Scalable Distributed Training of Large Neural Networks with LBANN

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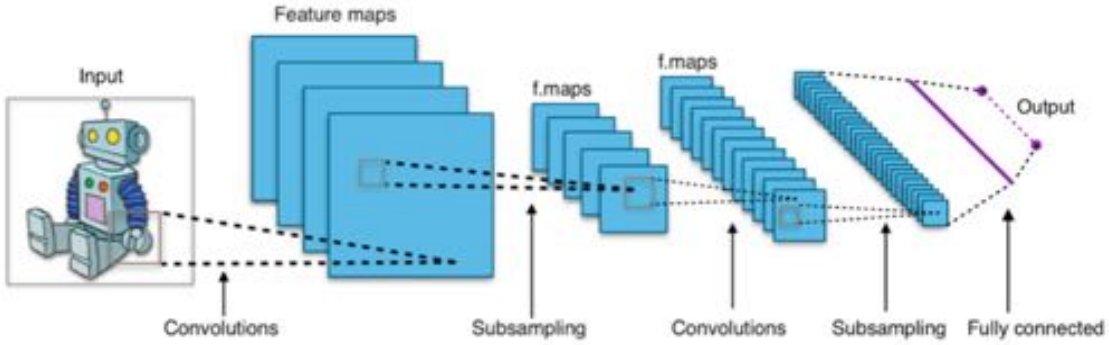
- LBANN Team

Training Deep Convolutional Neural Networks

- Iterative computations until error rate becomes sufficiently small
- Each iteration is a statically fixed DAG of matrix computations
  - Convolutions
  - Matrix multiplications
  - Element-wise filtering
  - Reductions
- Training sweeps a large collection of labeled samples by picking up a subset of samples ("mini-batch")



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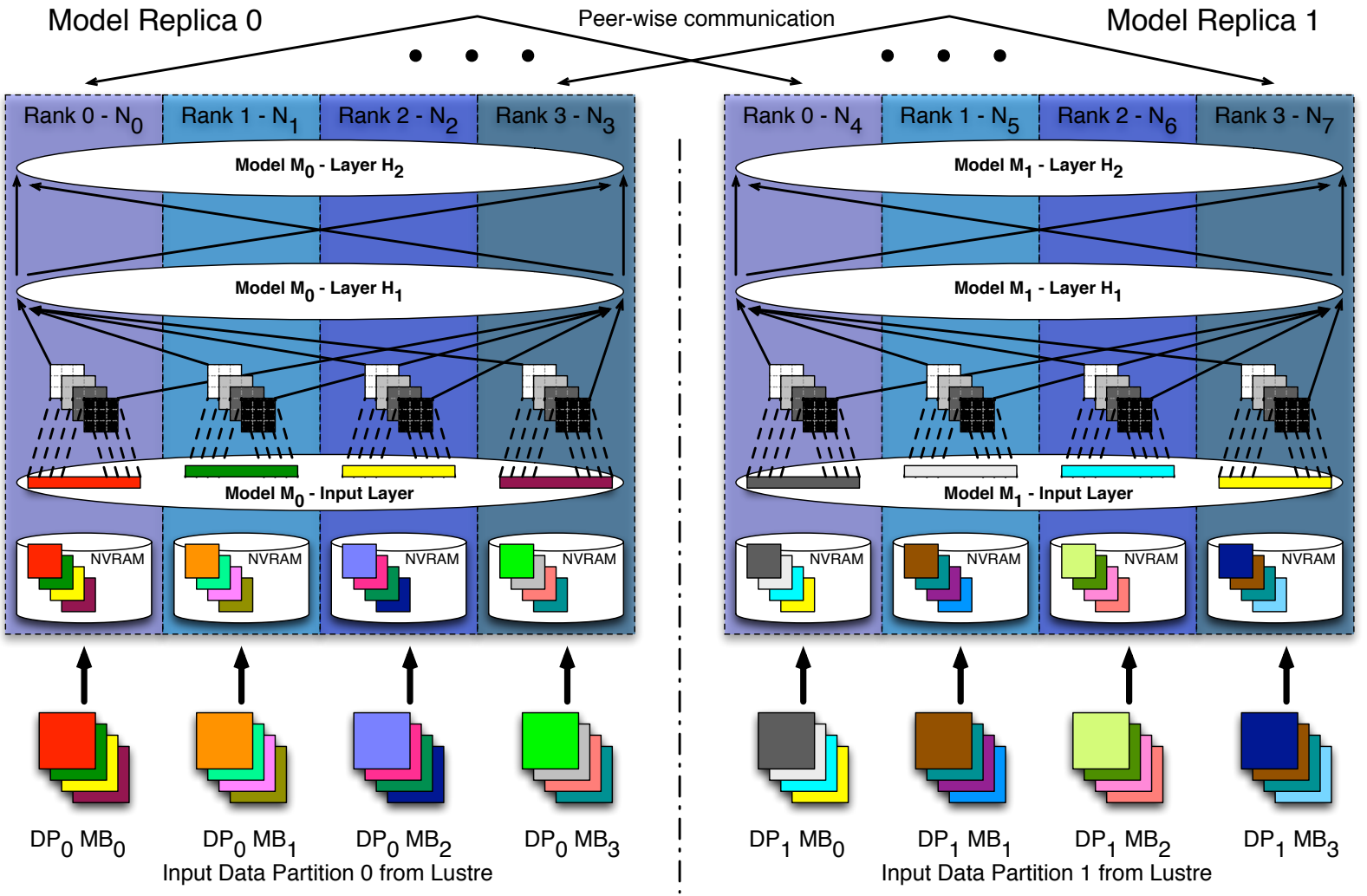
```
while unconverged
  pick a mini-batch
  traverse DAG from input to output
  traverse DAG from output to input
  adjusts network parameters
endwhile
```

LBANN: Livermore Big Artificial Neural Network Toolkit

- https://github.com/LLNL/lbann
- Deep Neural Network training / classification
  - Optimized distributed memory algorithms
    - Including spatially decomposed convolutions
  - Optimized asynchronous communication library
  - Compose parallelism at multiple levels
  - Optimize for strong & weak scaling
- Unique HPC resources at scale
  - InfiniBand or Omnipath interconnect
  - Tightly-coupled GPU accelerators
  - Node-local NVRAM
  - High bandwidth Parallel File System
  - State-of-the art distributed linear algebra library



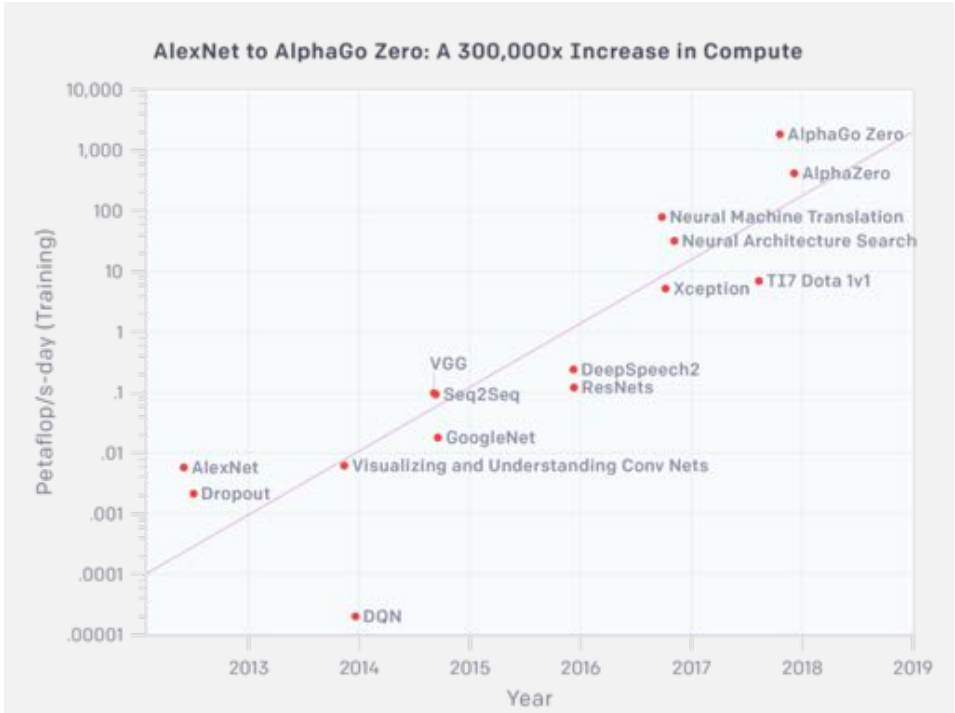
Parallel Training is Critical to Meet Growing Compute Demand

- Training is an extremely compute-intensive task
- And growing exponentially
  - Doubling every 3.5 months
- Distributed training is essential and is proven to be successful

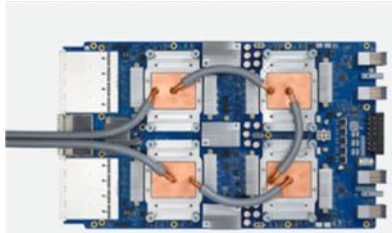
Table 1: Large-scale ResNet-50 training results.

	Hardware	Chips	Batch	Optimizer	BN	Accuracy	Time
Goyal et al. [6]	P100	256	8192	Momentum	Local	76.3%	1 hour
Smith et al. [16]	TPU v2	128	8192 → 16384	Momentum	Local	76.1%	30 mins.
Akiba et al. [2]	P100	1024	32768	RMS + Mom.	Local	74.9%	15 mins.
Jia et al. [10]	P40	1024	65536	LARS	Local	76.2%	8.7 mins.
Baseline	TPU v2	4	1024	Momentum	Local	76.3%	8.0 hours
Ours	TPU v2	256	16384	Momentum	Local	75.1%	10 mins.
Ours	TPU v2	256	32768	LARS	Local	76.3%	8.5 mins.
Ours	TPU v3	512	32768	LARS	Local	76.4%	3.3 mins.
Ours	TPU v3	1024	32768	LARS	Distributed	76.3%	**2.2 mins.**

Ying et al., "Image Classification at Supercomputer Scale," Systems for ML Workshop @ NIPS 2018

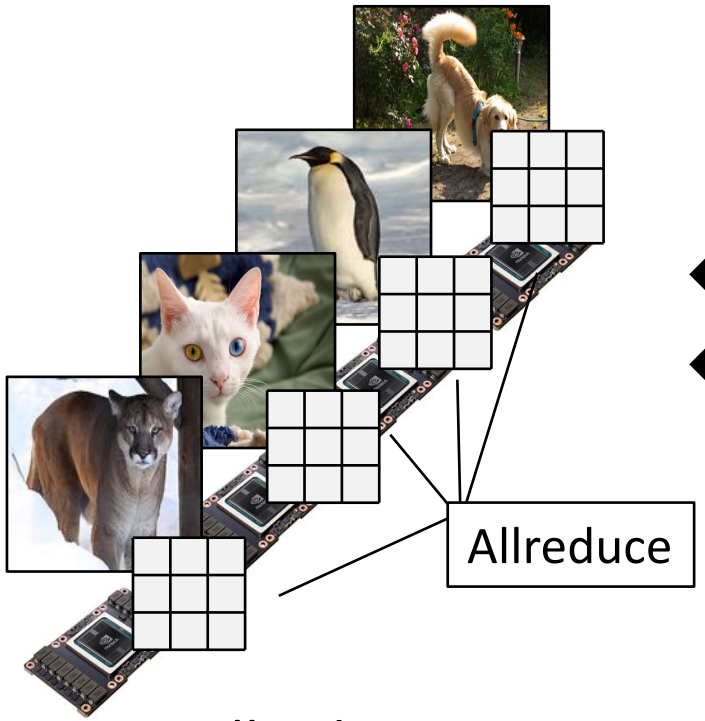


Source: OpenAI, https://blog.openai.com/ai-and-compute/



Generalized Parallel Convolution in LBANN

Sample (Data) Parallelism

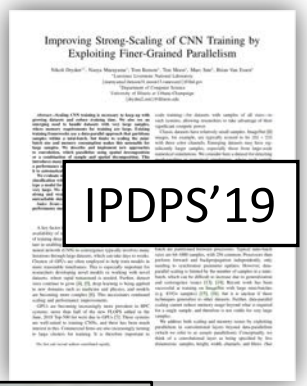


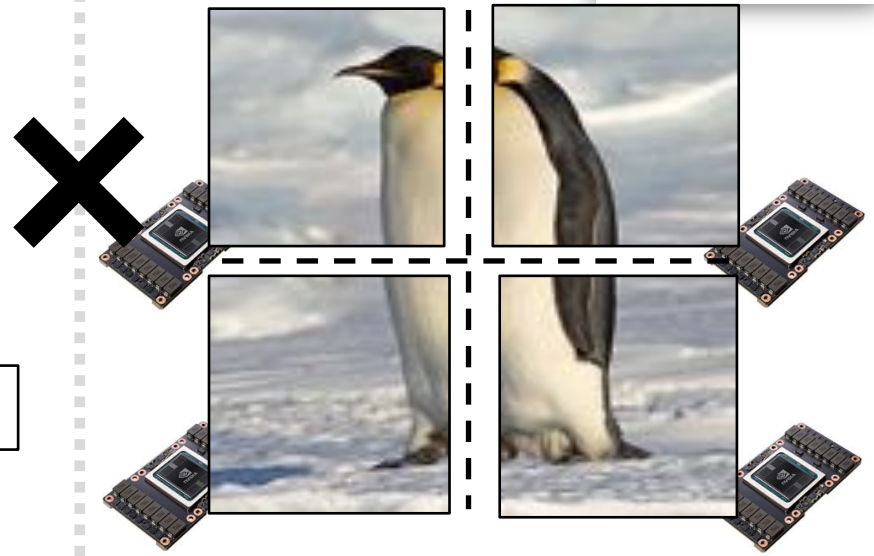
Allreduce

O(100-1000) GPUs

NCCL/MPI

Spatial Parallelism



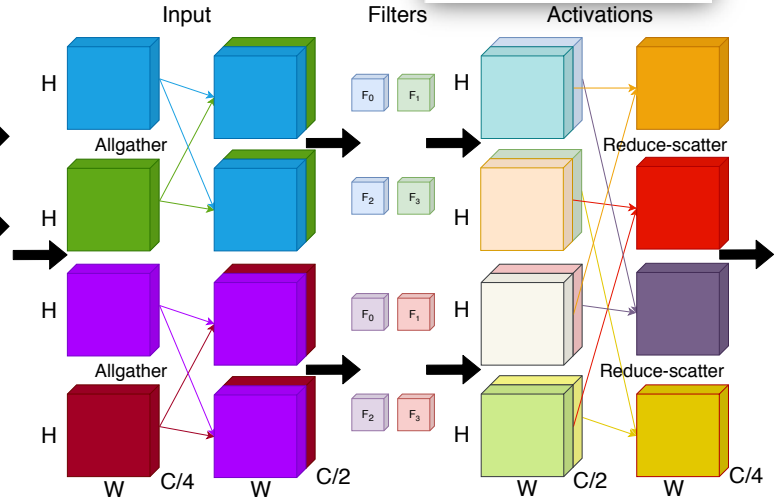


Halo exchange

O(10) GPUs

MPI/Custom

Channel/Filter Parallelism



Allgather/ReduceScatter

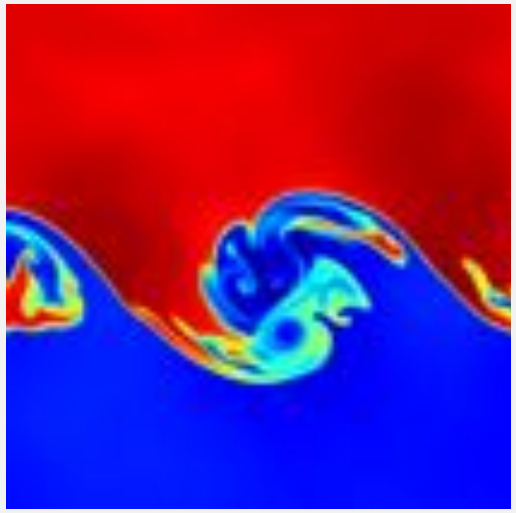
O(10) GPUs

NCCL/MPI

Scaling up Deep Learning for Scientific Data

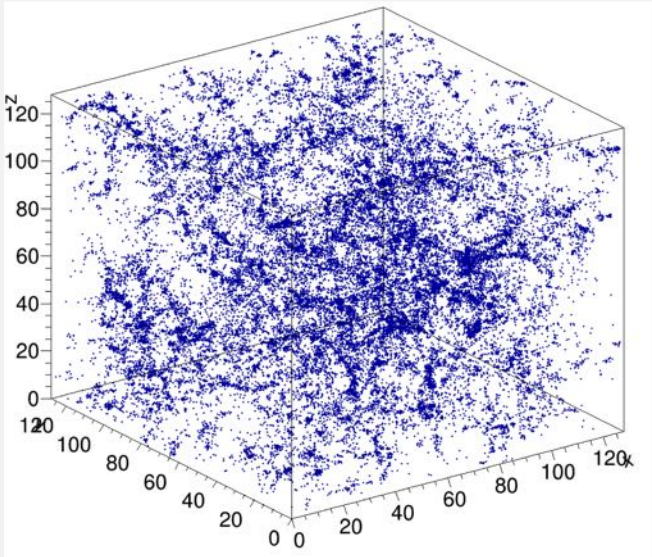
- The DOE has large scientific data sets that are unlike any commercial data set
  - May not be natural images
  - Large samples
  - May be generated by computational simulations
- Even a mini-batch with just one sample may require more than O(10) GB of memory → Does not fit in a single GPU memory

Mesh Tangling Detection



$O(1000)^2$ mesh

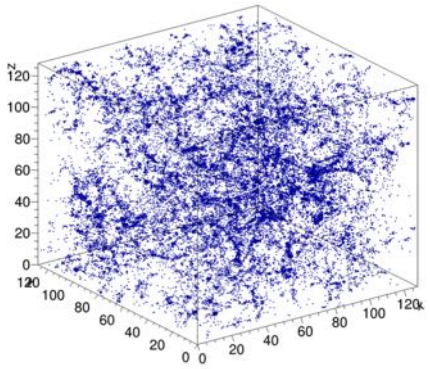
Cosmological Analysis



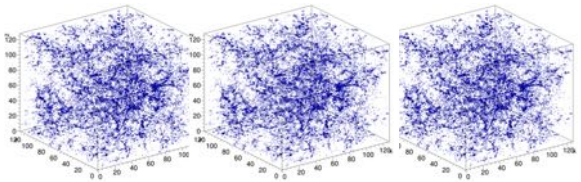
$O(100)^3$ volumetric data [Mathuriya18]

10x Better Prediction Accuracy with Large Samples

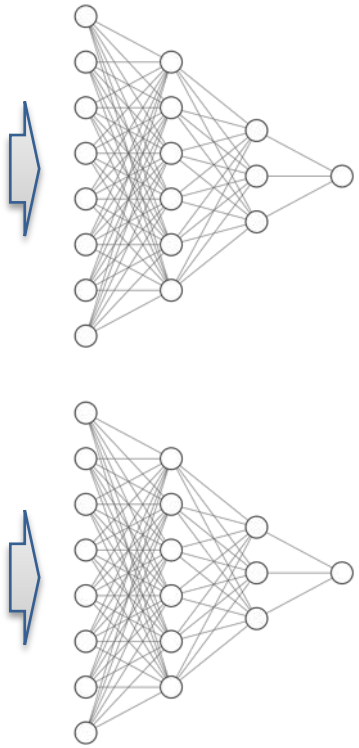
Cosmological Simulation

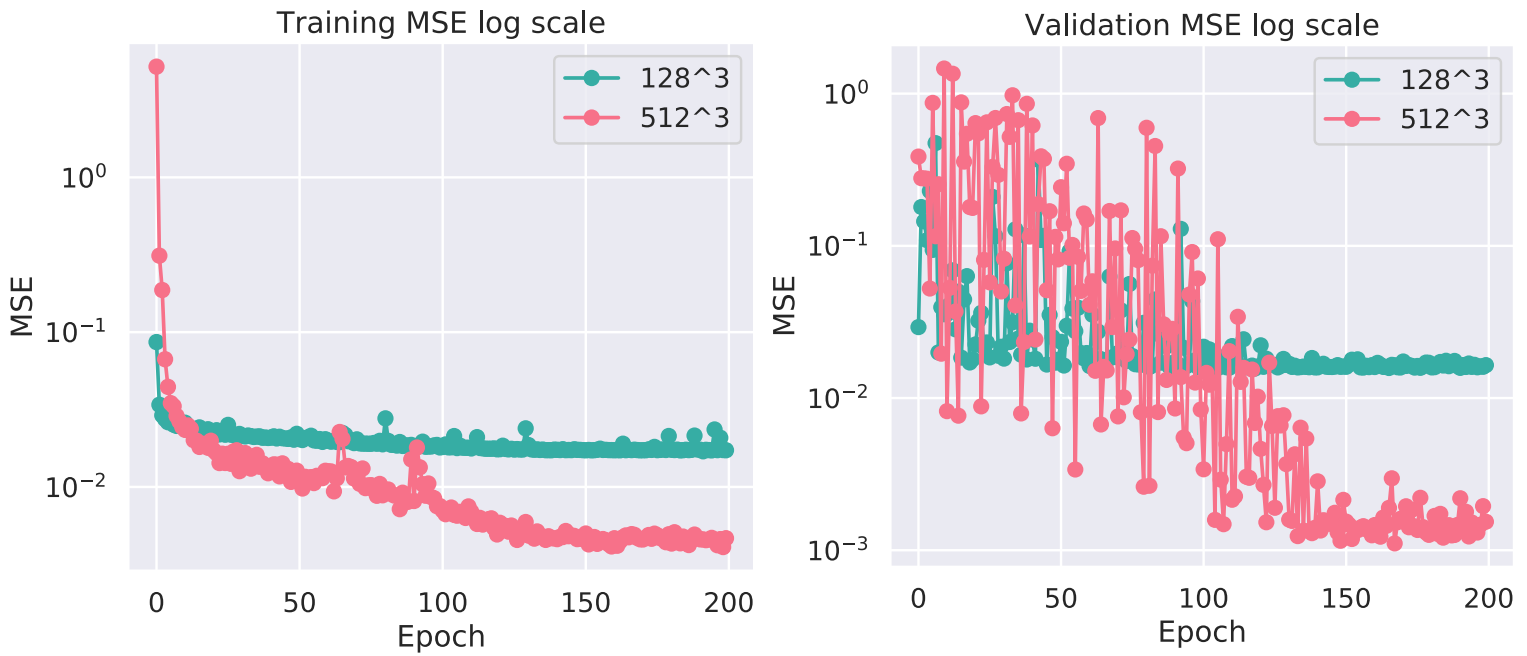


512^3 training samples



128^3 split samples

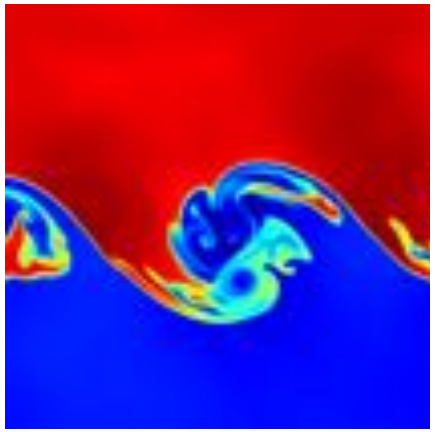




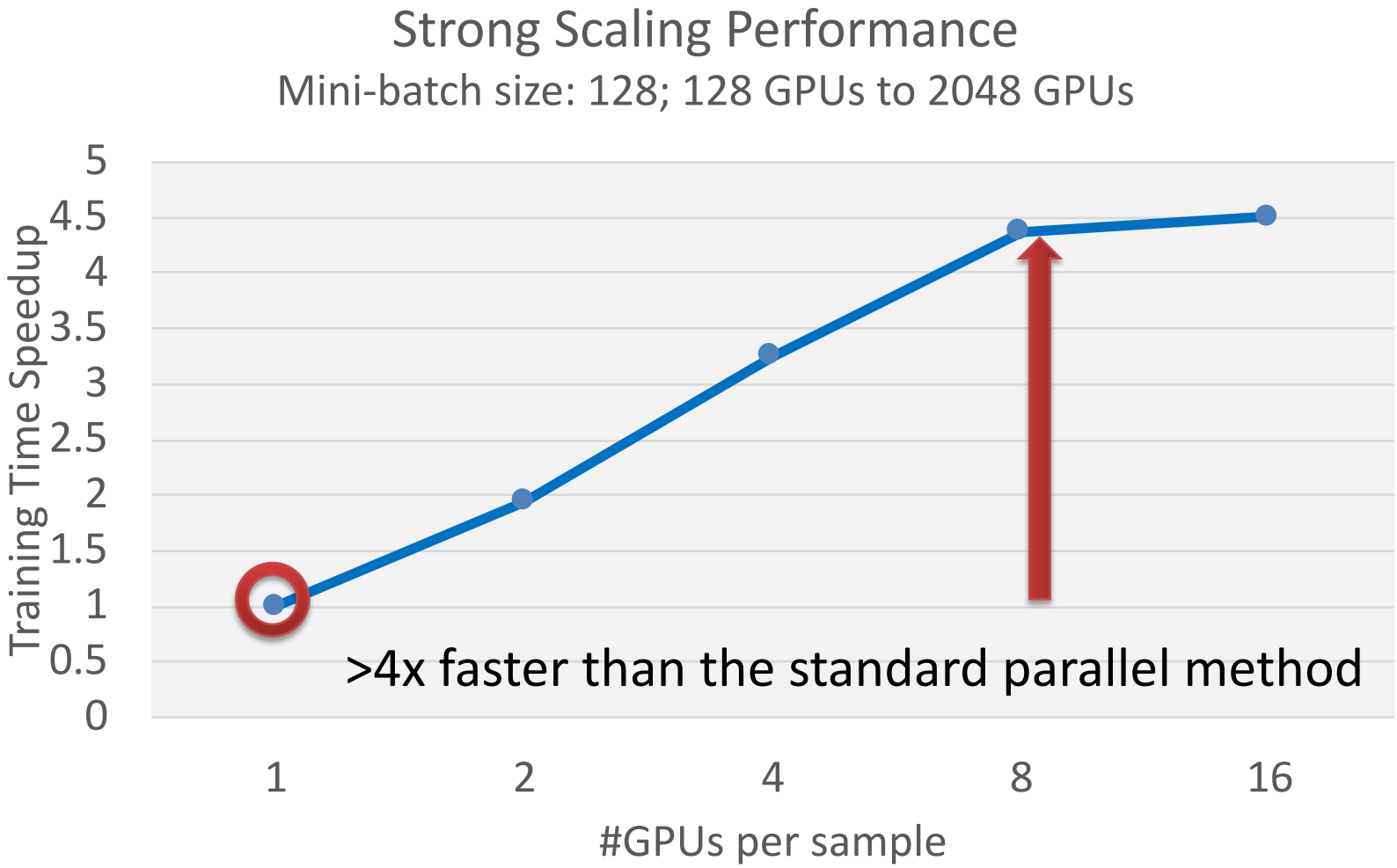
- Dataset: cosmoUniverse_2019_05_4pare
  - https://portal.nersc.gov/project/m3363/cosmoUniverse_2019_05_4parE)
- CosmoFlow model [Mathuriya18] + batchnorm
- Prediction of Omega_m

Scaling Performance beyond Data Parallel Training

1024^2 training samples



Lassen: Power 9 x 2 + Volta 100 x 4



Parallel Training

Not parallelizable with standard SGD

```
while unconverged
  pick a mini-batch
  traverse DAG from input to output
  traverse DAG from output to input
  adjusts network parameters
endwhile
```

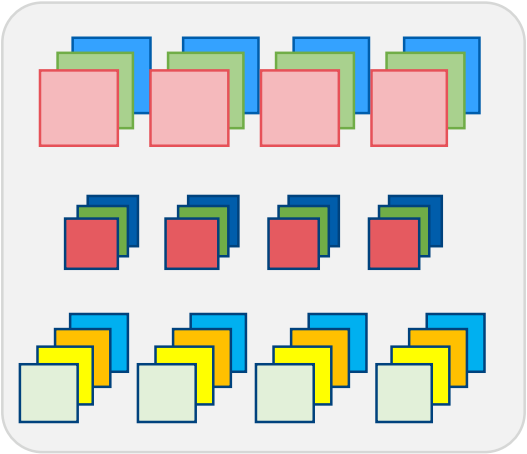
Parallelizable with some comm.

- Parallelism lies inside the training loop
- Parallel convolution
  - *N*: number of samples, *C*: number of channels, *F*: number of filters, *H*: height, *W*: width
  - Input: images of *N*x*C*x*H*x*W*
  - Filters: *F*x*C*x*K*x*K*
  - Output: *N*x*F*x*H*x*W*
  - Partitioning the samples is the most common approach

Images $N \times C \times H \times W$

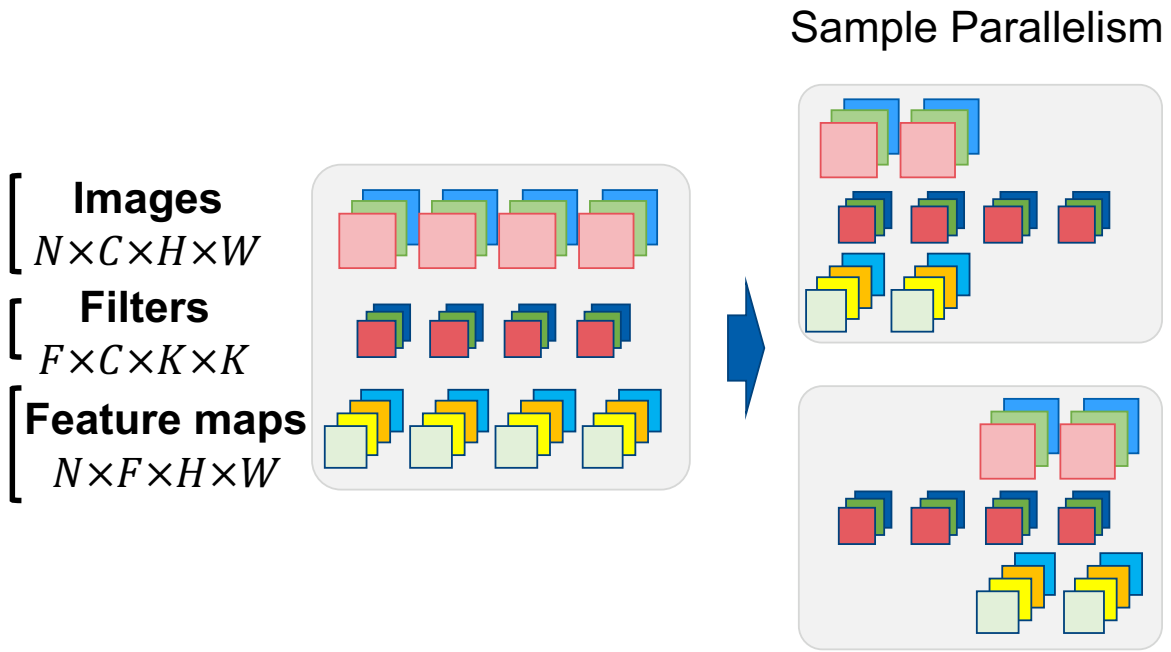
Filters $F \times C \times K \times K$

Feature maps $N \times F \times H \times W$



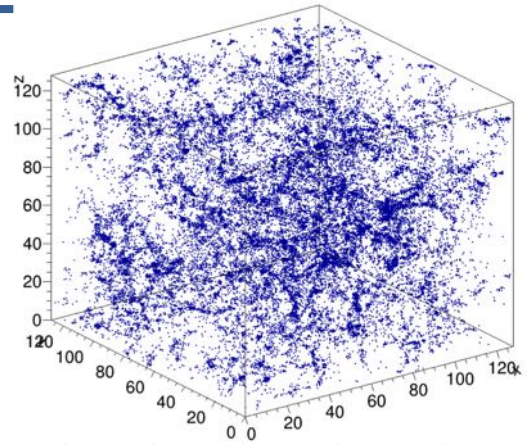
Sample-Parallel Convolution

- Split the samples of a mini-batch between processes (or GPUs)
- Each process computes independently with reductions of gradients
- Implemented in many of DL frameworks such as LBANN, TensorFlow, PyTorch, Chainer, etc.

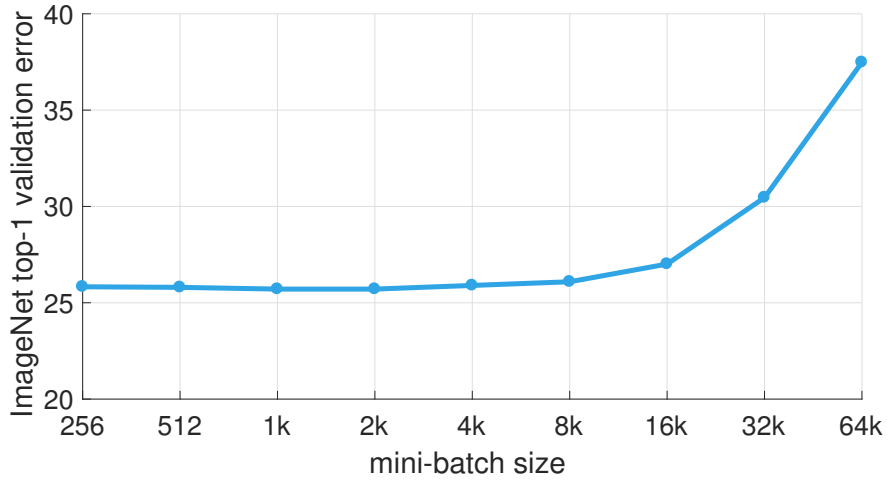


Scalability Limitations of Sample-Parallel Training

- Limited memory capacity
  - Neural networks are becoming deeper
  - Sample size is becoming bigger when dealing with scientific data rather than cats and dogs (^._.^)
  - Does not fit GPU memory
- Limited parallelism
  - The degree of parallelism depends on the number of samples in a mini-batch (i.e., *N*)
  - Can't make *N* arbitrary large as learning accuracy significantly drops
  - Usually, *N* is O(100)-O(1000)

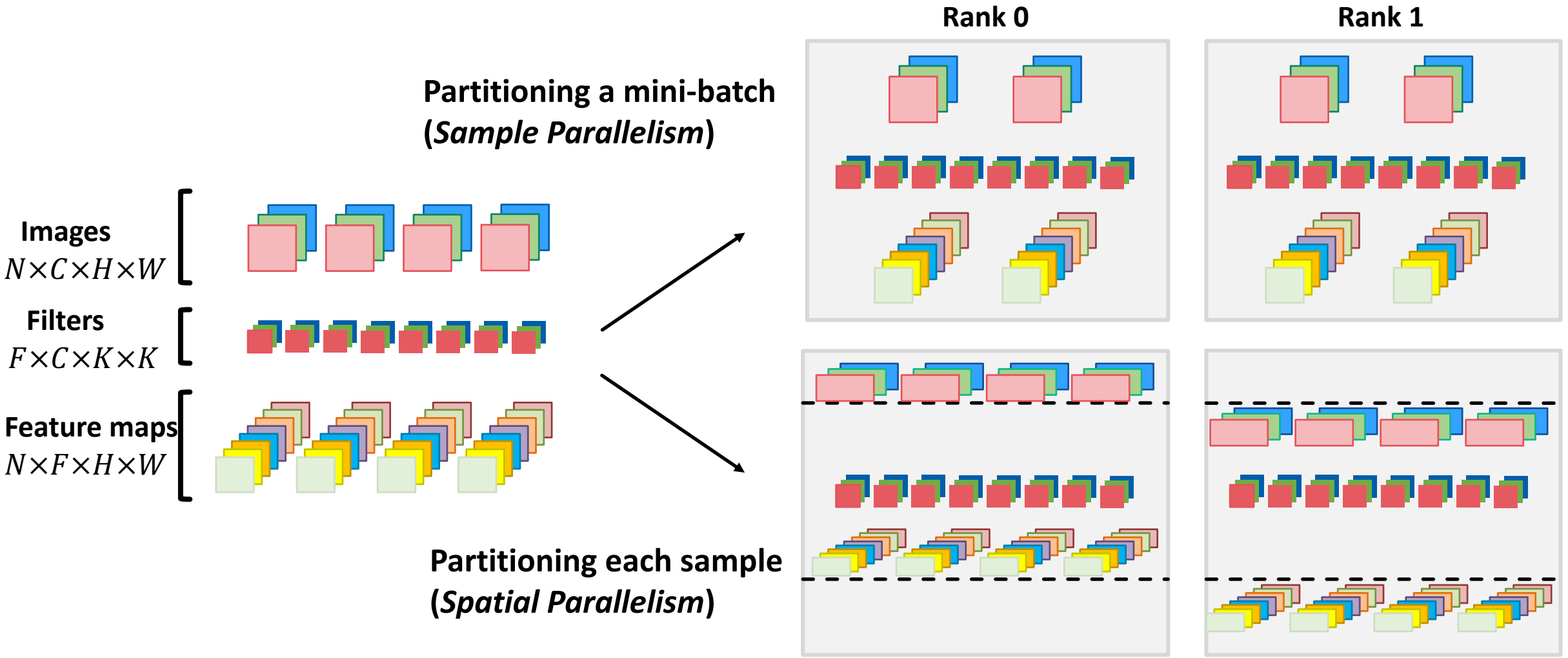


3D cosmological simulation by Mathuriya et al.



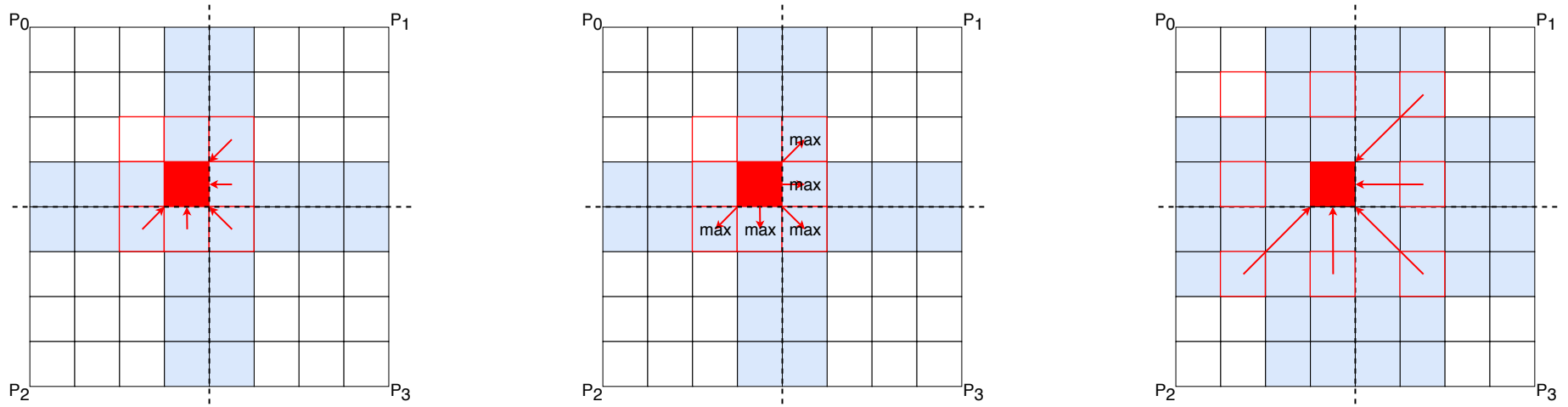
Goyal et al., Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour, 2017.

Parallelism is not Limited to the Sample Dimension



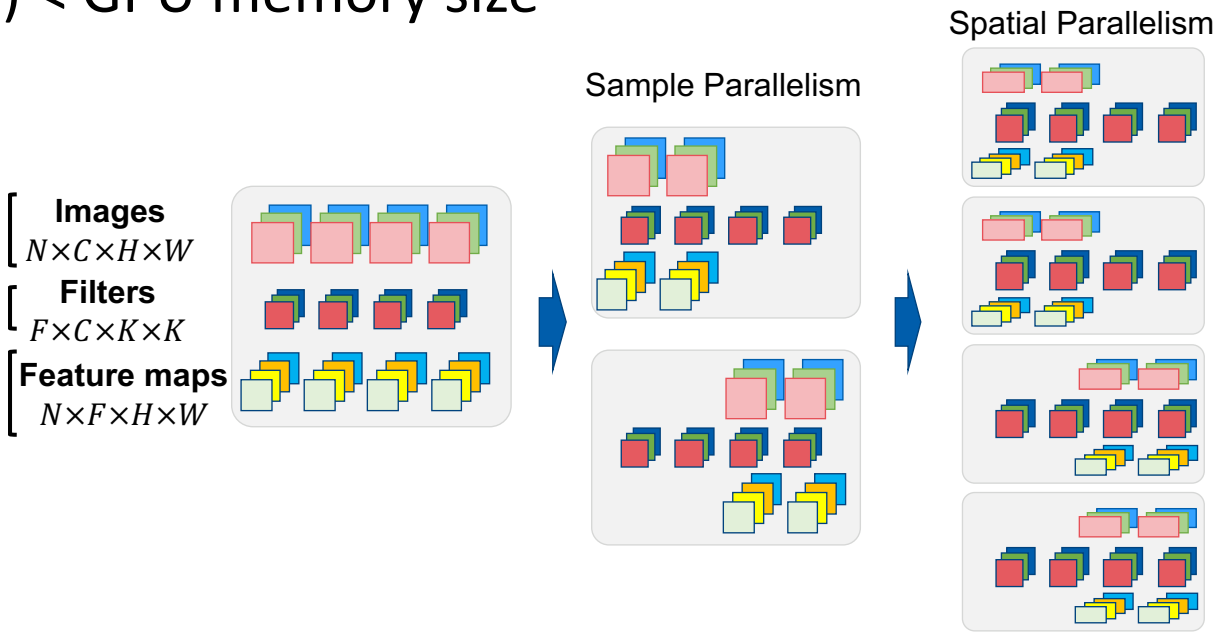
Boundary Data Exchange

- Convolution/pooling needs adjacent data for each point → *Halo exchange*
- Halo size depends on filter size and number of channels
- Also on stride and dilation
  - Does not depend on grouped convolution
- Pooling involves a “reverse halo exchange”
  - Push/accumulate values to remote



Hybrid Parallel Convolution

- Sample and spatial parallelisms are orthogonal and can be used simultaneously
- Can use $P_N * P_S$ GPUs
- If N > #GPUs && sizeof(activations+weights) < GPU memory size
  - Use sample parallel only
- Otherwise:
  - Spatial parallel to fit GPU memory
  - Sample parallel up to N
- Example
  - Spatial parallel with intra-node 4 GPUs of Sierra nodes
  - Sample parallel with as many nodes as the mini-batch size



An example case with nested partitioning along sample and spatial domains

Implementation

- Extend the LBANN toolkit (https://github.com/LLNL/lbann)
  - Annotate layers with parallel execution strategies
- Distconv: Custom distributed tensor library for convolution
  - Similar approach as stencil libraries
- Aluminum for communication (https://github.com/LLNL/Aluminum)
  - CUDA peer-to-peer intra-node
  - Aluminum's custom MPI+CUDA backend for inter-node
  - Collective routines with MPI and NCCL
- NVIDIA cuDNN for CNN GPU kernels

Optimizing Halo Exchange

- Standard MPI + CUDA communication model is inefficient for CNNs
  - GPU stream synchronization before MPI_Send is mandatory
  - GPU stream synchronization can be very costly
  - Can't keep issuing asynchronous GPU tasks, causing GPU kernel launch overhead (~10 us)
- Not an issue when doing weak scaling
  - Common in scientific computing
- Only strong scaling is possible with CNNs

Sending data from GPU

```
do_something<<<,,,st>>>(…)
(cudaMemcpyDeviceToHost)
cudaStreamSynchronize(st)
MPI_Send()
do_something<<<,,,st>>>(…)
```

Asynchronous Inter-Node Data Transfer

- CUDA stream memory operations allow GPU data transfer without GPU synchronization
- No GPU synchronization
- Implemented in the *Aluminum* communication library

Sendrecv with GPU buffers

Main thread

```
do_something<<<,,,st>>>(…)
(cudaMemcpyDeviceToHost)
cudaEventRecord(ev, st)
cuStreamWaitValue32(st, …)
do_something<<<,,,st>>>(…)
```

Comm thread

```
while (cudaEventQuery(ev)) {}
MPI_Sendrecv()
(cudaMemcpyHostToDevice)
cuStreamWriteValue32(st,…)
```

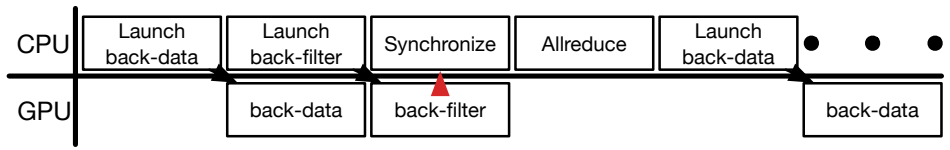
Aluminum: GPU-Centric Communication Library

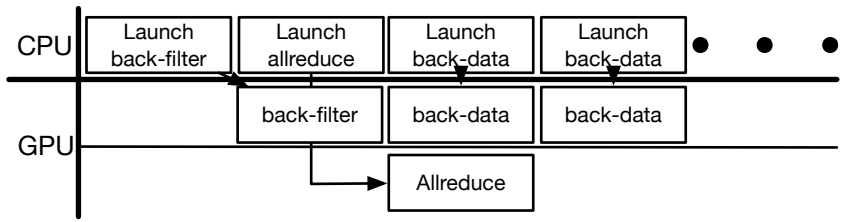
- Generic C++ interface to MPI, NCCL, custom algorithms
  - Asynchrony via dedicated communication engine
- Communication is “just another kernel” (GPU-centric, like NCCL)
  - Runtime handles all details (like non-blocking MPI– “progress is magic”)
- Associate a “stream of computation” with a communicator
  - CUDA stream; implicit on CPU, but could be a (lightweight) thread, …
  - Aluminum ensures communication does not begin until data on the stream is ready
- Blocking operations (like `MPI_Allreduce`):
  - Ensure no subsequent operations start until communication complete
  - Block only the associated stream
- Non-blocking operations (like `MPI_Iallreduce`):
  - Block no stream
  - Explicit completion operation (like `MPI_Wait`)
- https://github.com/llnl/aluminum

Aluminum

```
// Synchronous MPI:
for (int step = 0; step < num_steps; ++step) {
 load_mini_batch();
 for (auto&& layer : layers) layer.forward();
 for (auto&& layer : layers) {
  layer.backprop_data();
  if (layer.has_weights()) {
   layer.backprop_filter();
   cudaStreamSynchronize(stream);
   MPI_Allreduce(MPI_IN_PLACE, layer.weights,
    layer.size, MPI_FLOAT, MPI_SUM, comm);
   layer.sgd_step();
  }
 }
}
```

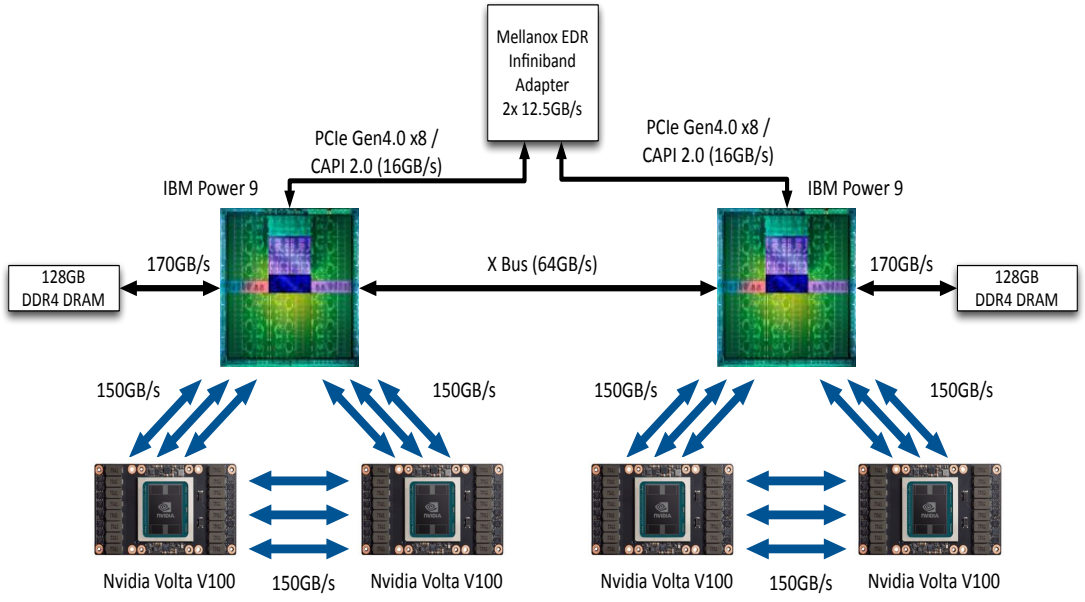
```
// Aluminum:
for (int step = 0; step < num_steps; ++step) {
 load_mini_batch();
 for (auto&& layer : layers) layer.forward();
 for (auto&& layer : layers) {
  if (layer.has_weights()) {
   layer.backprop_filter();
   Al::NonblockingAllreduce<Al::MPICUDABackend>(
    layer.weights, layer.size,
    Al::ReductionOperator::sum, comm, layer.req);
  }
  layer.backprop_data();
 }
 for (auto&& layer : layers) {
  Al::Wait<Al::MPICUDABackend>(layer.req);
  layer.sgd_step();
 }
}
```





Evaluation

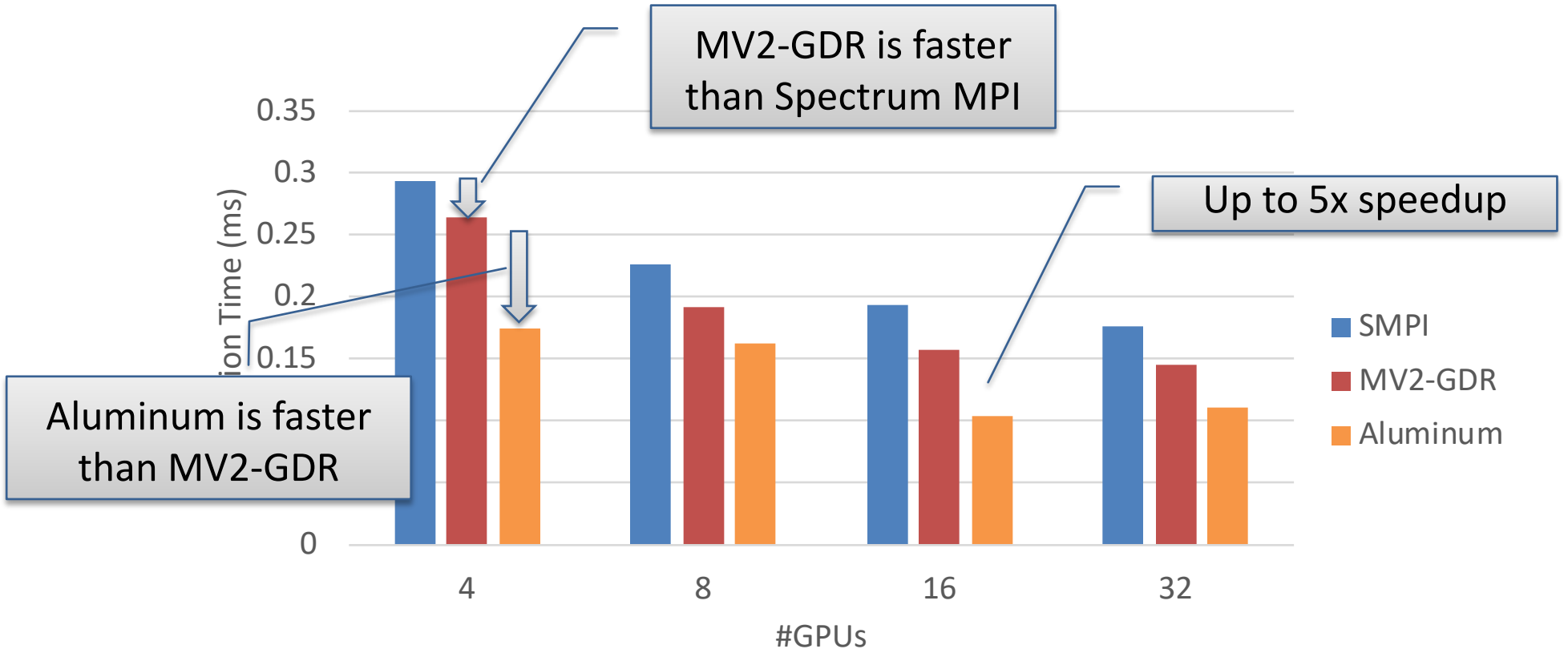
- Lassen - 700 nodes
  - 2x POWER9 + 4X V100 + NVLink2 + 2x InfiniBand EDR
  - Experiments use up to 2048 GPUs
- cuDNN v7.5.1
- MVAPICH2-GDR 2.3.2
- Spectrum MPI/2019.01.30
- Mesh tangling data:
  - 1K: 1024 x 1024 x 18
  - 2K: 2048 x 2048 x 18
- Same spatial distribution for all layers



Performance of Spatial-Parallel Convolution

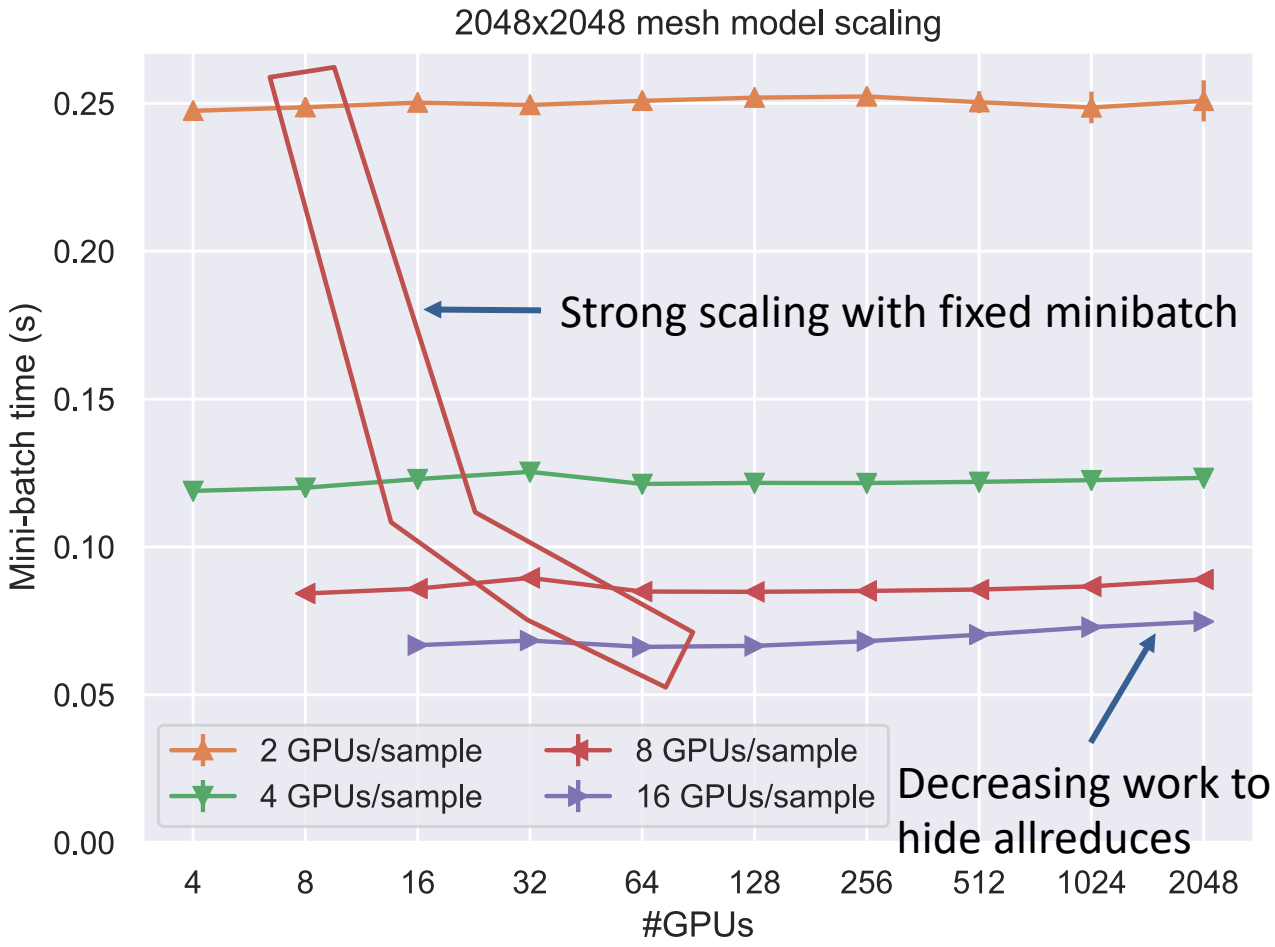
Convolution of a single 1024^2 image with 16 channels and 16 filters of 3x3 kernels

1GPU: 0.533 ms



End-to-End Hybrid Parallel Training of Mesh Model

- 2048^2 mesh tangling model
  - Needs 2 GPUs per sample at least
- Weak scaling with sample parallelism
  - Excellent scaling by overlapped gradient allreduces
  - Small increase at 2048 GPUs due to decreased work to hide allreduces
- Strong scaling with spatial parallelism
  - Close to 4x with 16 GPUs
  - Speedup is smaller at later layers due to decreasing spatial dimensions



Conclusion

- Generalized parallel convolution
  - Sample/spatial/channel/filter parallelism
  - Address memory capacity constraint → Enables more accurate models
  - Allow strong scaling → Faster training time
- LBANN: Scalable deep learning software stack for large-scale science and engineering problems
  - https://github.com/llnl/lbann
  - Aluminum: GPU-centric communication library (https://github.com/llnl/aluminum)
  - Implements the generalized parallel convolution algorithms

Ongoing Work

- Channel/filter parallelism
  - Early results to appear at SC19
- Performance modeling to identify optimal parallelization strategies
- Optimizing performance of reading training samples
- References
  - N. Dryden, N. Maruyama, T. Moon, T. Benson, A. Yoo, M. Snir, and B Van Essen, "Aluminum: An Asynchronous, GPU-Aware Communication Library Optimized for Large-Scale Training of Deep Neural Networks on HPC Systems," *Workshop on Machine Learning in HPC Environments (MLHPC'18),* 2018.
  - N. Dryden, N. Maruyama, T. Benson, T. Moon, M. Snir, and B Van Essen, "Improving Strong-Scaling of CNN Training by Exploiting Finer-Grained Parallelism," *International Parallel and Distributed Processing Symposium (IPDPS'19),* 2019
  - N. Dryden, N. Maruyama, T. Moon, T. Benson,, M. Snir, and B Van Essen, ”Channel and Filter Parallelism for Large-Scale CNN Training," *International Conference for High Performance Computing, Networking, Storage, and Analysis (SC’19)*, 2019 (to appear)

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