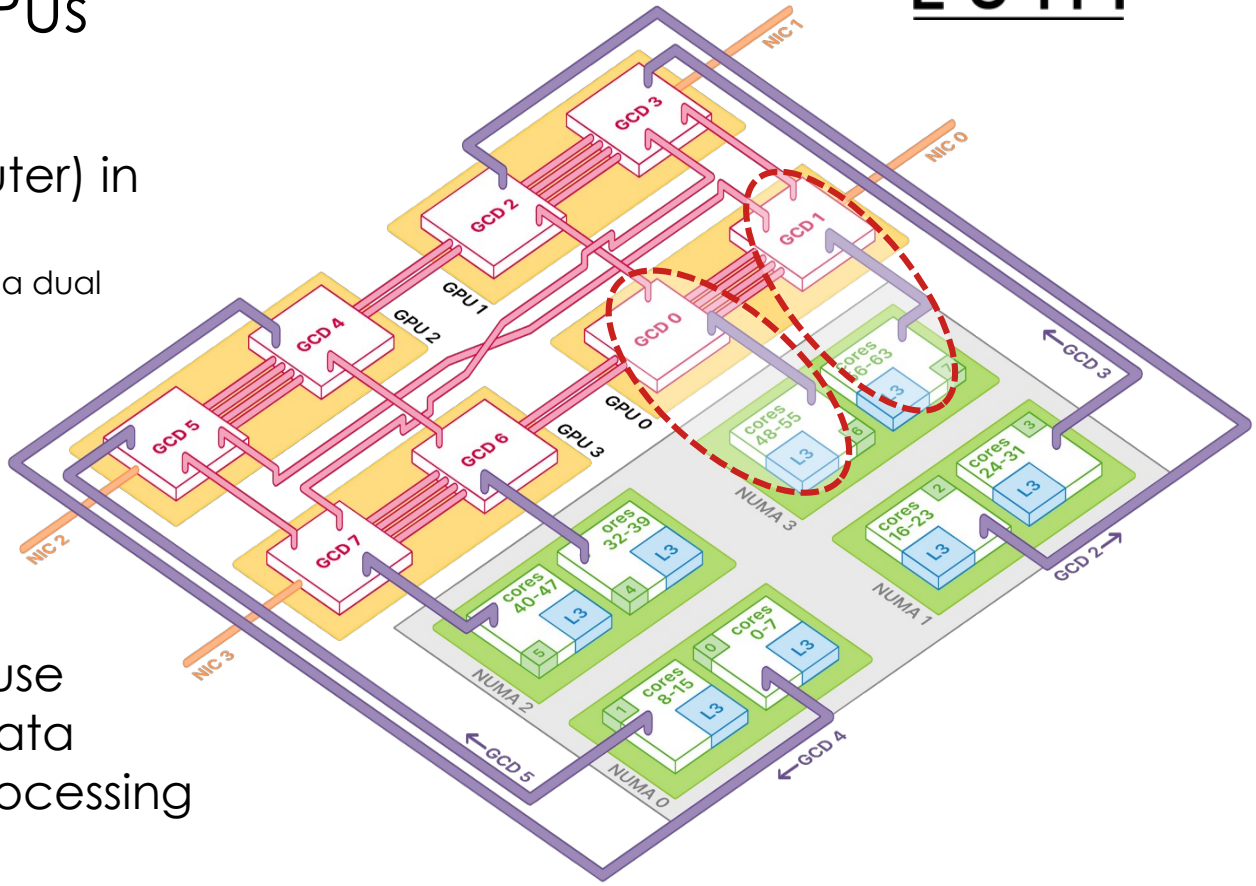
My model is too big to fit into one GPU
→ **model parallelism**



Using multiple GPUs

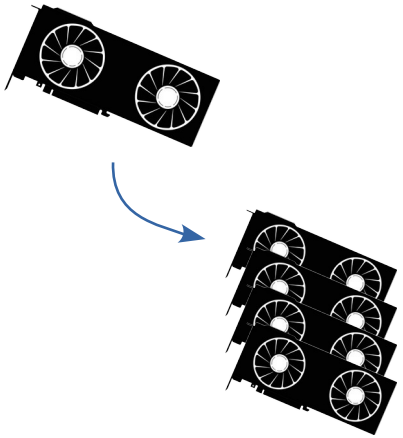
- Each node (computer) in LUMI has 8 GPUs
  (Actually 4 x MI250x, which is a dual chip card = 8 GCDs)

- 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



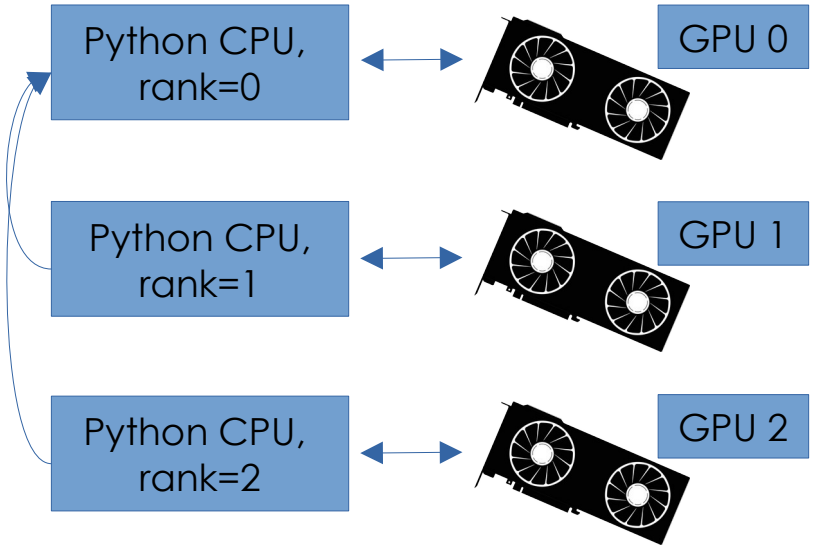
Multi-GPU resource allocation on LUMI

- Use **`--gpus-per-node=N`** where `N=1,…,8`
  - `--gpus-per-task` option not currently recommended due to bug in Slurm
- Max 8 GPUs in one node, for more GPUs, add more nodes: **`--nodes=M`**
  - More on multi-*node* jobs in the next lecture

Multi-GPU resource allocation on LUMI

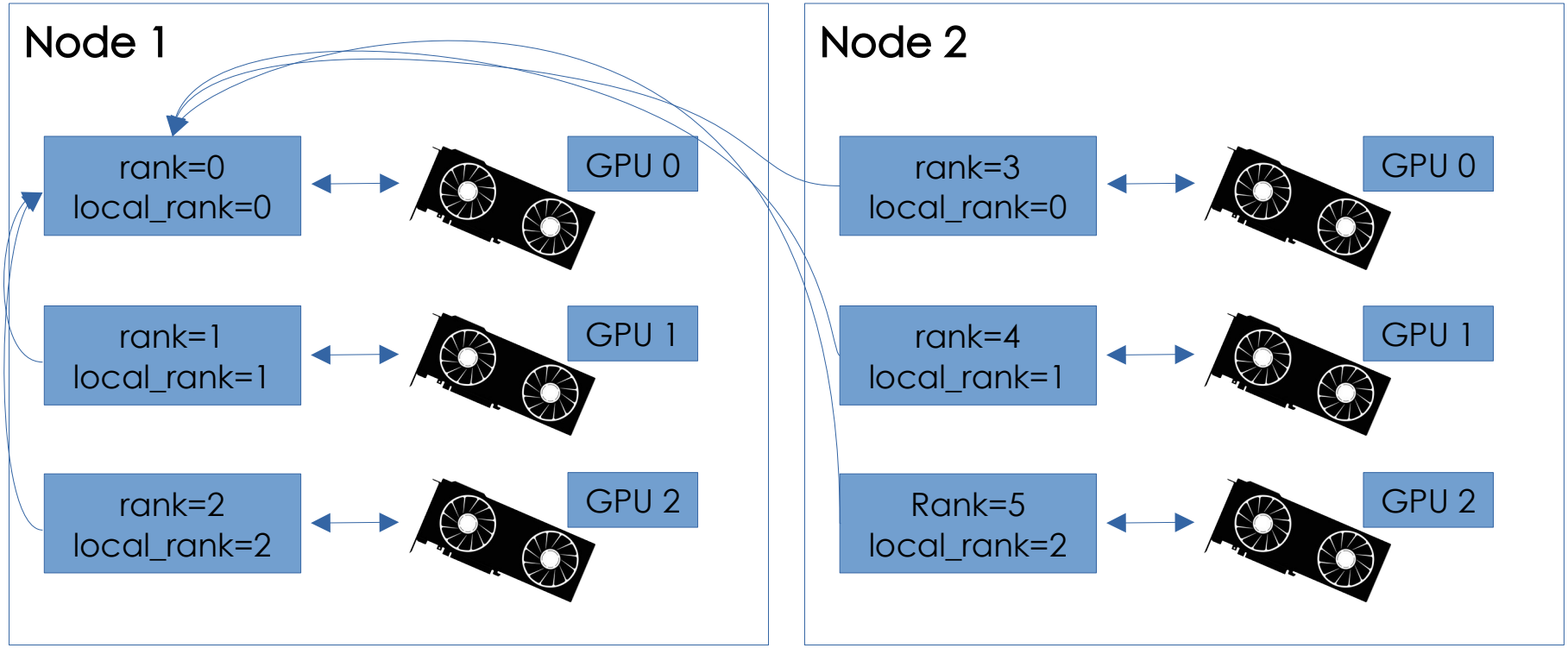
- Allocate a maximum of **1/8 of resources per GPU**:
  - 60 GB **CPU memory (RAM)** and 7 CPU cores per GPU
  - Full node: 480 GB and 56 cores
    (leaving some "slack" for the system)
  - Note: you **always get the full GPU memory (VRAM)** of 64 GB per GCD (no need to allocate that with Slurm options)
  - Resources billed in GPUh according to 1/8 slice

One Python CPU control process per GPU



- We start one Python process (CPU) per GPU
- Each process needs to know which GPU it should talk to, given by the process **rank**
- The first process (rank=0) is the main process, and the others connect back to it

Multiple nodes: rank and local_rank



Example: one full node, 8 GPUs

```
#!/bin/bash
#SBATCH --account=project_NNNNNNNN
#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_NTASKS

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

Where to connect to?

How many processes are there?

Which process am I?

*The line with **srun** will be launched multiple times according to the number of **tasks***

In the Python code:

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

Example: 2 nodes, 2×8=16 GPUs in total

```
#!/bin/bash
#SBATCH --account=project_NNNNNNNN
#SBATCH –partition=standard-g
#SBATCH --nodes=2
#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_NTASKS

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

Example: one full node, 8 GPUs, *with torchrun*

LUMI

```
#!/bin/bash
#SBATCH --account=project_NNNNNNNN
#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
```

Torchrun will take care of launching multiple processes, Slurm just needs to start one torchrun

Example: 2 nodes, 2×8=16 GPUs in total, with torchrun

```
#!/bin/bash
#SBATCH … < skipping some common Slurm options >
#SBATCH --nodes=2
#SBATCH --gpus-per-node=8
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=56
#SBATCH --mem=480G
## < module loading part as before – removed for readability>

export RDZV_HOST=$(hostname)
export RDZV_PORT=29400

srun singularity exec $CONTAINER \
    torchrun --rdzv_id=${SLURM_JOB_ID} --rdzv_backend=c10d
             --rdzv_endpoint="$RDZV_HOST:$RDZV_PORT" \
             --nnodes=${SLURM_JOB_NUM_NODES} \
             --nproc-per-node=${SLURM_GPUS_PER_NODE} \
```

srun is needed again, as we want Slurm to start ONE torchrun PER node

Torchrun has it's own rendezvous mechanism for connecting to the main node, essentially we again need to tell it the hostname and port

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)

LUMI

1) Initialize PyTorch distributed:

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

2) Wrap your model:

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

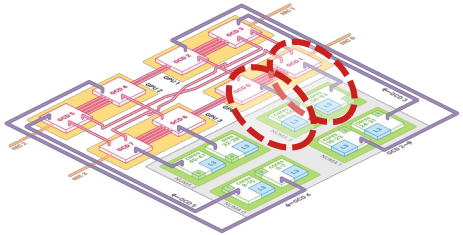
3) Use the distributed sampler:

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

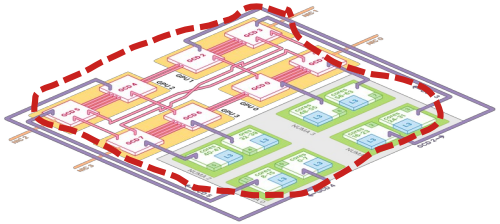
Check that you are actually using all GPUs!

Check GPU utilization

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



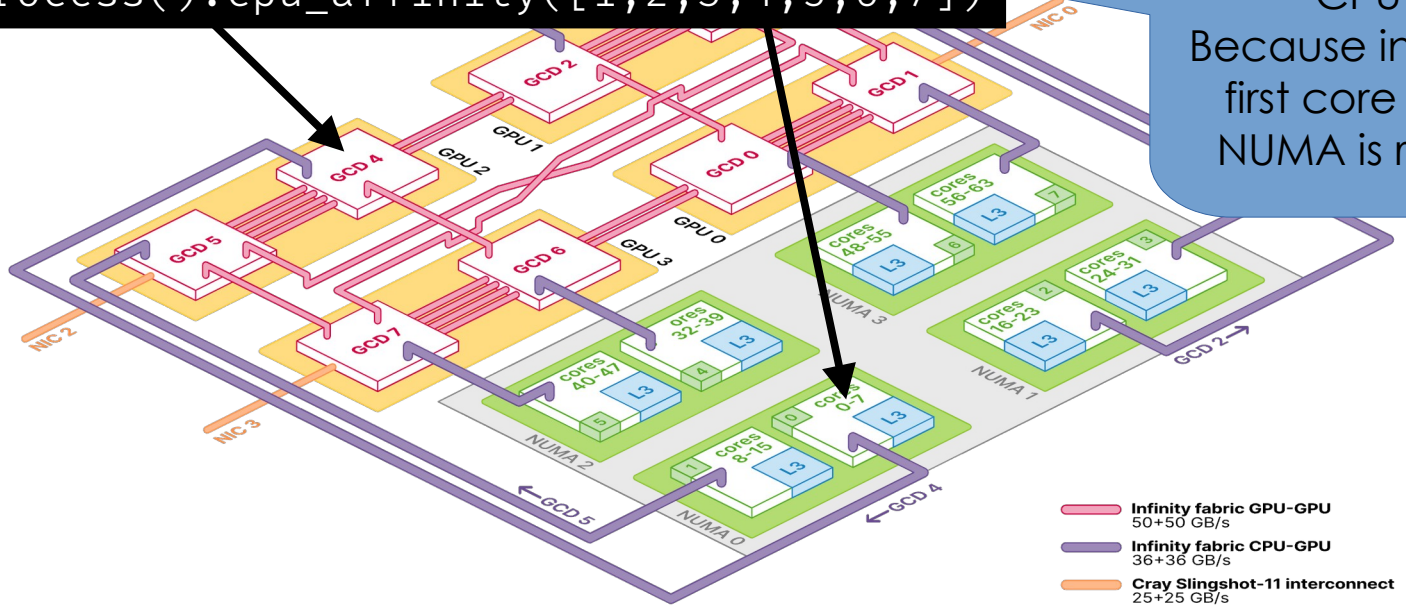
- Utilization should be > 0% for all requested GPUs
- Note: showing high utilization is a **necessary, but not sufficient** condition for it actually doing something useful!
  - Refer back to lecture 4 yesterday *Understanding GPU activity & checking jobs*
  - Check GPU power and use profiling



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