# DISTRIBUTED DEEP LEARNING

#### NATHAN NICHOLS & KAUSHIK VELUSAMY

AI/ML Team
Argonne National
Laboratory





### OUTLINE

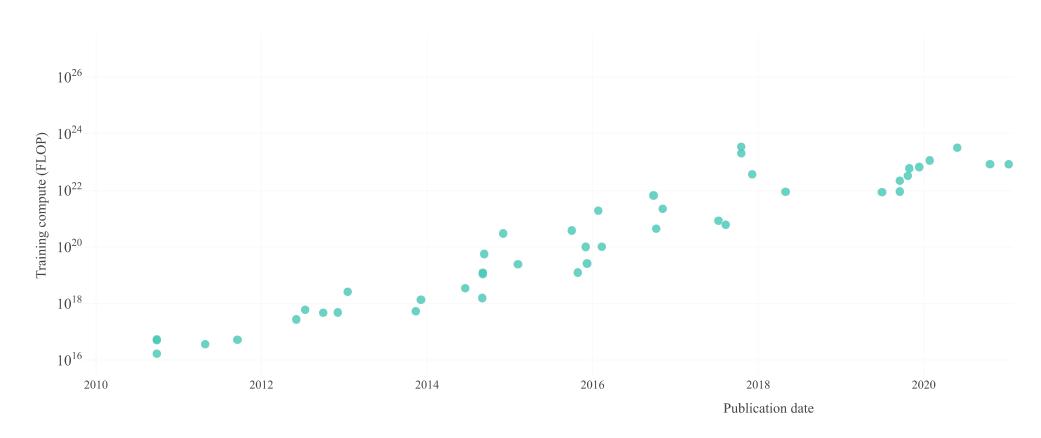
- The need for distributed training
- Communication libraries
- State-of-the-art parallelization schemes
- Data-parallel training in detail
- I/O and data management in distributed training
- Hands-on

# THE NEED FOR DISTRIBUTED TRAINING ON HPC

"Since 2012, the amount of compute used in the largest AI training runs has been increasing exponentially with a 3.4-month doubling time (by comparison, Moore's Law had a 2-year doubling period)."

Dario Amodei & Danny Hernandez, **Al and compute**, OpenAl Blog, May 16 2018

# TRAINING COMPUTE OF FRONTIER MODELS



Epoch Al: Key Trends and Figures in Machine Learning

# TRANSFORMER ARCHITECTURE INTRODUCED!

#### ATTENTION IS ALL YOU NEED

- Introduced by Vaswani et al. at NeurIPS 2017
- Replaced recurrence/convolutions with self-attention
- Enabled massive parallelization & modeling of long contexts

# MODEL SIZE OF FRONTIER MODELS



Epoch AI: Key Trends and Figures in Machine Learning

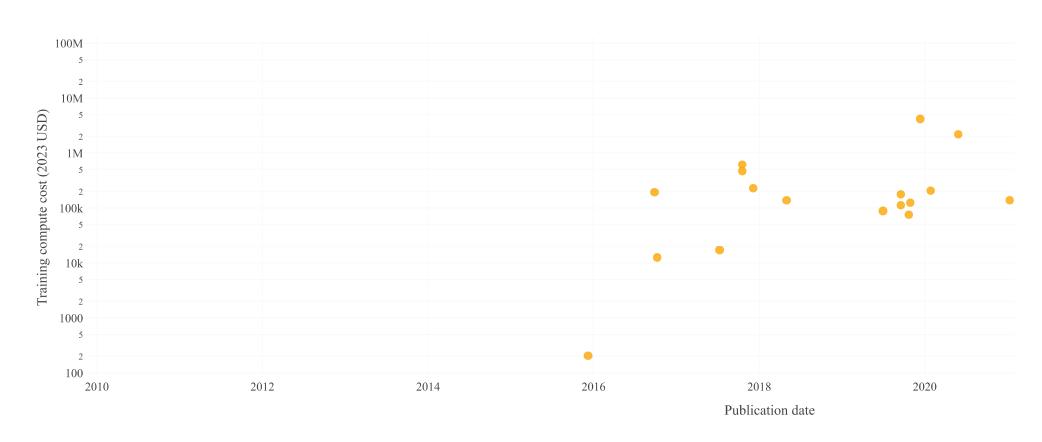
### **DISTRIBUTED TRAINING: RESNET-50**

#### YET ANOTHER ACCELERATED SGD

Scaling data-parallel SGD slashes ResNet-50/ImageNet training from days to seconds.

Year	Batch Size	Hardware	Library	Time	Accuracy
2015	256	P100 × 8	Caffe	29 hrs	75.3 %
2017	8,192	P100 × 256	Caffe2	1 hr	76.3 %
2018	8,192 → 16,384	Full TPU × Pod	TensorFlow	30 mins	76.1 %
2017	32,768	P100 × 1,024	Chainer	15 mins	74.9 %
2018	65,536	P40 × 2048	TensorFlow	6.6 mins	75.8 %
2018	65,536	TPU v3 × 1,024	TensorFlow	1.8 mins	75.2 %
2019	55,296	V100 × 3,456	NNL	2.0 mins	75.29 %
2019	81,920	V100 × 2048	MXNet	1.2 mins	75.08 %

# TRAINING COST OF FRONTIER MODELS



Epoch Al: Key Trends and Figures in Machine Learning

#### WHY DISTRIBUTED TRAINING?

- Exascale compute: 10<sup>18</sup> FLOP workloads need multi-node parallelism.
- Model scale: Millions → trillions of parameters—beyond single-device RAM.
- **Data volumes:** Petabyte-scale datasets saturate node I/O and storage.
- HPC & ML: Coupling large simulations with AI drives heterogeneous scaling.
- Efficiency: Distributed frameworks maximize utilization and power on exascale systems.

ALCF, Aurora Exascale Supercomputer

### SCIENTIFIC DL AT SCALE

- Climate Analytics: Exascale DL for extreme weather modeling (2018)
- Cancer Research: Accelerating cancer pathology analysis (2019)
- Inverse Problems: Exascale DL for inverse problems (2019)
- Flood-Filling Networks: Scaling FFN training on HPC (2019)
- Dark Energy Survey: DL at scale for galaxy catalogs (2019)
- Megatron-LM: Large-scale transformer training (2021)

Representative publications showcasing scientific deep learning at exascale.

### **COMMUNICATION LIBRARIES**

- Collective ops (all-reduce, all-gather) underpin distributed DL.
- Latency & bandwidth optimizations dictate scaling efficiency.
- Plugins bridge DL frameworks to HPC fabrics transparently.

#### ONECCL IN DISTRIBUTED TRAINING

- Intel oneAPI Collective Communications Library (oneCCL).
- Optimized for Intel GPUs and CPUs.
- Implements MPI-like collectives with Level Zero & SYCL/DPC++ back-ends.
- Deep integration with PyTorch, TensorFlow, Horovod, IPEX.
- High-throughput collectives over OFI & MPI transport layers.

#### ONECCL — FEATURE HIGHLIGHTS

- Default hierarchical algorithm (topo) optimizes intra-node (scale-up) and inter-node (scale-out) communication
- Collective operations on low-precision datatypes
- Asynchronous progress threads overlap computation and communication
- Unified C and C++ API for host (CPU) and device (GPU) memory buffers

```
// Minimal C++ all-reduce with oneCCL
#include <oneapi/ccl.hpp>

int main(int argc, char** argv) {
   ccl::init();
   auto comm = ccl::create_communicator();
   std::vector send(1024, comm.rank()), recv(1024);
   comm.allreduce(send, recv, ccl::reduction::sum).wait();
   return 0;
}
```

#### **COMMUNICATION LIBRARY LANDSCAPE**

- MPI: Portable, mature; rich semantics;
   CPU-centric.
- NCCL: NVIDIA GPU collectives; PCIe/NVLink topology-aware.
- **RCCL:** AMD ROCm counterpart to NCCL; HIP-enabled.
- Gloo: Simple API; CPU/GPU; best < 1 k ranks.</li>

# LIBRARY TRADE-OFFS & SELECTION GUIDE

- Vendor lock-in: NCCL (NVIDIA), RCCL (AMD), oneCCL (Intel).
- Heterogeneous support: MPI/UCX & oneCCL span
   CPU + GPU.
- **Ease of integration:** Gloo simple; NCCL/oneCCL have framework plugins.
- Scalability: MPI & \*CCL proven to 10 k+ GPUs;
   Gloo ≤ 1 k.

# STATE-OF-THE-ART PARALLELISM SCHEMES

- Data Parallelism
  - Distributed Data-Parallel (DDP)
- Model Parallelism
  - Tensor (intra-layer) Parallelism
  - Pipeline (inter-layer) Parallelism
- Hybrid ("3D") Parallelism

### MODEL PARALLELISM OVERVIEW

Splits a model's parameters or ops across devices to handle very large networks.

- Tensor Parallelism: shard weight tensors within each layer; all devices work on the same batch.
- Pipeline Parallelism: cut the model into sequential stages; devices process different micro-batches in flight.

# TENSOR (INTRA-LAYER) PARALLELISM

- Shards each layer's weight tensors across multiple GPUs.
- GPUs collaborate on the same mini-batch.
- Fine-grained all-reduce ops.
- Key benefits:
  - Train layers too large for a single device.
  - Maintains low pipeline latency (no bubbles).
- Best for models with extremely large dense layers.

### PIPELINE PARALLELISM

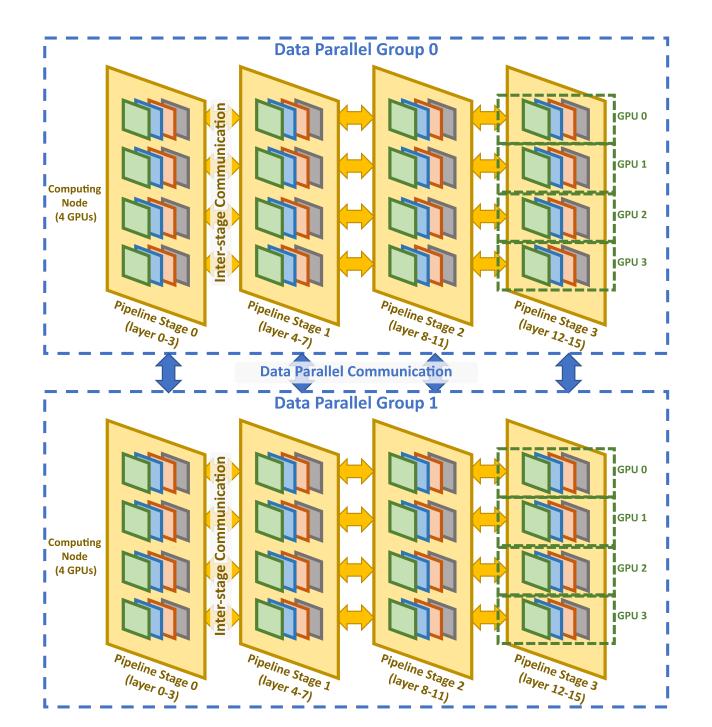
- **Stages:** e.g., layers 1–10 on GPU 0, 11–20 on GPU 1, ...
- Micro-batches: chunk the batch and stream pieces through stages.
- Overlap: compute on one micro-batch overlaps communication of another.
- **Pipeline bubbles:** startup/shutdown idle periods when ramping up/down.

# COMPARING PARALLELISM FORMS

Aspect	Tensor Parallelism	Pipeline Parallelism	
Granularity	Per-layer shards; sync every op	Only at stage boundaries	
Concurrency	All devices on same batch	Different micro-batches on each stage	
Overhead	Fine-grained all-reduces	Startup/drain bubbles	
Best for	Huge layers, heavy tensor ops	Deep models, balanced stage compute	

#### DATA PARALLEL

- Replicate full model on each worker.
- Each rank processes unique mini-batch shard.
- Gradients all-reduced after backward pass.
- Simple; scales to 10 k+ GPUs.
- Bandwidth-bound at very large scale.



# DATA PARALLEL TRAINING: PYTORCH DDP

### LINEAR SCALING RULE

When global batch size multiplies by *k*, scale the learning rate by *k*.

$$w_{t+1} = w_t - \eta rac{1}{|B|} \sum_{x \in B} 
abla L(x, w_t)$$

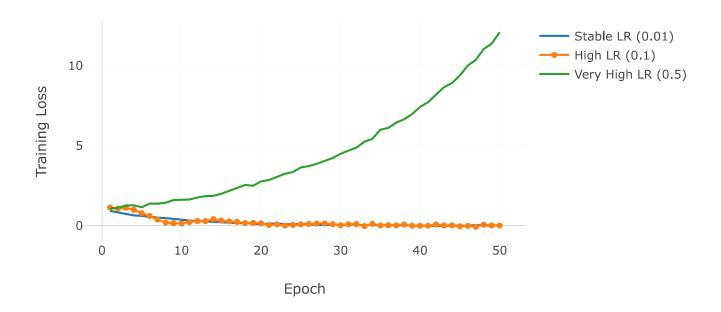
- Keep local batch size per worker.
- Increase global batch size & learning rate proportionally.

# LARGE-BATCH CHALLENGES & SOLUTIONS

- Optimization Instability use LR warm-up (cosine or linear).
- Generalization Gap apply LR decay, regularization, longer warm-up.

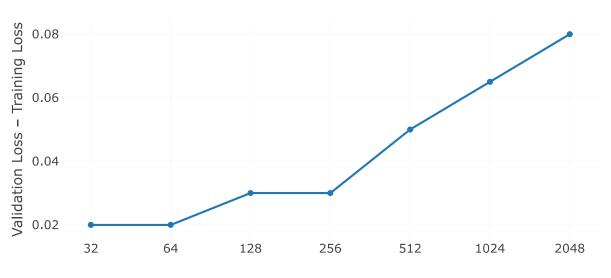
### **OPTIMIZATION INSTABILITY**

Optimization Instability: Training Loss vs Epochs



## GENERALIZATION GAP (LOG SCALE)

Generalization Gap vs Batch Size



Batch Size (log scale)

### PYTORCH DDP WORKFLOW

```
import torch
import torch.distributed as dist
from torch.nn.parallel import DistributedDataParallel as DDP

dist.init_process_group('nccl')

model = DDP(MyModel().cuda(), device_ids=[local_rank])
optimizer = torch.optim.Adam(model.parameters(), lr=base_lr * world_

for inputs, targets in loader:
    outputs = model(inputs.cuda())
    loss = criterion(outputs, targets.cuda())
    loss.backward()
    ontimizer_sten()
```

# DATA MANAGEMENT & I/O CHALLENGES

- Growing data volumes (TB-PB) demand efficient ingestion pipelines.
- Complex workflows: preprocessing, augmentation, caching, staging.
- Balancing throughput, latency & compute utilization.

### DL I/O TRAITS

#### **Read-Intensive:**

Sustained high-throughput reads.

### **Metadata-Hungry:**

Millions of small files & frequent directory ops.

### Random & Sparse Access:

Non-sequential reads across dataset.

#### **Multi-format:**

Images, JSON, TFRecord, HDF5, custom archives.

### **Hierarchical Storage:**

Leveraging DRAM, SSD/NVMe, parallel file systems.

# I/O VS COMPUTE BOTTLENECKS IN DL WORKLOADS

#### **UNet3D**

3-D convolutional U-Net for volumetric data.

#### **BERT**

Transformer-based language model pre-training on large text corpora.

# UNET3D I/O BOTTLENECK ON GPFS

- I/O-bound: Storage limits throttle sustained reads.
- **GPU/CPU idle:** Frequent I/O stalls leave compute under-utilized.
- Weak scaling: Throughput plateaus as cluster size increases.

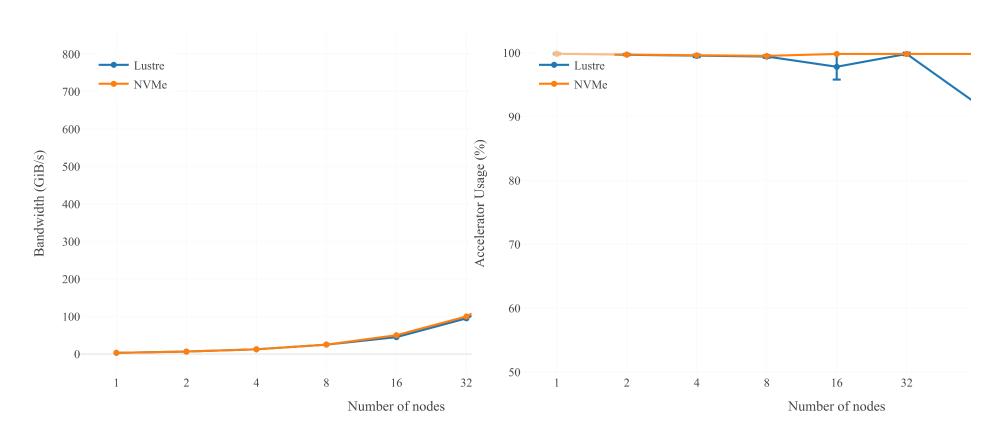
### BERT PRE-TRAINING SCALING

- Compute-bound: Floating-point workloads saturate GPUs before I/O.
- Linear weak scaling: Performance grows nearly linearly with GPUs.
- I/O overhead: Well below storage limits, so not the bottleneck.

# COMPUTE VS I/O BOUND: KEY TAKEAWAYS

- Data-intensive (UNet3D): Prioritize I/O optimizations—caching, parallel reads.
- Compute-intensive (BERT): Scale GPU capacity & optimize kernels.
- Choose your focus: Storage tuning vs hardware/algorithmic scaling.

# UNET3D I/O THROUGHPUT & UTILIZATION



ALCF, **DLIO Benchmark** (Polaris)

### **OPTIMIZING DATA PIPELINES**

- Efficient Formats: preprocess to TFRecord/LMDB or binary archives.
- Sharding & Layout: pack samples per file, bucket by size, shard across workers.
- Parallel I/O: async prefetch, multi-thread/process workers.
- Caching & Staging: in-memory buffers, SSD/NVMe lanes, burst buffers.
- Filesystem Tuning: stripe count/size, object-store optimizations.

### **SUMMARY**

- Scaling: Multi-node training for ever-larger models
- Communication: Optimized collectives & hybrid parallelism
- Best Practices: LR scaling, overlap & lowprecision ops
- Data Pipeline: Sharding, caching & parallel I/O