Parallel and Distributed Deep Learning

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Outline

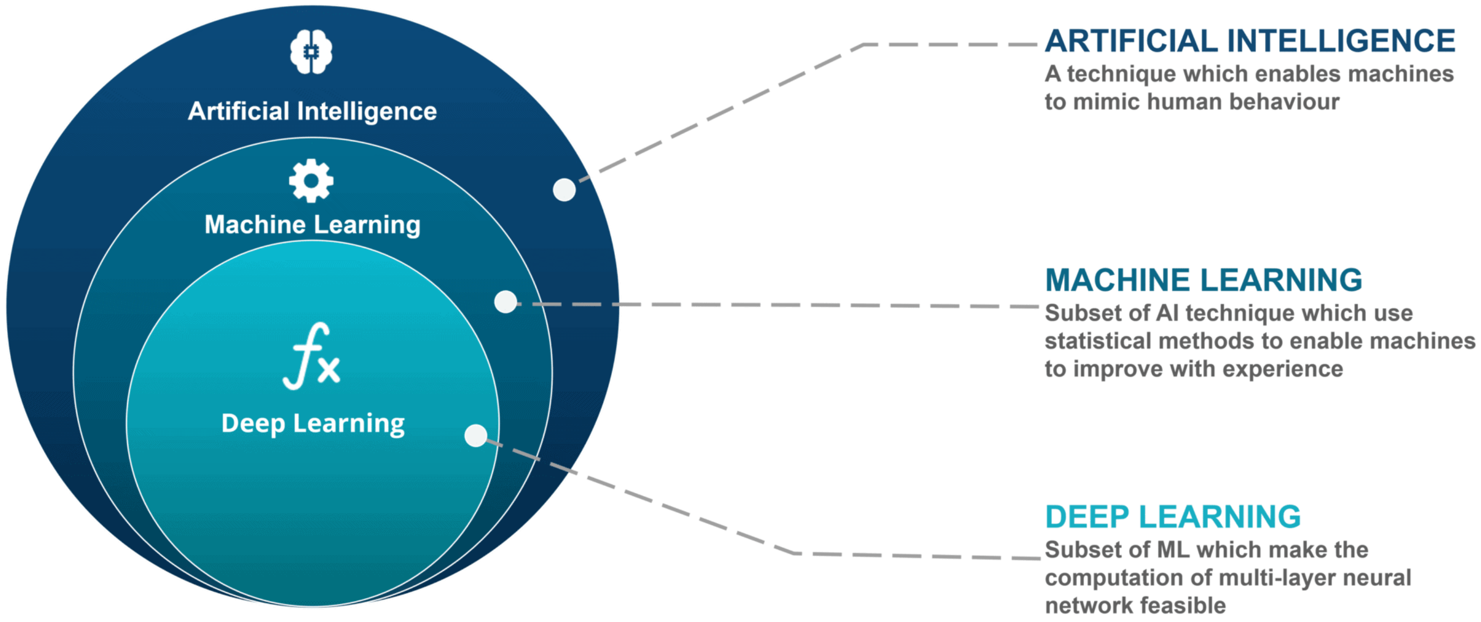
- ❑ Basics of deep learning
- ❑ Parallel deep learning on a GPU
- ❑ Distributed deep learning on multiple GPUs
- Data parallelism
  -- Zero Redundancy Optimizer
- Model parallelism
  -- Pipeline parallelism
  -- Tensor parallelism

Machine learning and deep learning

- Artificial intelligence
- Machine learning

  Statistical algorithms

  Learn from data
- Supervised learning: classification, regression
- Unsupervised learning: clustering



- Deep learning: deep neural network
- Cornerstones of DL: learning algorithms, big data, and high-performance computing.
- Computer vision: Convolutional Neural Network (CNN)
- Natural Language Processing (NLP): Large Language Model (LLM), transformer architecture

Access to ORCD clusters

- Get started

https://orcd-docs.mit.edu/getting-started/

- Log in Engaging

```
ssh <user>@eofe10.mit.edu
```

- Get an interactive session and set up environment

```
srun -t 120 -n 4 --gres=gpu:4 -p mit_normal_gpu --pty bash
module load miniforge/23.11.0-0
```

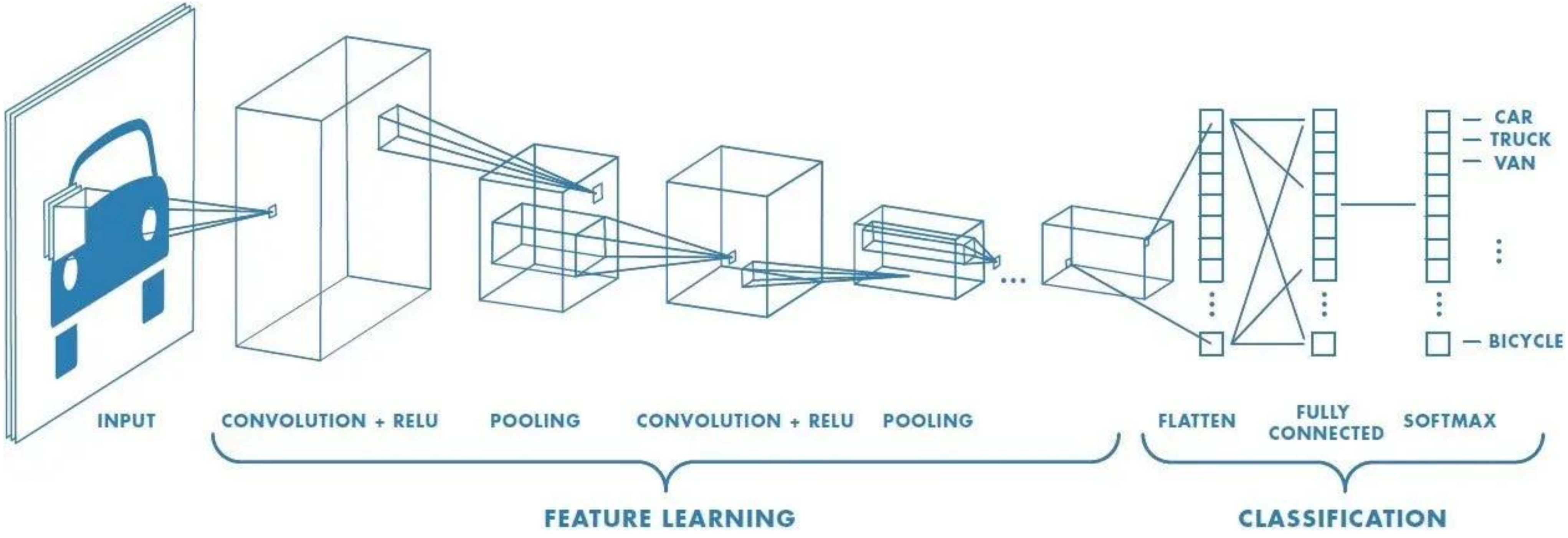
Install PyTorch and Deepspeed

- Install PyTorch, Deepspeed, and dependencies.

```
conda create -n ds
source activate ds
conda install PyTorch==2.4.1 torchvision==0.19.1 torchaudio==2.4.1 pytorch-cuda=12.4 -c PyTorch -c
nvidia
pip install deepspeed
pip install datasets  tensorboard transformers
pip install fire loguru sh matplotlib
```

Convolutional Neural Network (CNN)

- CNN for CIFAR10 in PyTorch
- Load training and test datasets: CIFAR10, normalize, using torchvision
- Define a CNN: convolutional layers, nonlinear ReLU activation, pooling, fully connected layers, softmax



https://saturncloud.io/blog/a-comprehensive-guide-to-convolutional-neural-networks-the-eli5-way/

Train a neural network

- Training: adjust the model to minimize a loss function.
- Loss function: cross entropy

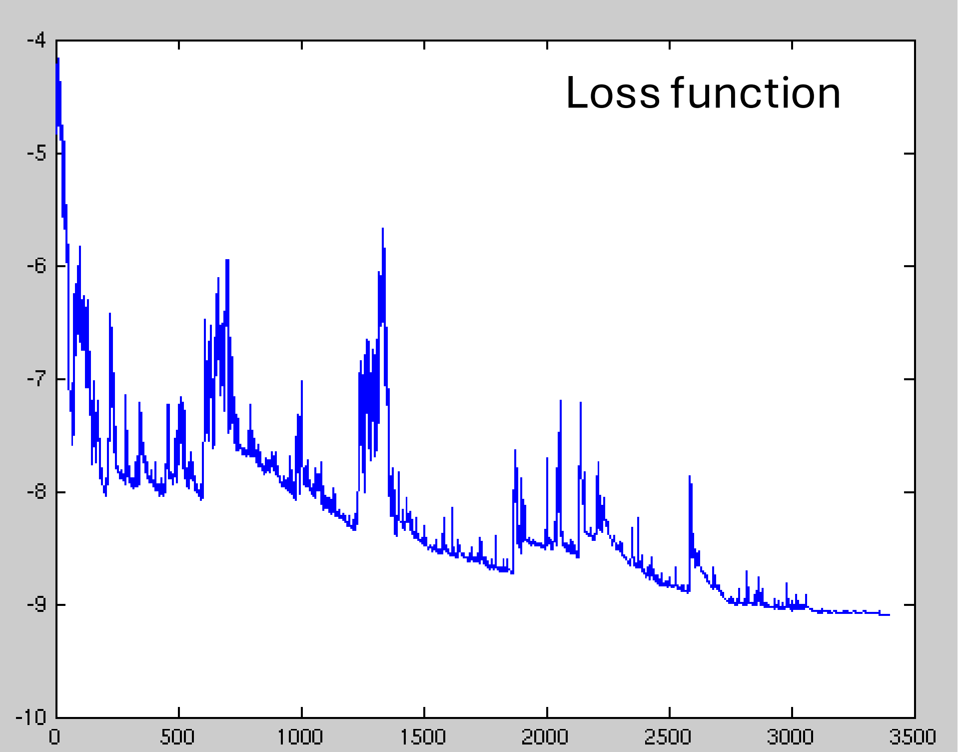
$$-\frac{1}{N}\sum_{n=1}^{N}\left[y_n \log \hat{y}_n + (1-y_n)\log(1-\hat{y}_n)\right]$$

- Optimizer: Stochastic Gradient Descent (SGD)
- Training data: batch or mini-batch (a randomly-picked subset of data), epoch (loop over all data).
- Train the network on the training data:

-- forward + backward + optimize

-- Backpropagation: computes the gradient of the loss function with respect to the weights, one layer at a time, iterating backward from the last layer to avoid redundant calculations of intermediate terms in the chain rule of derivatives.

- Test the network on the test data



https://en.wikipedia.org/wiki/Stochastic_gradient_descent

Training on a GPU with PyTorch

- Define a CUDA device

```
device = torch.device('cuda:0' if torch.cuda.is_available() else 'cpu')
```

- Send the model to the GPU

```
net.to(device)
```

- Training process:

```
for epoch in range(2):  # loop over the dataset multiple times
    running_loss = 0.0
    for i, data in enumerate(trainloader, 0):   # get a batch of data

        # Send a batch of data to the GPU at every step
        inputs, labels = data[0].to(device), data[1].to(device)

        optimizer.zero_grad()     # initialize gradients
        outputs = net(inputs)     # forward pass
        loss = nn.CrossEntropyLoss(outputs, labels) # define loss function
        loss.backward()           # backward pass
        optimizer.step()          # optimize
```

What happens under the hood?

What about parallel?

- Training a neural network involves large-scale linear algebra computations.
- When PyTorch is built with CUDA support, it dynamically links to cuDNN and cuBLAS libraries.
- Linear algebra computations are optimized and parallelized in cuBLAS and thus accelerated on GPUs.

What about other platforms or libraries?

- Tensorflow: Python or C API, a steeper learning curve, less friendly to researchers, easier with Keras integration, better performance optimizations, better for developers.
- cuDNN: C API, a bridge between deep-learning platforms and GPUs.

Distributed Parallelism for Deep Learning

- Distributed on multiple GPUs.

- Data Parallelism

Each GPU gets a different batch of data

Process more data at the same time period.

Universal to different models. The model must fit within GPU memory.

- Model Parallelism

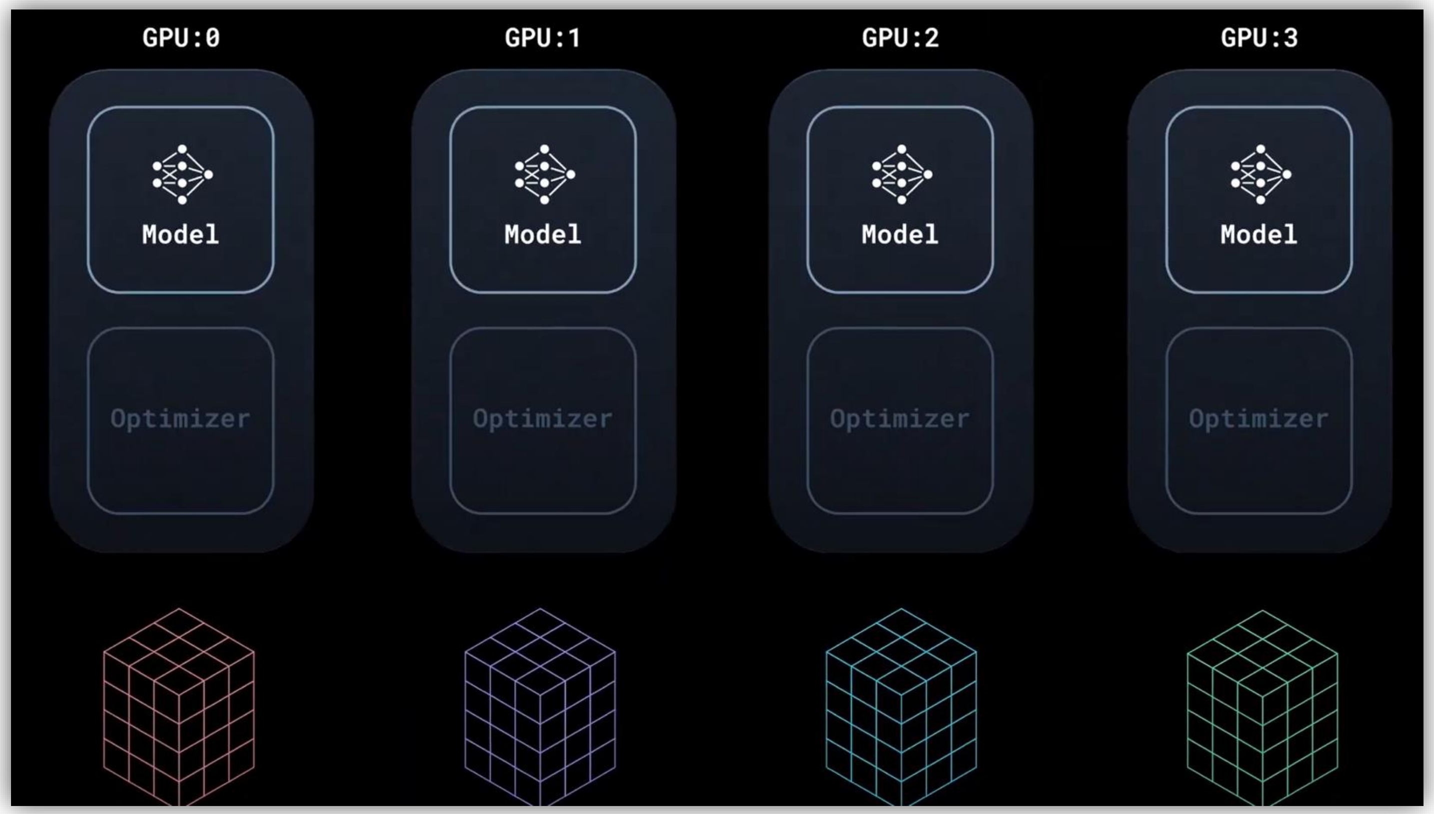
A model is too big to be stored on a GPU.

Partition the model on multiple GPUs.

Tricky to design and implement.

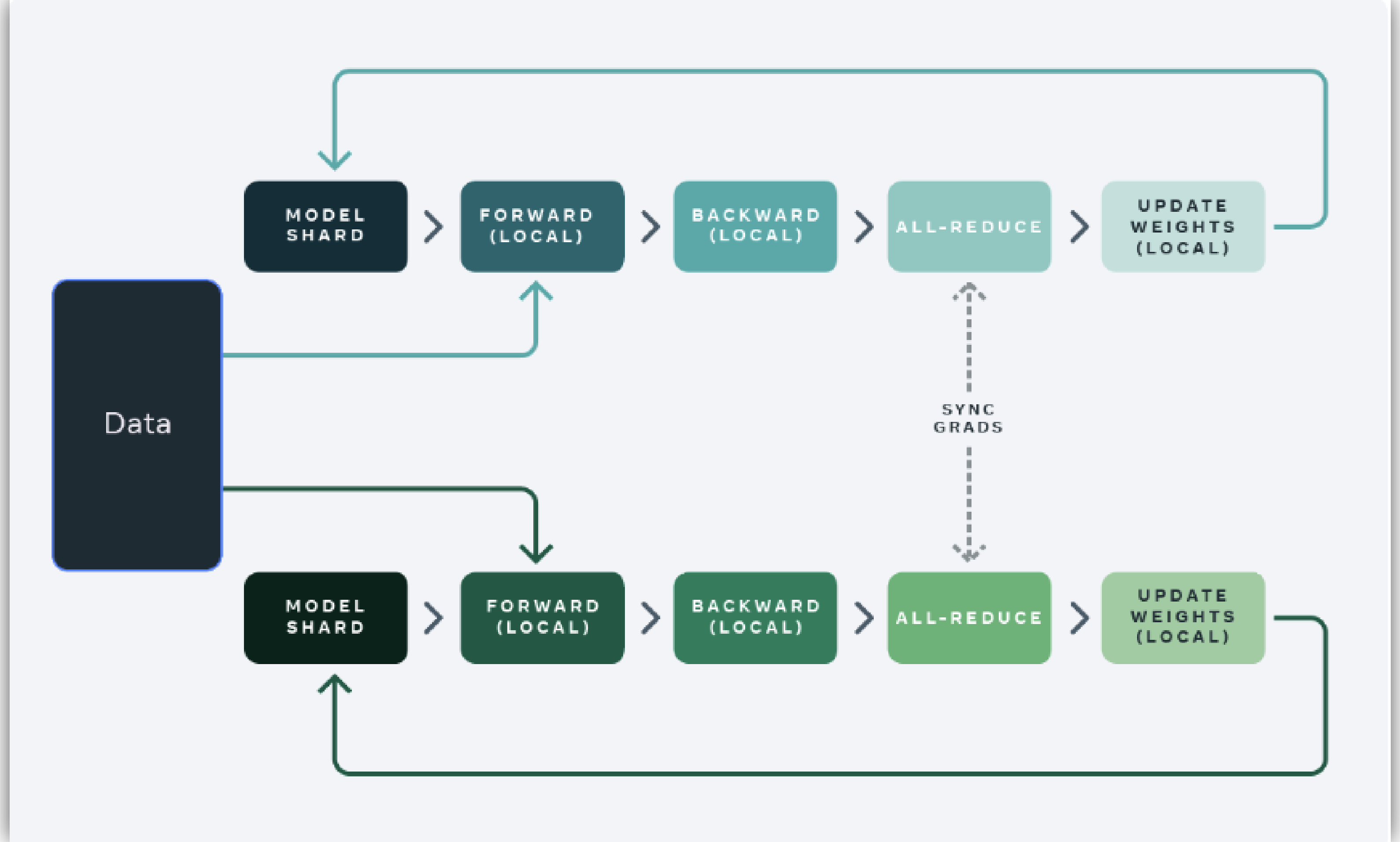
Data Parallelism

- Each GPU has a copy of the model
- Each GPU gets a different batch of data
- Data sampling is handled by a Distributed Sampler
- Concurrently processing multiple batches of data



Data Parallel training at large scale may affect model quality

Communication in data parallel



- Gradients on each GPU are different because the input data is different.
- Gradients from each GPU are synchronized before the update.
- Synchronization is done with a bucketed Ring-AllReduce algorithm.
- Each GPU gets the averaged gradient, then models are updated locally.
- Overlap gradient computation with communication so GPUs are utilized efficiently.

Scaling with data parallel introduces communication overhead when syncing gradients

Distributed Data Parallel with PyTorch

- Linear neural network $y = xA^T + b$

```
model = torch.nn.Linear(20, 1)
```

- Set up GPU ID

```
torch.cuda.set_device(rank)
```

- Apply DDP

```
self.model = DistributedDataParallel(model, device_ids=[gpu_id])
```

- Spawn training processes on multiple GPUs

```
world_size = torch.cuda.device_count()
mp.spawn(main, args=(world_size, args.save_every, args.total_epochs, args.batch_size), nprocs=world_size)
```

- Communication is under the hood. PyTorch calls NCCL.

https://PyTorch.org/tutorials/beginner/ddp_series_multigpu.html , https://PyTorch.org/docs/stable/notes/ddp.html

Why big models?

- Transformer architecture

  -- Remove the sequential processing dependency of RNNs, such as Long Short-term Memory (LSTM).

  -- Enable language models to be trained with parallelism

- A dramatic increase in model sizes after the birth of Transformer.

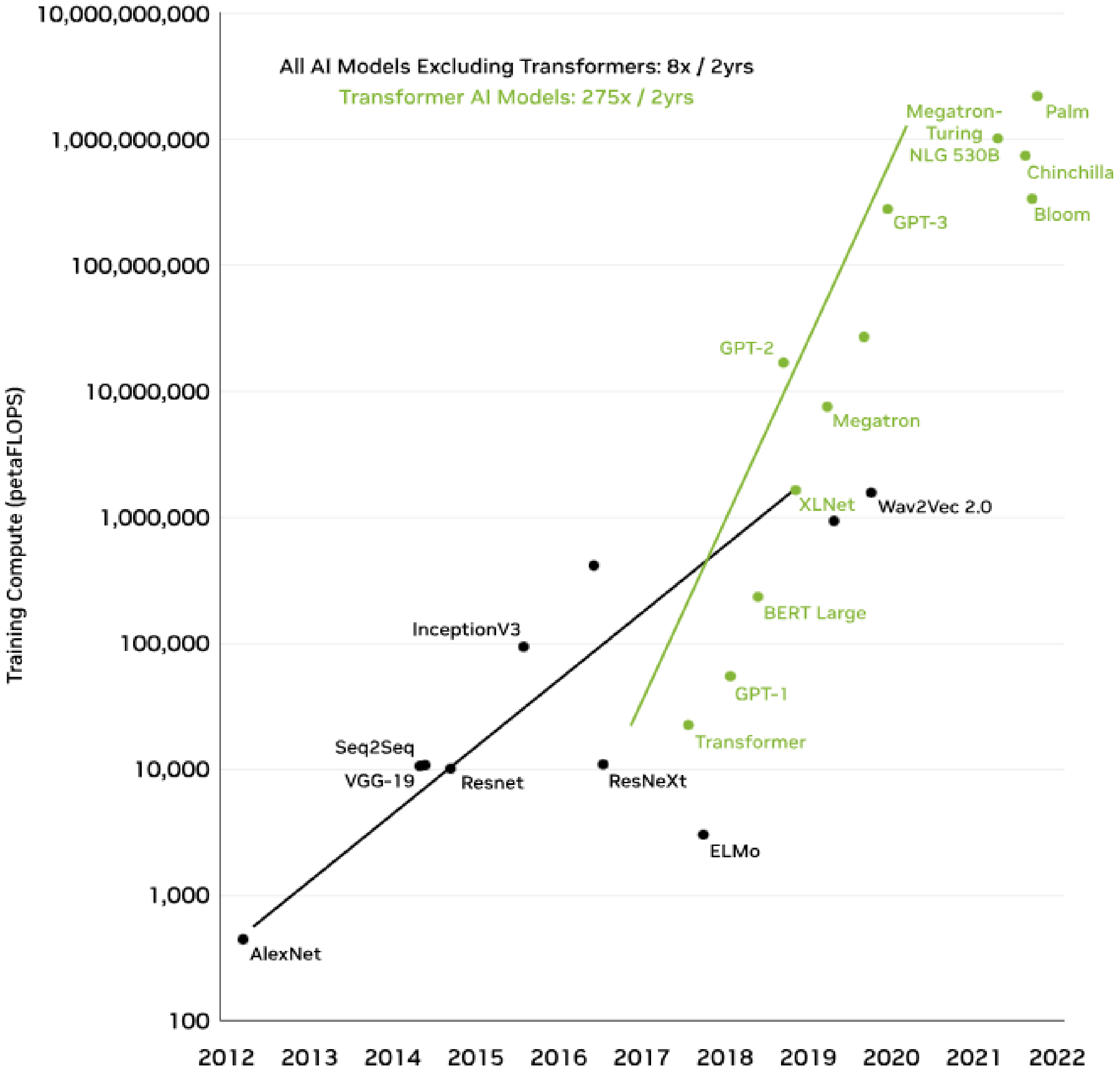


Figure 3. Compute required for training transformer models.

Memory requirements by big models

- Adam optimizer: 24 bytes per parameter for FP32

States	Bytes per parameter
Model parameters (weights)	4 bytes per parameter
Adam optimizer (2 states)	8 bytes per parameter
Gradients	4 bytes per parameter
Activations and temp memory (variable size)	8 bytes per parameter (high-end estimate)
TOTAL	**= 4 + 20 bytes per parameter**

- 1 billion parameters:

  24 GB for FP32, 12 GB for FP16, 16 GB for mixed-precision (FP32 for optimizer states, FP16 for the rest)

https://www.oreilly.com/library/view/generative-ai-on/9781098159214/ch04.html#:~:text=Quantization%20from%20fp32%20to%20fp16,shown%20in%20Figure%204%2D6

https://www.geeksforgeeks.org/adam-optimizer/

https://www.determined.ai/blog/act-mem-2

Scale of compute with big models

Model size	Attention heads	Hidden size	Number of layers	Number of parameters (billion)	Model-parallel size	Number of GPUs	Microbatch size	Batch size	Achieved teraFlOP/s per GPU	Percentage of theoretical peak FLOP/s	Achieved aggregate petaFLOP/s
1.7B	24	2304	24	1.7	1	32	16	512	137	44%	4.4
3.6B	32	3072	30	3.6	2	64	16	512	138	44%	8.8
7.5B	32	4096	36	7.5	4	128	16	512	142	46%	18.2
18B	48	6144	40	18.4	8	256	8	1024	135	43%	34.6
39B	64	8192	48	39.1	16	512	4	1536	138	44%	70.8
76B	80	10240	60	76.1	32	1024	2	1792	140	45%	143.8
145B	96	12288	80	145.6	64	1536	2	2304	148	47%	227.1
310B	128	16384	96	310.1	128	1920	1	2160	155	50%	297.4
530B	128	20480	105	529.6	280	2520	1	2520	163	52%	410.2
1T	160	25600	128	1008.0	512	3072	1	3072	163	52%	502.0

Weak scaling throughput for GPT models ranging from 1 billion to 1 trillion parameters.

~6 weeks on 1 x DGX A100
~2 weeks on 4 x DGX A100

~65 weeks on 1 x DGX A100
~16 weeks on 4 x DGX A100

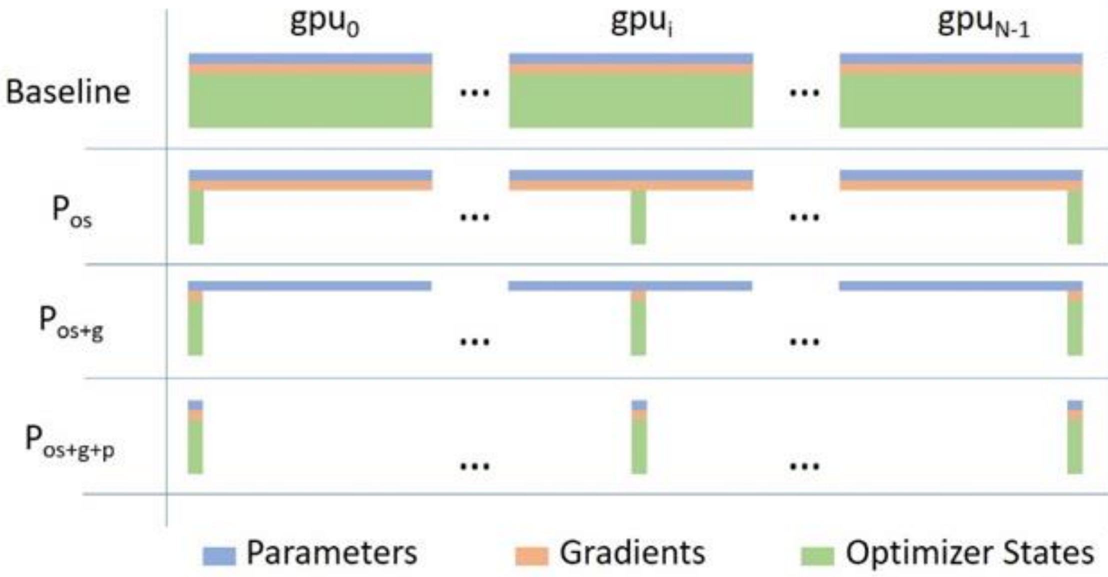
~5 years on 1 x DGX A100
~1 year on 4 x DGX A100

~69 years on 1 x DGX A100
~17 year on 4 x DGX A100

Narayanan, Deepak, et al. "**Efficient large-scale language model training on GPU clusters using megatron-LM**." *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*. 2021.

Zero Redundancy Optimizer (1)

- Operate within the data parallel framework, optimizing memory usage by distributing model states across data parallel workers.
- Partition tensors similar to tensor parallel. Each GPU stores only a slice of model parameters, gradients, and optimizer states.
- Communication: Each GPU receives other slices of parameters from other GPUs during the forward and backward pass.



	Memory Consumption		Comm Volume
	Formulation	Specific Example $K=12$ $\Psi=7.5B$ $N_d=64$	
Baseline	$(2+2+K)*\Psi$	120GB	1x
P_{os}	$2\Psi+2\Psi+\frac{K*\Psi}{N_d}$	31.4GB	1x
P_{os+g}	$2\Psi+\frac{(2+K)*\Psi}{N_d}$	16.6GB	1x
P_{os+g+p}	$\frac{(2+2+K)*\Psi}{N_d}$	1.9GB	1.5x

https://www.microsoft.com/en-us/research/blog/zero-deepspeed-new-system-optimizations-enable-training-models-with-over-100-billion-parameters/

Zero Redundancy Optimizer (2)

- Further save GPU memory

  -- Mixed precision: weights and gradients stored in FP16, optimizer states stored in FP32

  -- Offloading to CPU

  -- Checkpointing activations

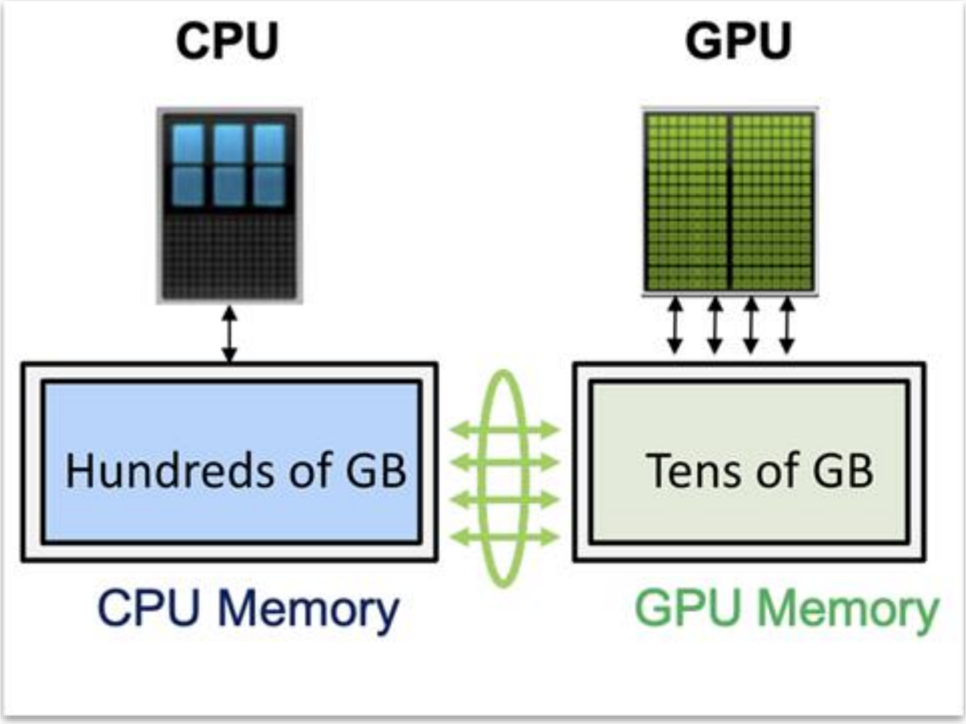
- ZeRO is implemented in Deepspeed.
- Quick and easy: only need to change a few configurations in the configuration JSON.

  Does not require a code redesign or model refactoring.

- ZeRO may or may not be faster depending on the situation and configuration.
- Fully Sharded Data Parallel (FSDP): another name for the ZeRO concept, implemented in PyTorch.

https://www.deepspeed.ai/tutorials/zero/ https://pytorch.org/blog/introducing-pytorch-fully-sharded-data-parallel-api/

Offloading to CPU



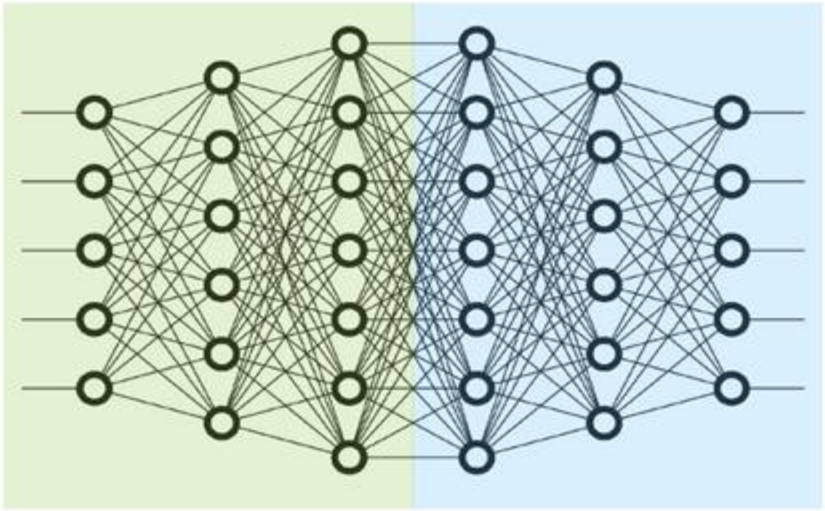
Offload CPU tensors not used in computation form GPU to CPU

- Training times will be slower due to slow data movement.
- Overlap communication with computation.

Model Parallelism

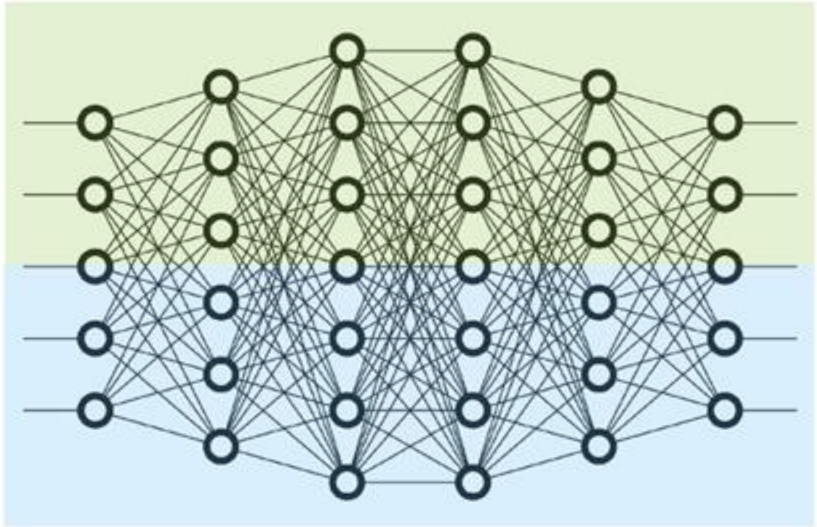
❑ Pipeline (Inter-Layer) Parallelism

- Split the model vertically
- Only one or several layers of the model are placed on a single GPU.
- Each GPU processes in parallel different stages of the pipeline and works on a small chunk of the batch.



❑ Tensor (Intra-Layer) Parallelism

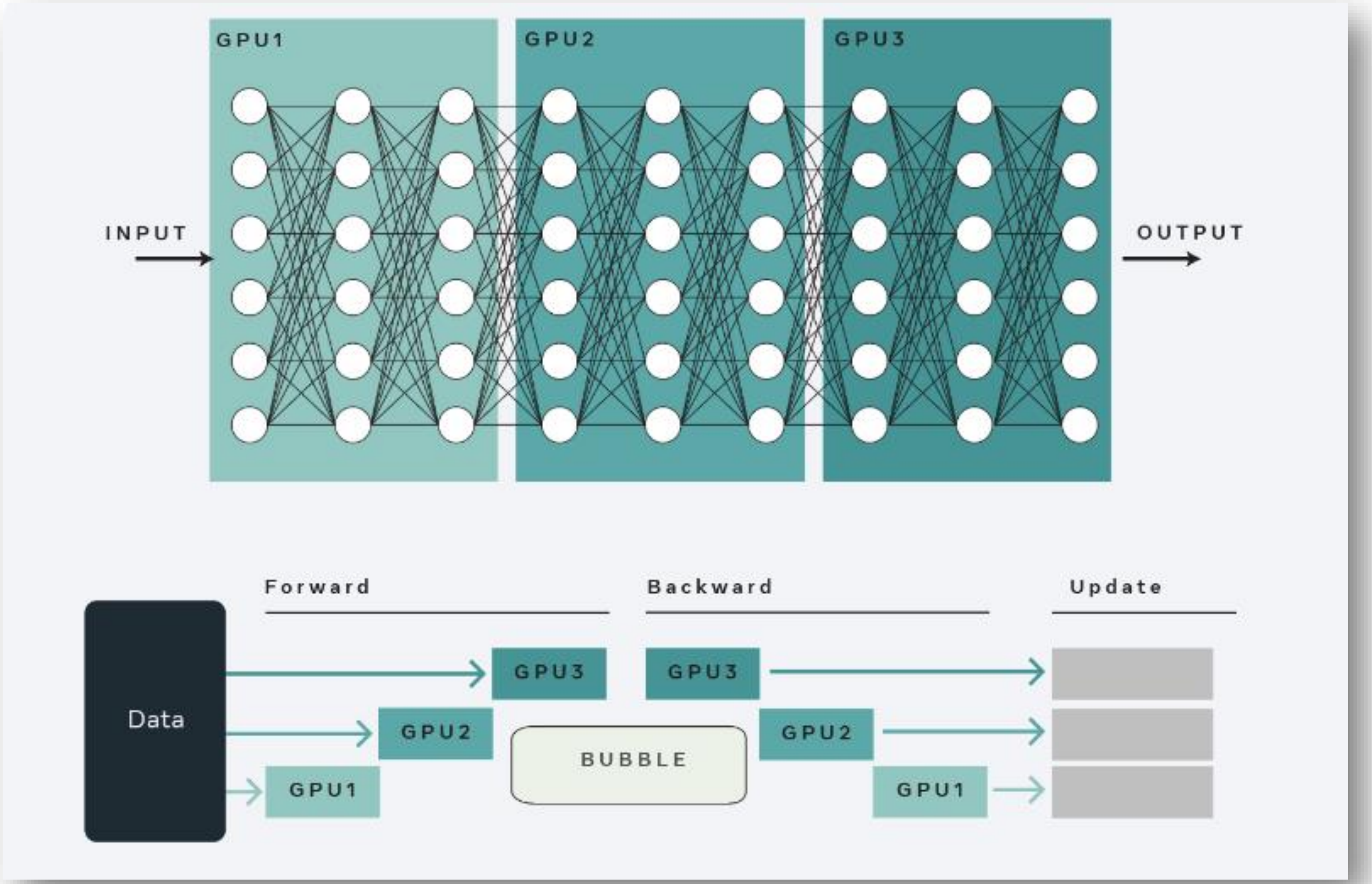
- Split the model horizontally
- Each tensor is split into multiple shards, and each shard resides on its designated GPU.
- Each shard is computed in parallel on different GPUs and the results are synced at the end of the step.



https://huggingface.co/docs/transformers/v4.13.0/en/parallelism

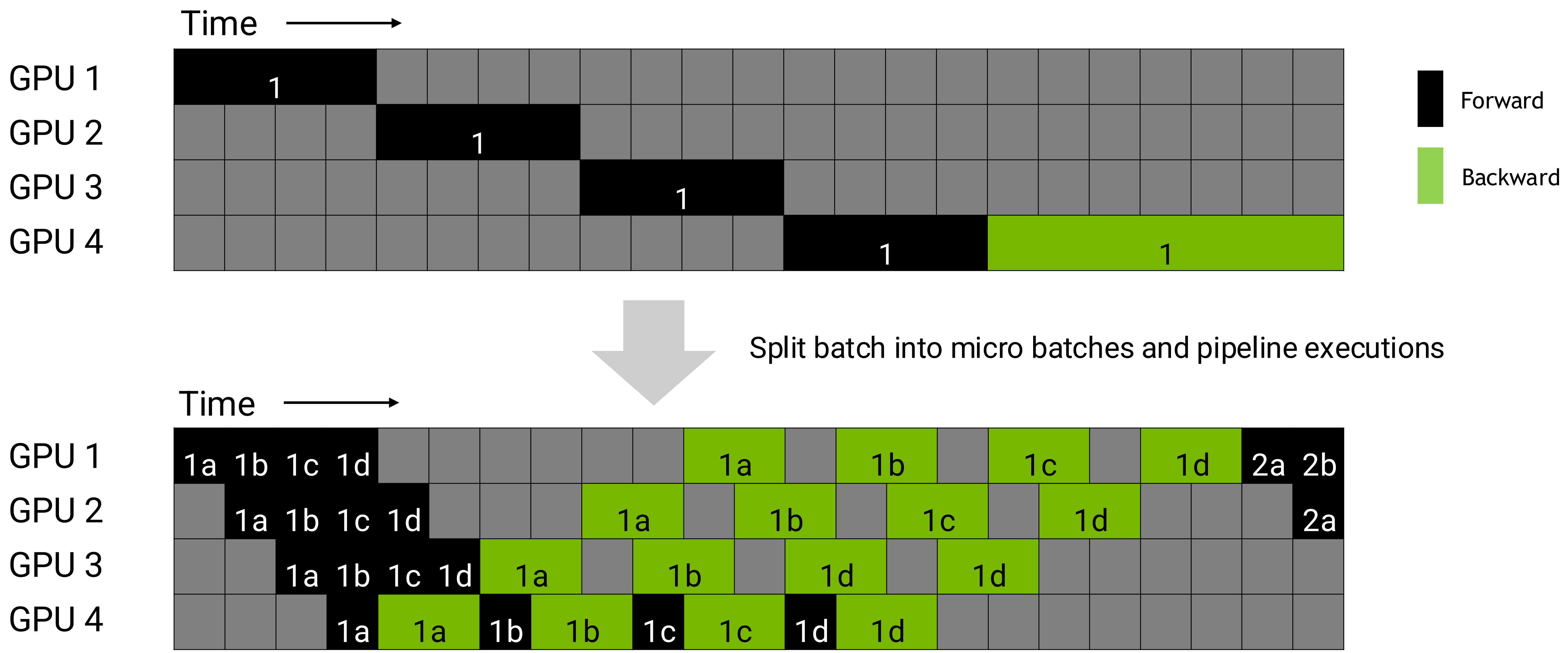
Pipeline Parallelism (1)

- Naive pipeline parallel is sequentially processed.
- Leads to GPU underutilization.



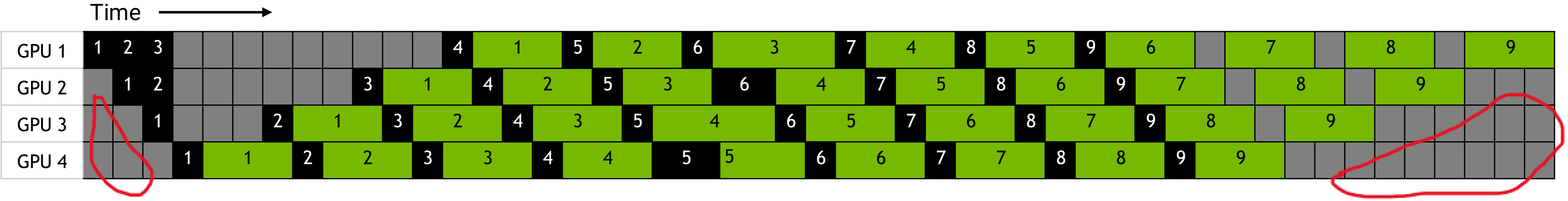
https://fairscale.readthedocs.io/en/latest/deep_dive/pipeline_parallelism.html

Pipeline Parallelism (2)



Pipeline Parallelism (3)

Split batch into micro batches and pipeline executions to increase GPU utilization.



$$\text{total time} = (m + p - 1) \times (t_f + t_b)$$
$$\text{ideal time} = m \times (t_f + t_b)$$
$$\text{bubble time} = (p - 1) \times (t_f + t_b)$$

$$\text{bubble time overhead} = \frac{\text{bubble time}}{\text{ideal time}} = \frac{p-1}{m}$$

p : number of pipeline stages

m : number of micro batches

t_f : forward step time

t_b : backward step time

$$speedup = \frac{t_1}{t_p} = \frac{m*p*(t_f+t_b)}{(m+p-1)(t_f+t_b)} = \frac{m*p}{m+p-1}$$

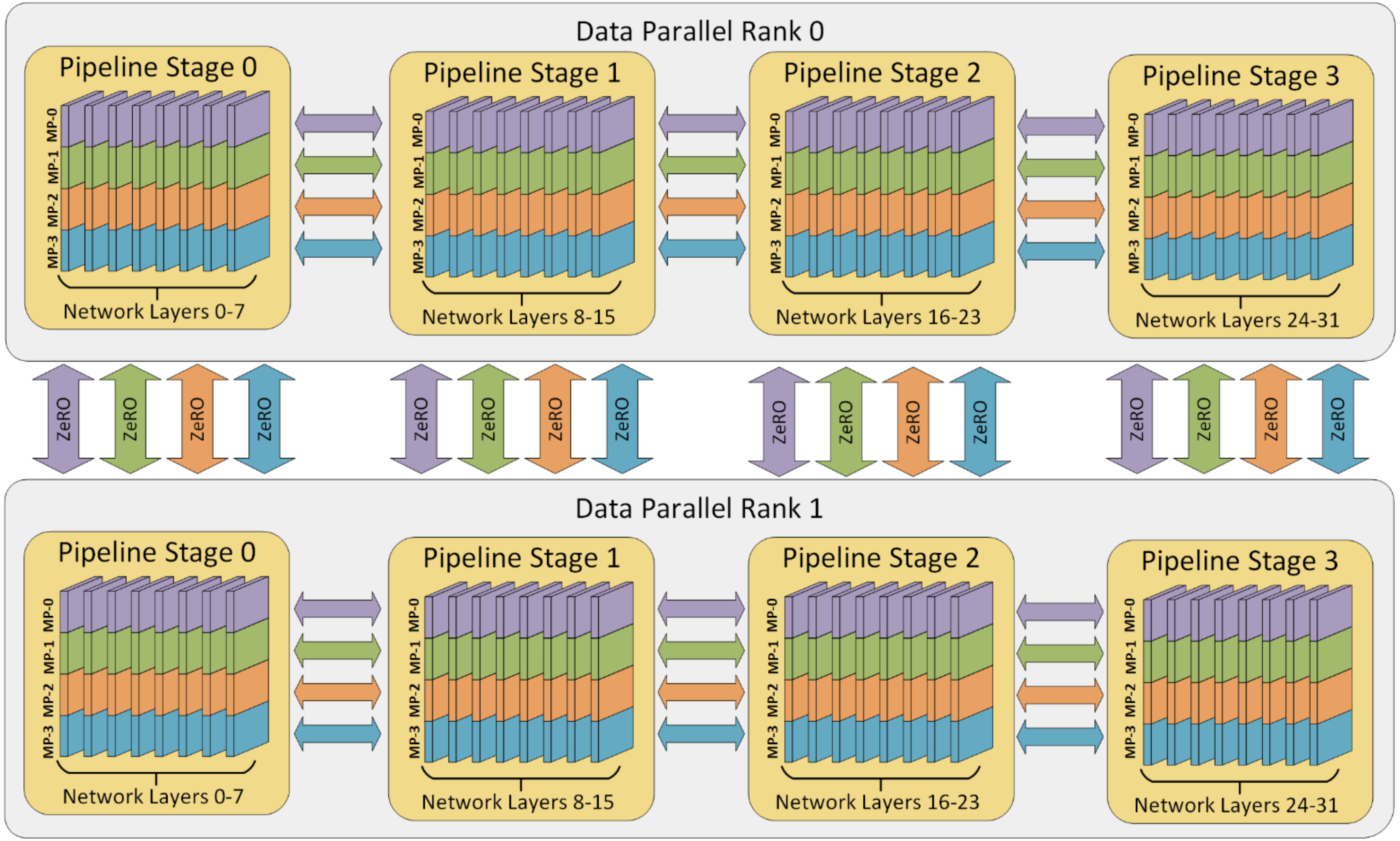
3 times speedup with 4 pipeline stages and 9 micro batches.

Data and Pipeline Parallel (1)

❑ Hybrid parallel: model parallel is applied with data parallel to obtain further acceleration.

- Data parallel

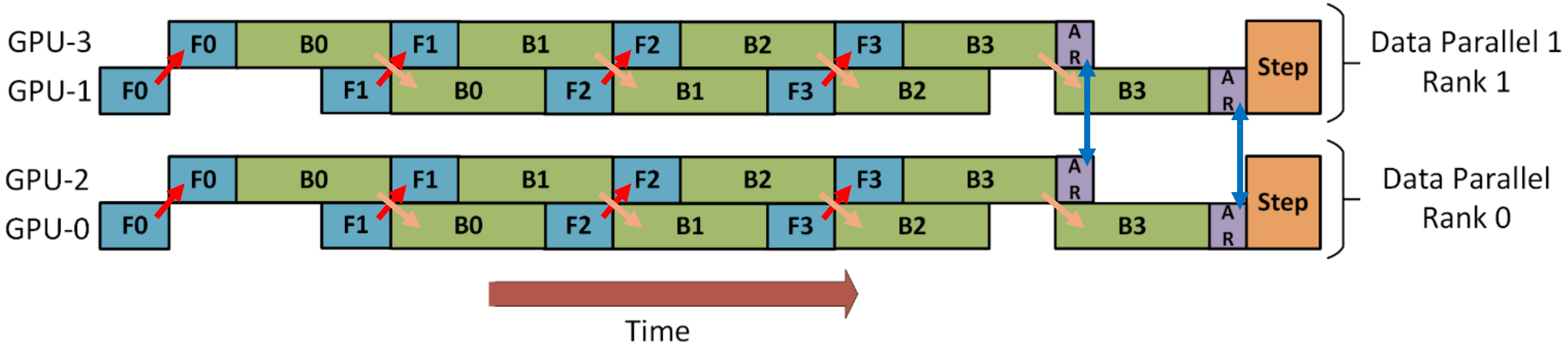
  \+ pipeline parallel



https://www.deepspeed.ai/tutorials/pipeline/

Data and Pipeline Parallel (2)

- Strategy for 4 GPUs: two-way data parallel, two pipeline stages, and eight micro-batches.
- GPUs 0 and 2 are arranged in a pipeline and alternate forward (F) and backward (B) passes — the same for GPUs 1 and 3.
- In the forward pass on a micro-batch, the activation is communicated to the next pipeline stage.
- In the backward pass on a micro-batch, the gradient with respect to the activation is communicated to the next pipeline stage.
- Each backward pass accumulates gradients locally, then a GPU will all-reduce (AR) gradients with its data-parallel counterpart (0 - 1, 2 - 3).
- Finally, the two pipeline stages update their model weights.



Data and Pipeline Parallel with Deepspeed

- Alexnet: 5 convolutional layers + 2 fully connected hidden layers + 1 fully connected output layer.

```
net = AlexNet(num_classes=10)
```

- Set up a pipeline module

```
net = PipelineModule(layers=join_layers(net),
                     loss_fn=torch.nn.CrossEntropyLoss(),
                     num_stages=args.pipeline_parallel_size,
                     partition_method=parameters,
                     activation_checkpoint_interval=0)
```

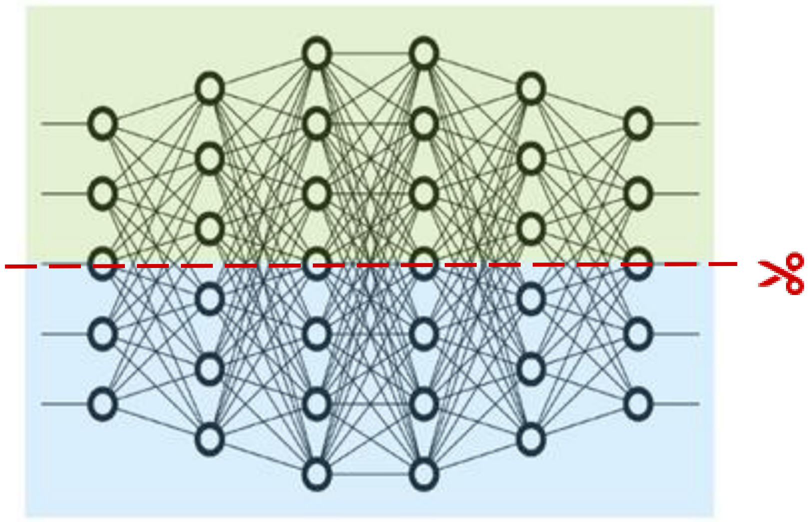
- Set the micro batch size in the configuration JSON

```
"train_micro_batch_size_per_gpu" : 8,
```

- Run the program. The total number of GPUs must be divisible by the number of pipeline stages.

```
deepspeed train.py --deepspeed_config=ds_config.json -p 2 --steps=200
```

Tensor Parallelism

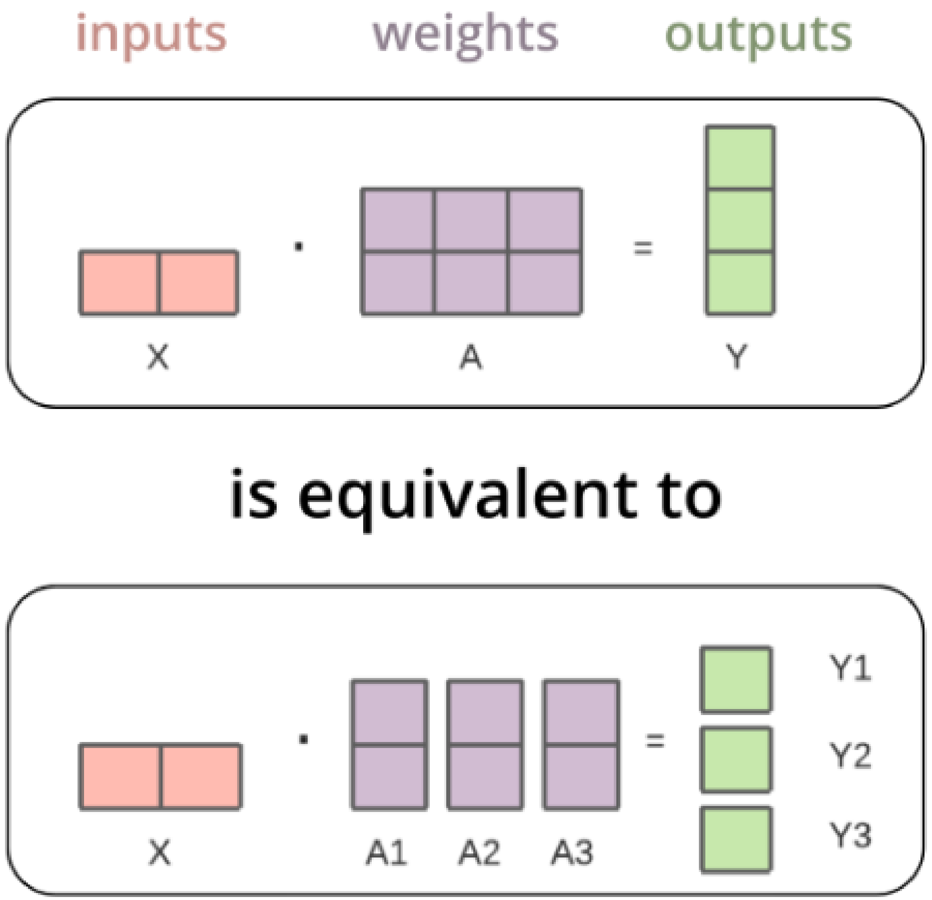


- Use to scale beyond data parallelism
- Less restrictive on the batch size (avoids bubble issue in pipelining)
- Reduces memory proportional to the number of workers (model dependent)
- Sharded computations work well for large matrices (e.g. Transformers)
- Large communication overhead. Does not scale well beyond the node boundary.

The implementation of TP depends on the neural network architecture.

A simple example of tensor parallelism

- When multiplying the input tensors with the first weight tensor, the matrix multiplication is equivalent to splitting the weight tensor column-wise, multiplying each column with the input separately, and then concatenating the separate outputs.
- The outputs are then transferred from the GPUs and concatenated together to get the final result.

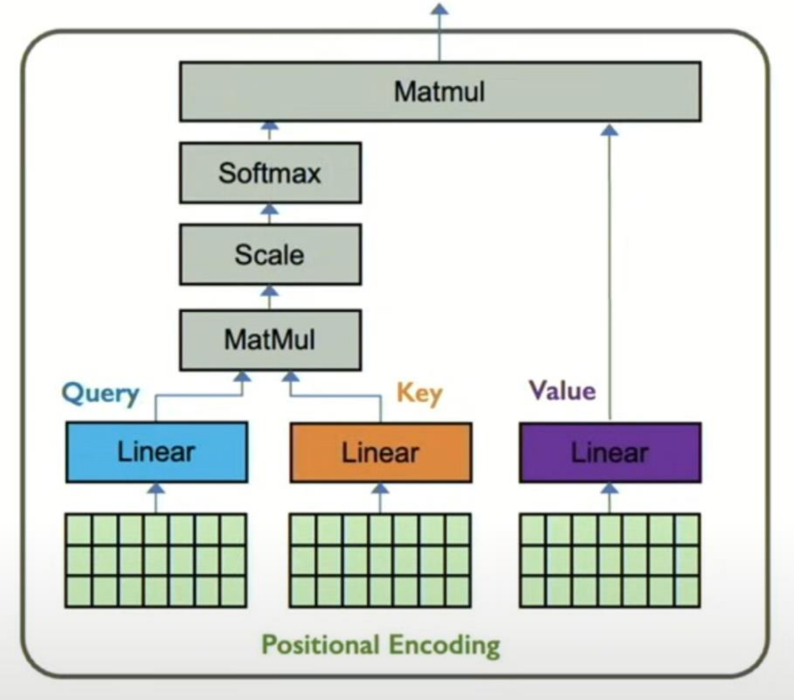


https://huggingface.co/docs/text-generation-inference/en/conceptual/tensor_parallelism

Transformer architecture

Attention is all you need

- Positional embedding. A word → A vector in high-dimensional space.
- Extract Query, Key, and Value for search.
- Attention weighting/mask: cosine similarity between query and key
- Extract features with high attention: multiply attention mask and value.
- A self-attention head.
- Transformer: a neuro network built on multiple self-attention heads.



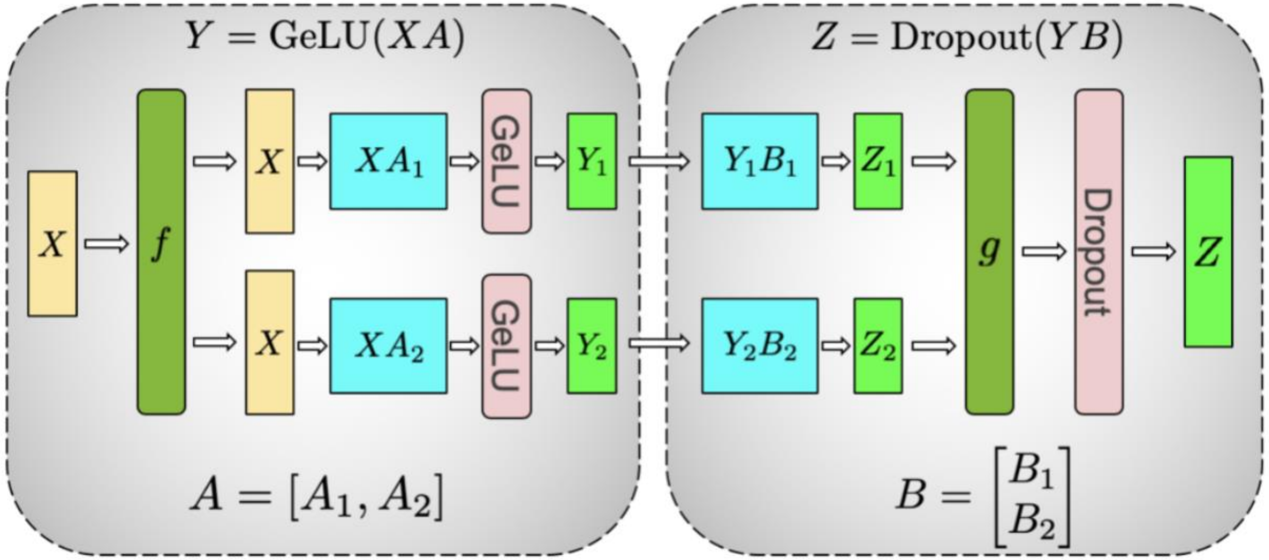
Successful in sequence modeling problems

- LLM: predict the next word. Bidirectional Encoder Representations from Transformers (BERT), Generative pre-trained transformer (GPT)
- Predict protein structure from DNA sequence (AlphaFold)
- Video/audio production

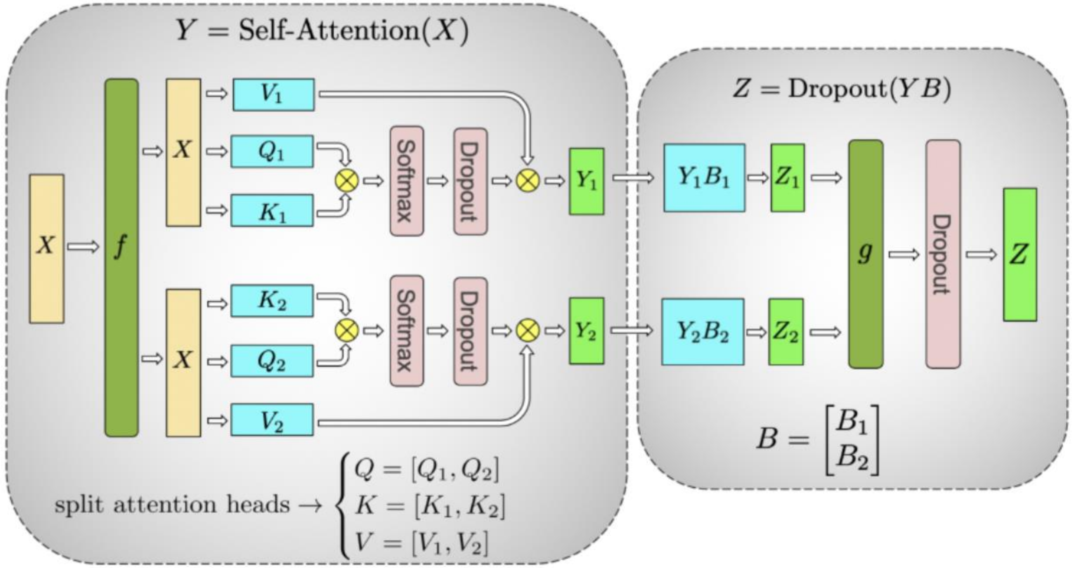
MIT course: https://www.youtube.com/watch?v=dqoEU9Ac3ek

Tensor Parallel for Transformer (1)

- A transformer block consists of a feed-forward (MLP) layer and a self-attention layer.
- Split matrices in the MLP and self-attention layers.
- The matrix multiplications in both attention and MLP happen through sharded computations.



Multilayer perceptron (MLP)

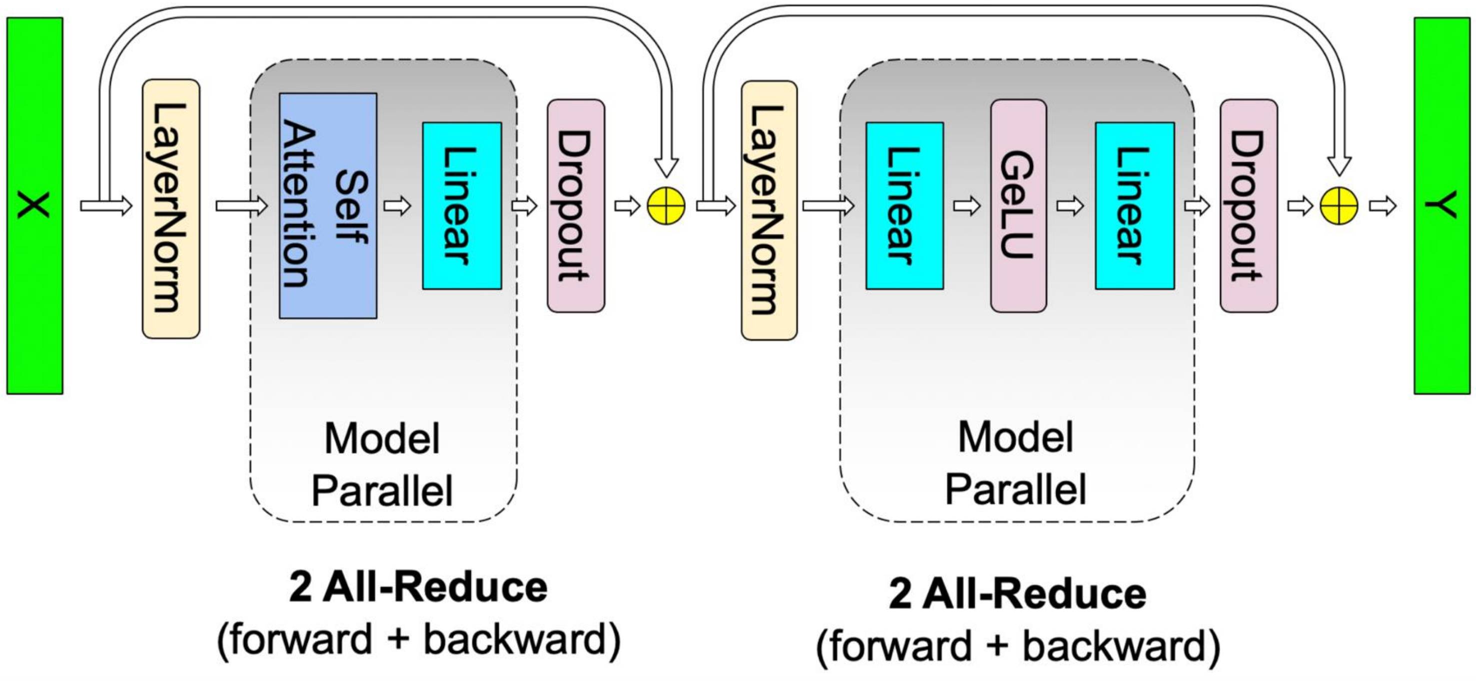


Self-attention

https://arxiv.org/abs/1909.08053

Tensor Parallel for Transformer (2)

- Minimal communication: 4 x all-reduce in the forward and backward pass of a single tensor parallel transformer layer.



- Larger communication overhead than DP or PP: more frequently.

https://arxiv.org/abs/1909.08053

Data and Tensor Parallel with PyTorch (1)

- Llama2 (Large Language Model Meta AI): built on transformer architecture.
- Hybrid parallel: Tensor Parallel within each node + Fully Sharded Data Parallel (FSDP) across nodes.
- Group GPUs for TP and DP

```
device_mesh = init_device_mesh("cuda", (dp_size, tp_size), mesh_dim_names=("dp", "tp"))
```

- Create the model and send it to GPUs

```
model = Transformer.from_model_args(simple_llama2_config).to("cuda")
```

- Set up a tensor parallel module

```
Parallelize_module(
   module=transformer_block,
   device_mesh=tp_mesh,
   parallelize_plan=layer_tp_plan
)
```

- Apply FSDP to the model

```
sharded_model = FSDP(model, device_mesh=dp_mesh, use_orig_params=True)
```

https://PyTorch.org/tutorials/intermediate/TP_tutorial.html

Data and Tensor Parallel with PyTorch (2)

- TP plan: specify how to shard feed-forward and self-attention layers, column-wise or row-wise.

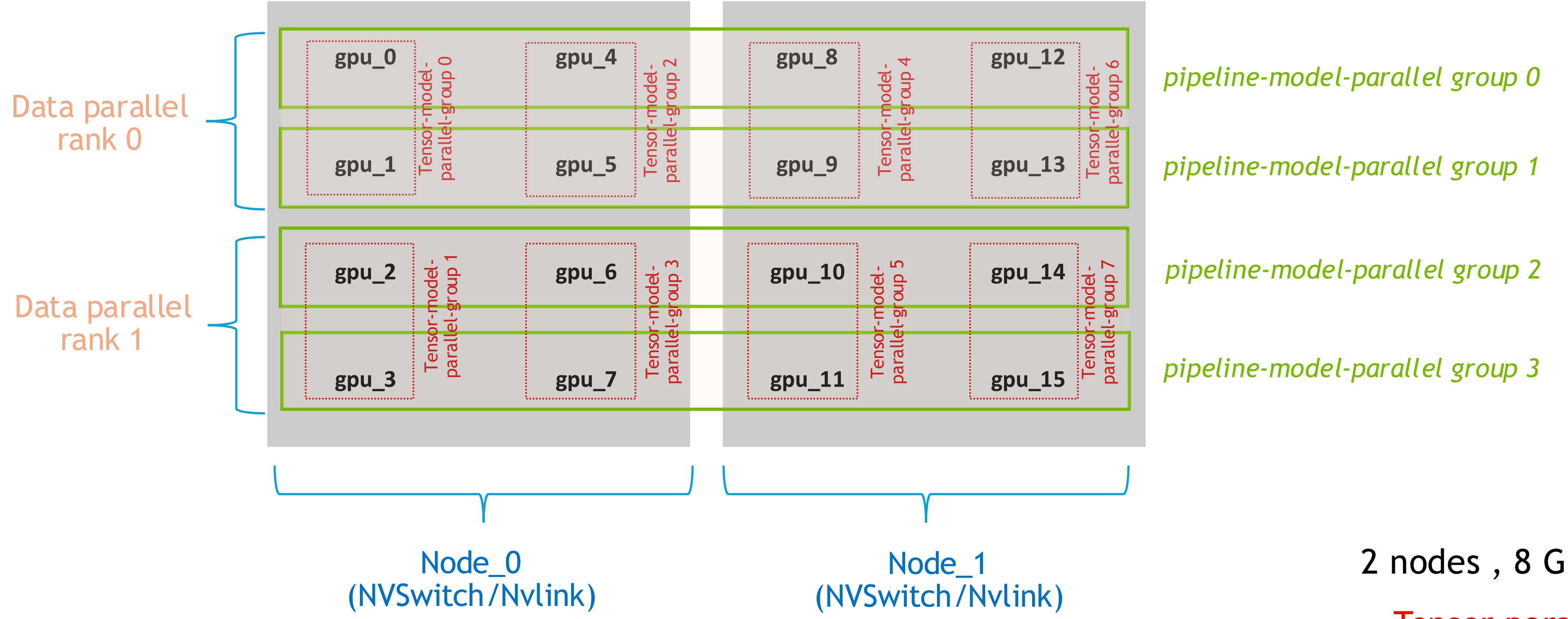
```
layer_tp_plan = {
    "attention_norm": SequenceParallel(),
    "attention": PrepareModuleInput(
        input_layouts=(Shard(1), None),
        desired_input_layouts=(Replicate(), None),
    ),
    "attention.wq": ColwiseParallel(),
    "attention.wk": ColwiseParallel(),
    "attention.wv": ColwiseParallel(),
    "attention.wo": RowwiseParallel(output_layouts=Shard(1)),
    "ffn_norm": SequenceParallel(),
    "feed_forward": PrepareModuleInput(
        input_layouts=(Shard(1),),
        desired_input_layouts=(Replicate(),),
    ),
    "feed_forward.w1": ColwiseParallel(),
    "feed_forward.w2": RowwiseParallel(output_layouts=Shard(1)),
    "feed_forward.w3": ColwiseParallel(),
}
```

- Sequence parallel: a variant of TP that performs sharded computations on layer normalization.
- Communications (e.g. allreduce) will happen under the hood.

https://PyTorch.org/tutorials/intermediate/TP_tutorial.html

Hybrid model parallelism

GPU Affinity grouping example for PP + TP + DP



2 nodes , 8 GPUs per node

- Tensor parallel = 2
- Pipeline parallel = 4
- Data parallel = 2

- Communication overhead: PP < DP < TP
- Network: fast Nvlinks within a node, Infiniband across nodes

https://docs.nvidia.com/nemo-framework/user-guide/latest/nemotoolkit/features/parallelisms.html

Which Strategy To Use When

❑ Single-node Multi-GPU

- The model fits into a single GPU: DP (distributed DP)
- The model doesn't fit into a single GPU: PP, TP, ZeRO, PP + DP, or TP + DP
- The largest layer does not fit into a single GPU: TP or ZeRO.

❑ Multi-node Multi-GPU

- ZeRO (easy)
- PP + TP + DP (tricky but faster)

➢ Best to experiment to find the winner on your particular setup.

https://huggingface.co/docs/transformers/v4.13.0/en/parallelism

What is not covered ...

- Mixed-precision training
- Save GPU memory by offloading to CPU
- Activation Checkpointing
- Sequence parallelism
- Hybrid model parallelism: PP + TP + DP
- Distributed inference