MVAPICH
MPI, PGAS and Hybrid MPI+PGAS Library

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HiDL
High-Performance Deep Learning

Boosting Performance of Deep Learning, Machine Learning, and Dask with MVAPICH2

Tutorial at MUG '21

by

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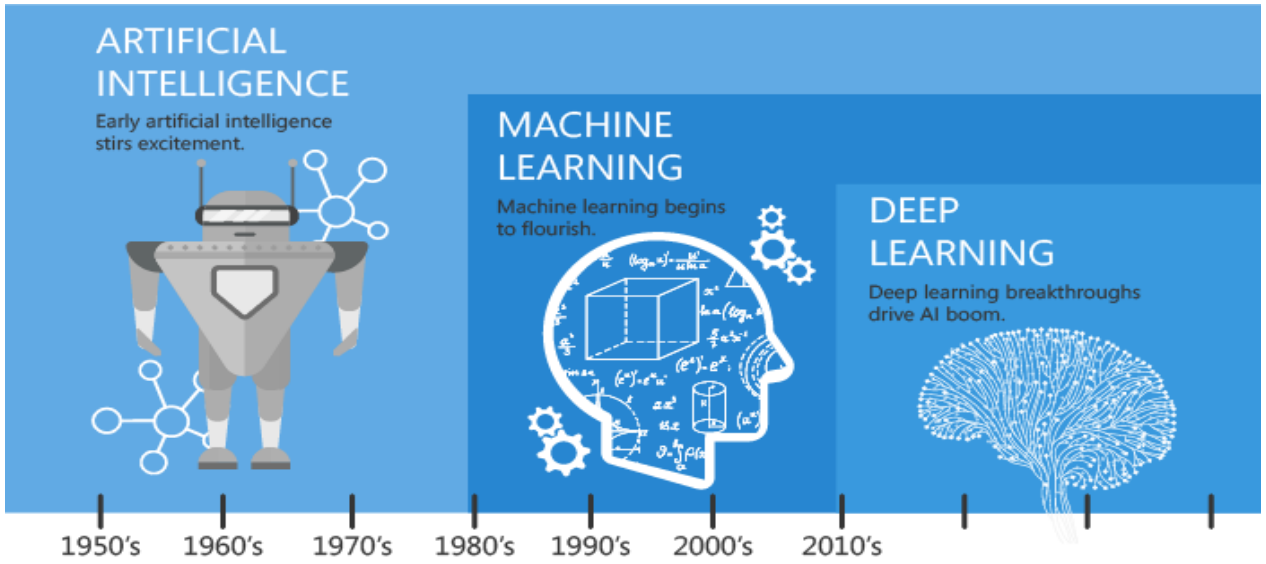
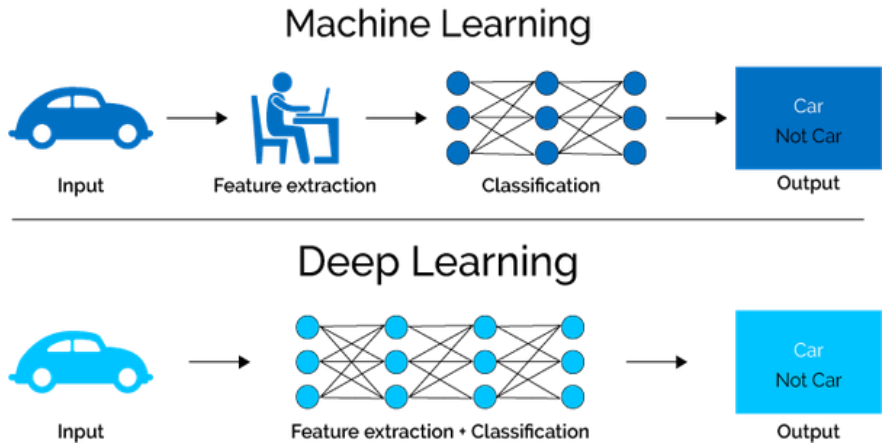
Outline

- **Introduction**
- Deep Neural Network Training and Essential Concepts
- Parallelization Strategies for Distributed DNN Training
- Machine Learning
- Data Science using Dask
- Conclusion

What is Machine Learning and Deep Learning?

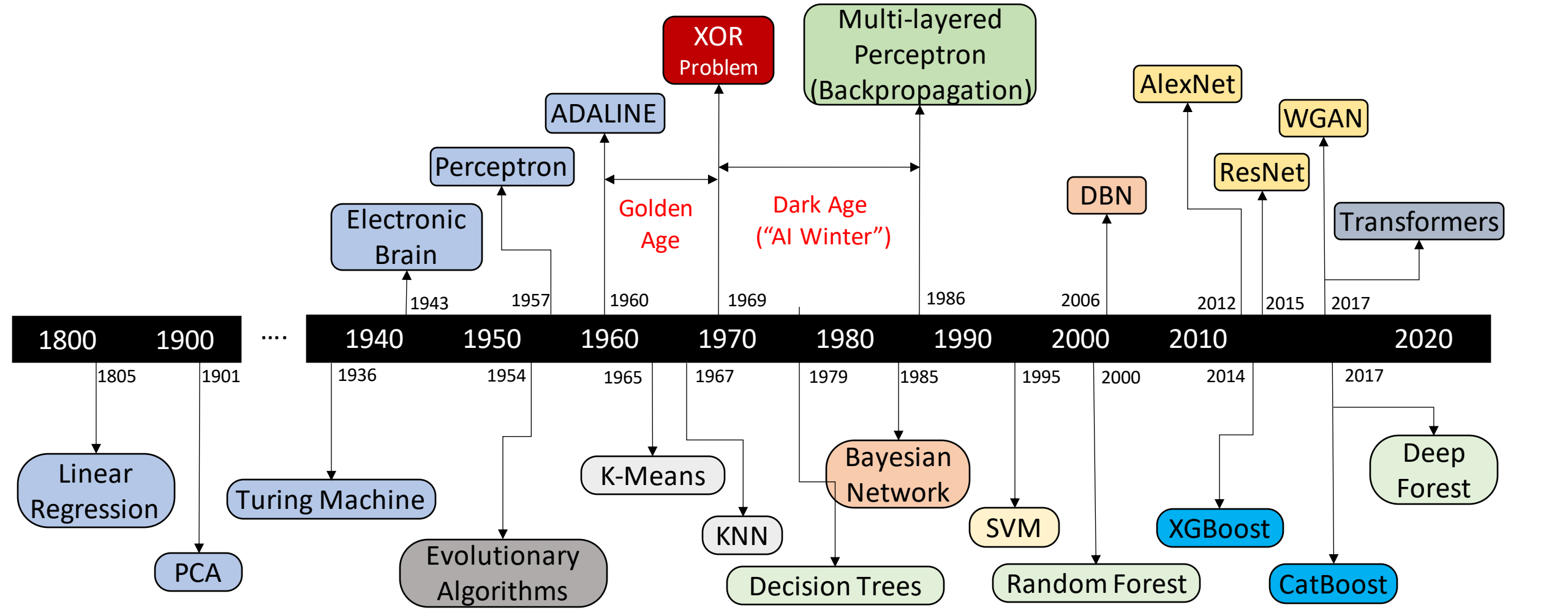
- Machine Learning (ML)
  - "the study of computer algorithms to improve automatically through experience and use of data"
- Deep Learning (DL) – a subset of ML
  - Uses Deep Neural Networks (DNNs)
  - **Perhaps, the most revolutionary subset!**
- Based on learning data representation
- DNN Examples: Convolutional Neural Networks, Recurrent Neural Networks, Hybrid Networks
- Data Scientist or Developer Perspective for using DNNs
  1. Identify DL as solution to a problem
  2. Determine Data Set
  3. Select Deep Learning Algorithm to Use
  4. Use a large data set to train an algorithm





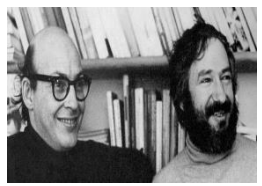
Courtesy: https://hackernoon.com/difference-between-artificial-intelligence-machine-learning-and-deep-learning-1pcv3zeg, https://blog.dataiku.com/ai-vs.-machine-learning-vs.-deep-learning, https://en.wikipedia.org/wiki/Machine_learning

History: Milestones in the Development of ML/DL



A. Legendre – J. Gauss K. Pearson

A. Turing S. McCulloch – W. Pitts F. Rosenblatt B. Widrow – M. Hoff



M. Minsky – S. Papert

J. Pearl

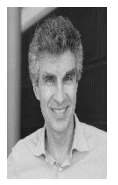
D. Rumelhart – G. Hinton – R. Wiliams

V. Vapnik – C. Cortes

A. Krizhevsky

A. Ng

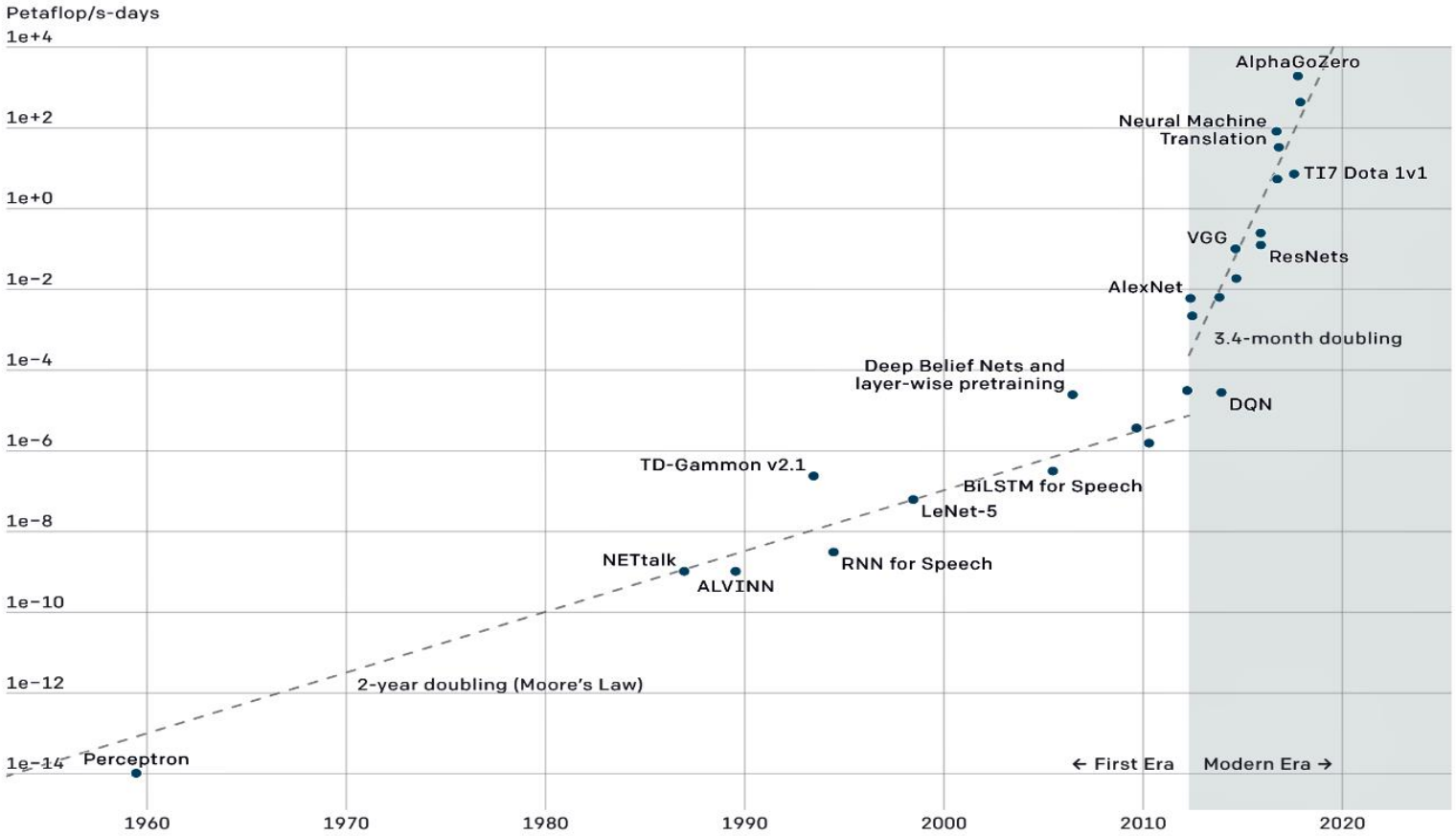
Y. LeCun



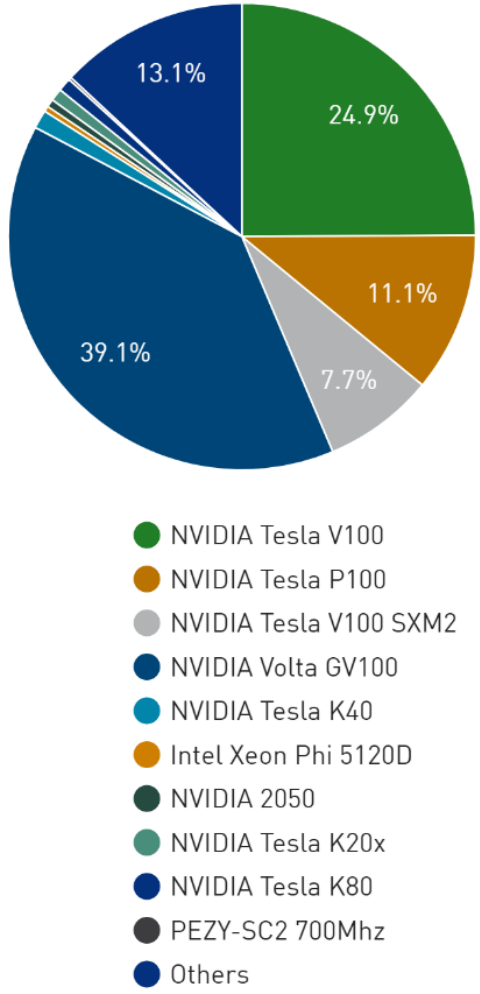
Y. Bengio

Deep Learning meets Super Computers

- Computation requirement is increasing exponentially
  - CPUs still dominates HPC arena and can be used for Deep Learning



Accelerator/CP Family Performance Share



www.top500.org

Courtesy: https://openai.com/blog/ai-and-compute/

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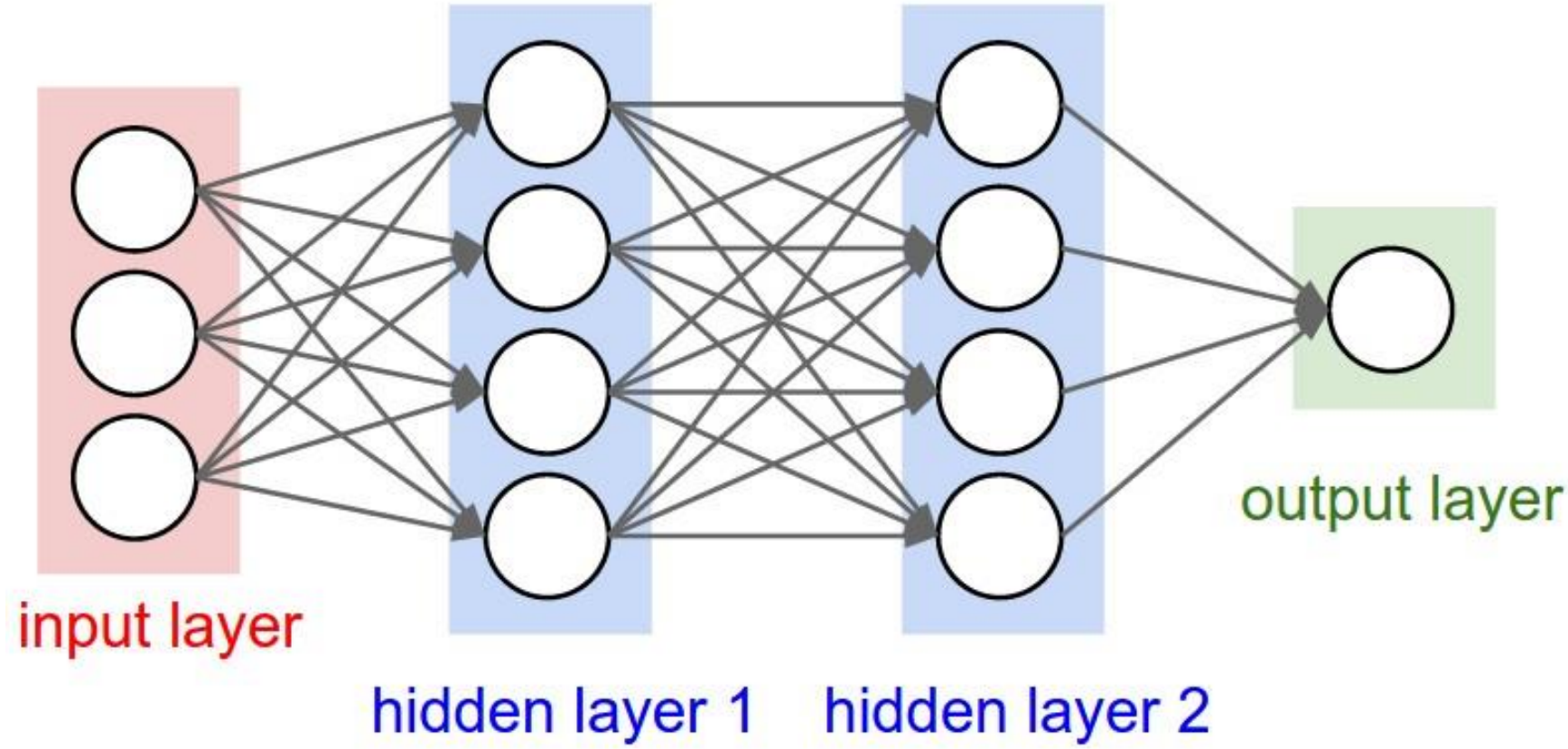
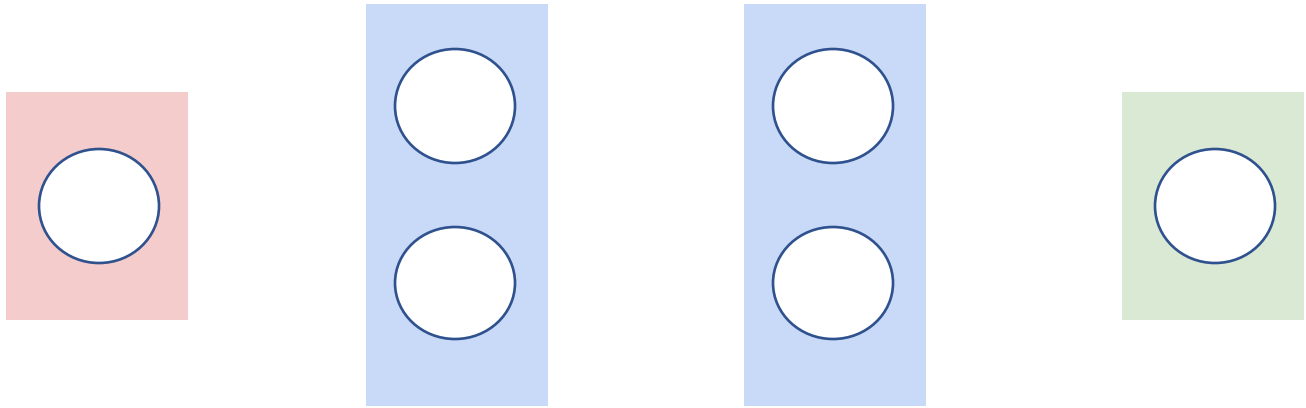
So what is a Deep Neural Network?

- Example of a 3-layer Deep Neural Network (DNN) – (input layer is not counted)



Courtesy: http://cs231n.github.io/neural-networks-1/

DNN Training: Forward Pass



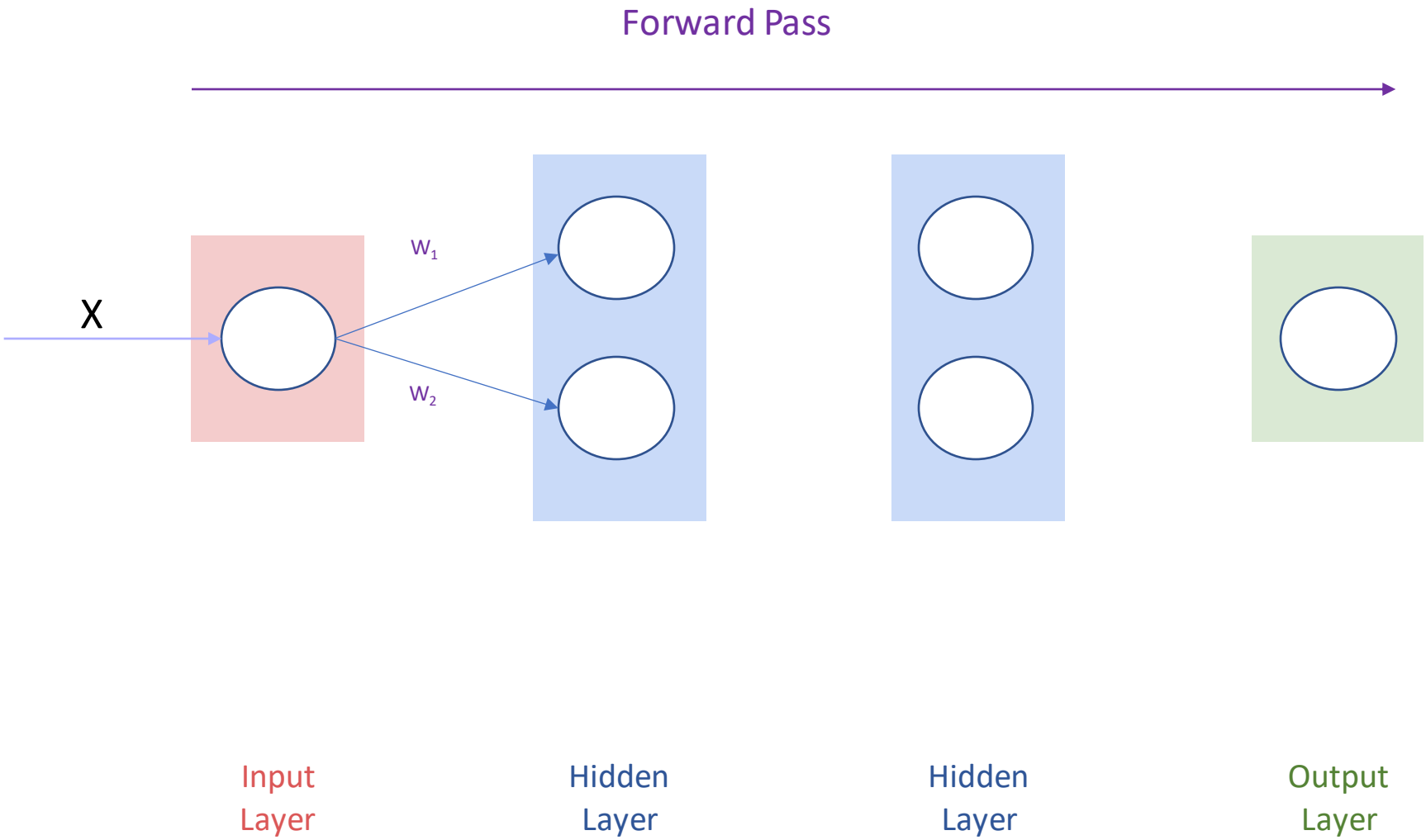
Input Layer

Hidden Layer

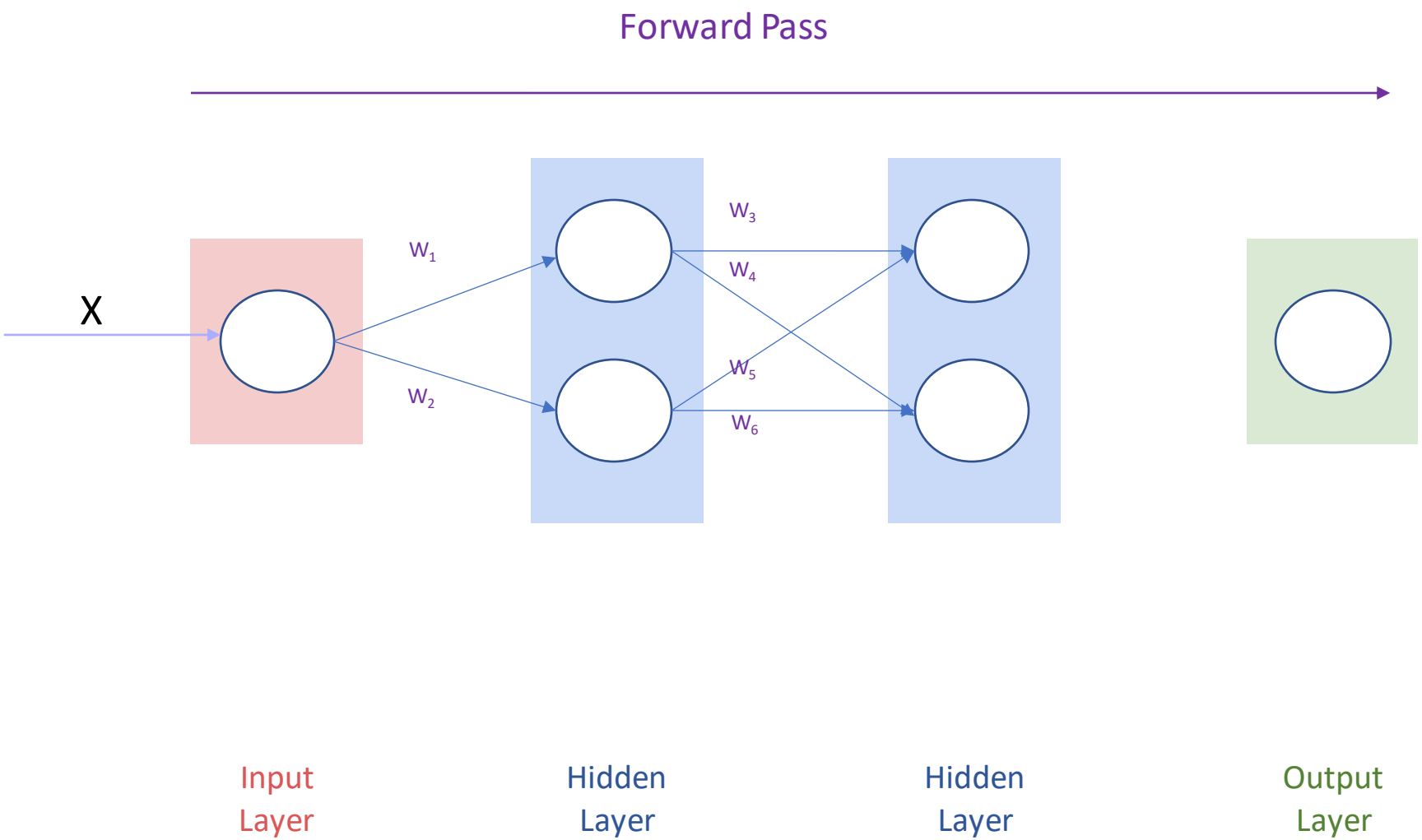
Hidden Layer

Output Layer

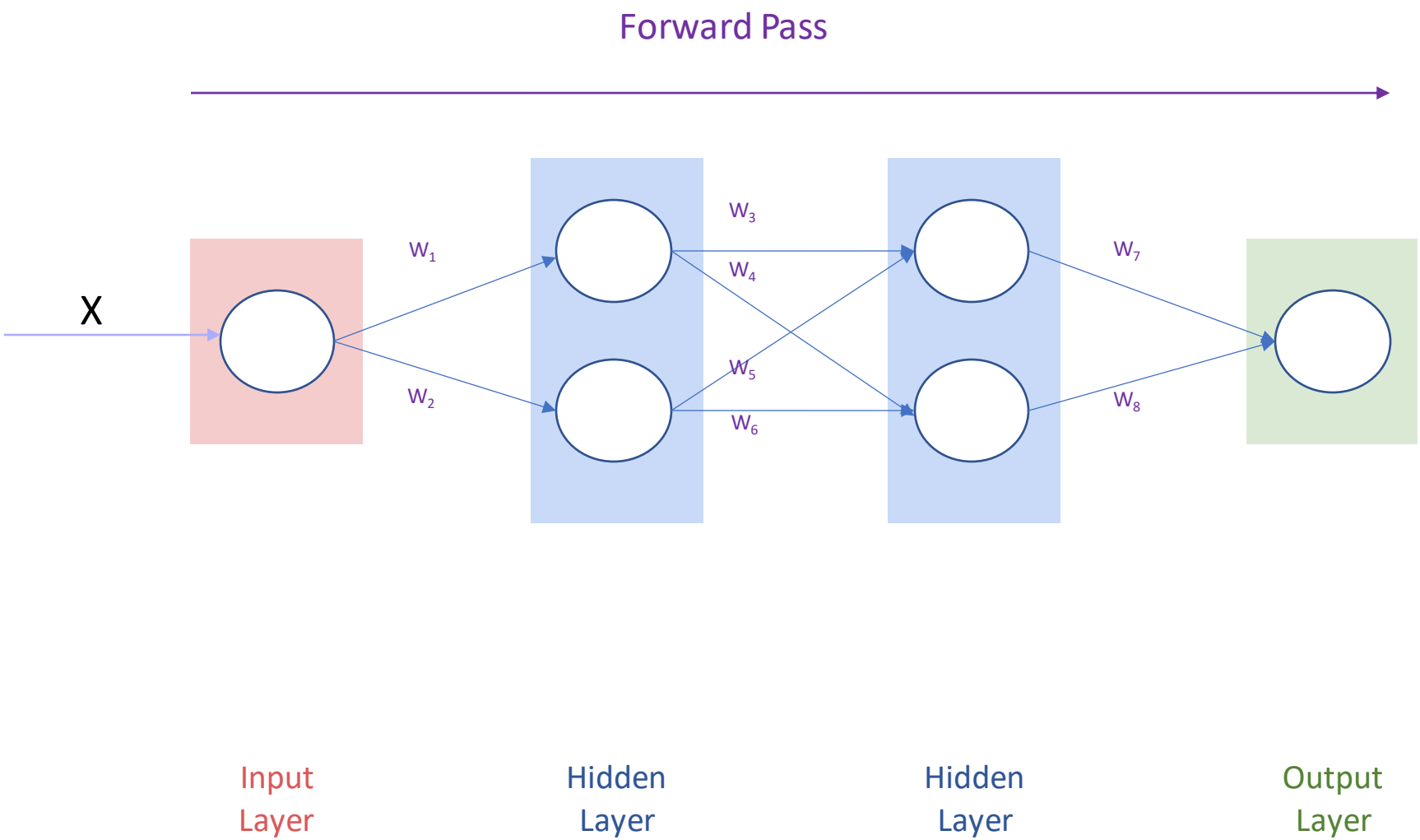
DNN Training: Forward Pass



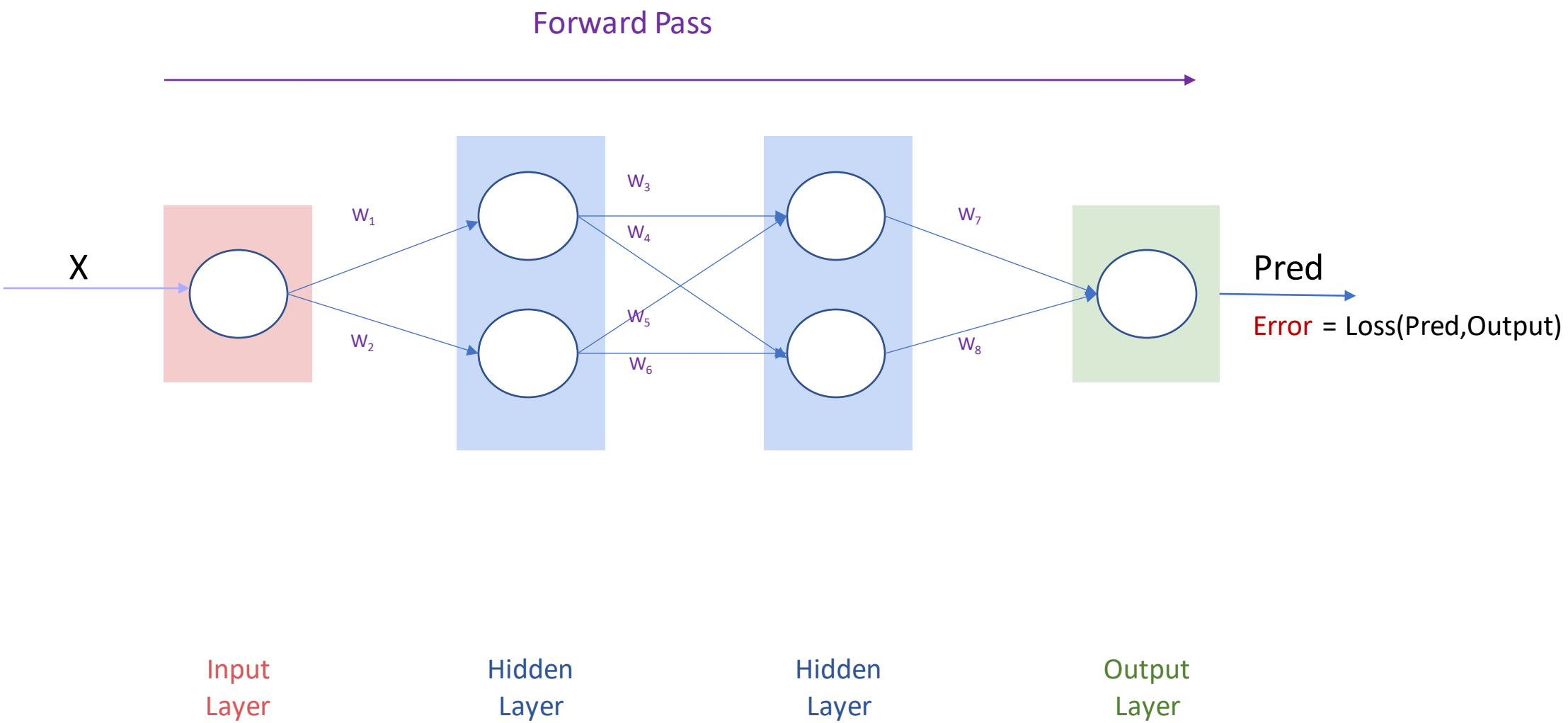
DNN Training: Forward Pass



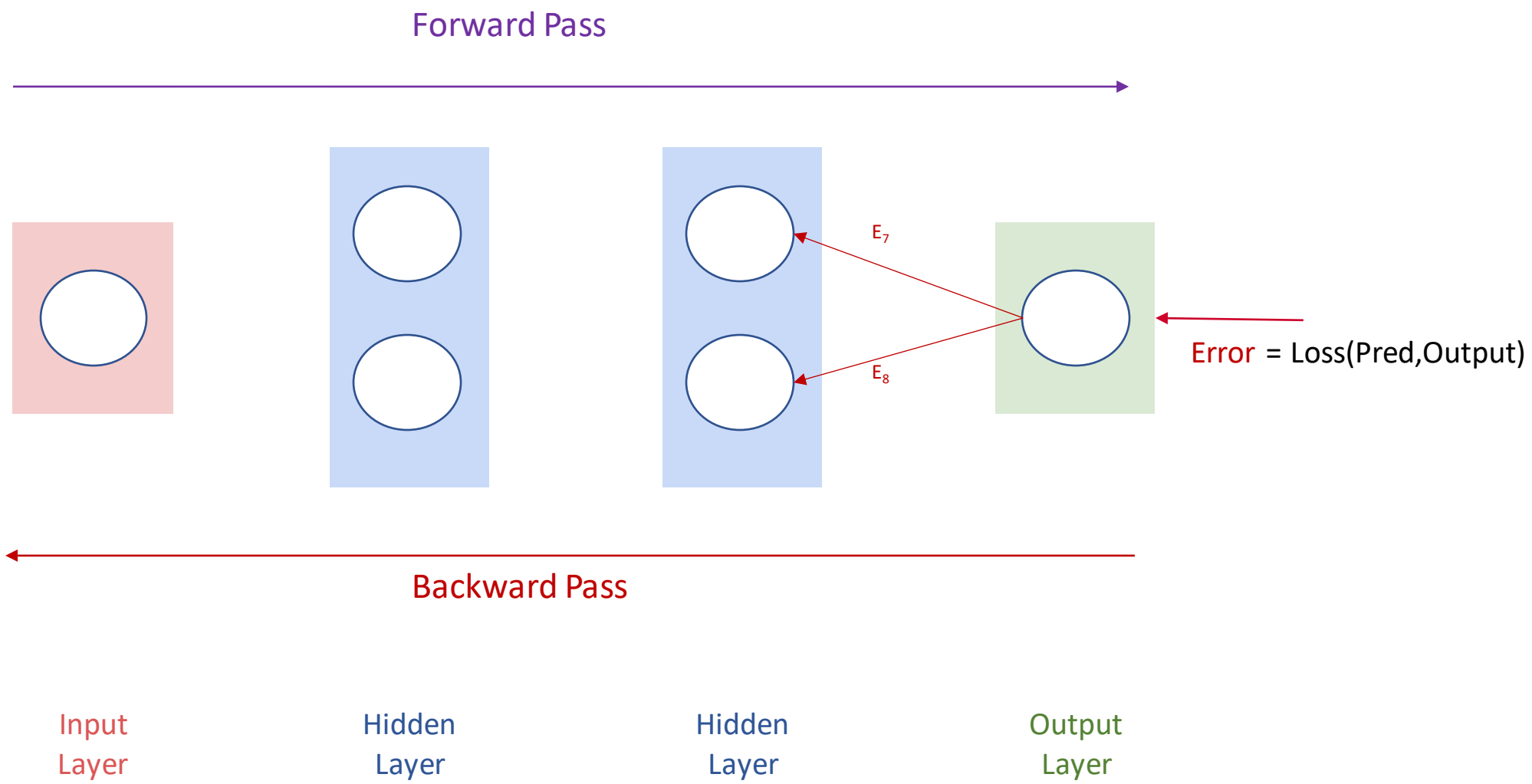
DNN Training: Forward Pass



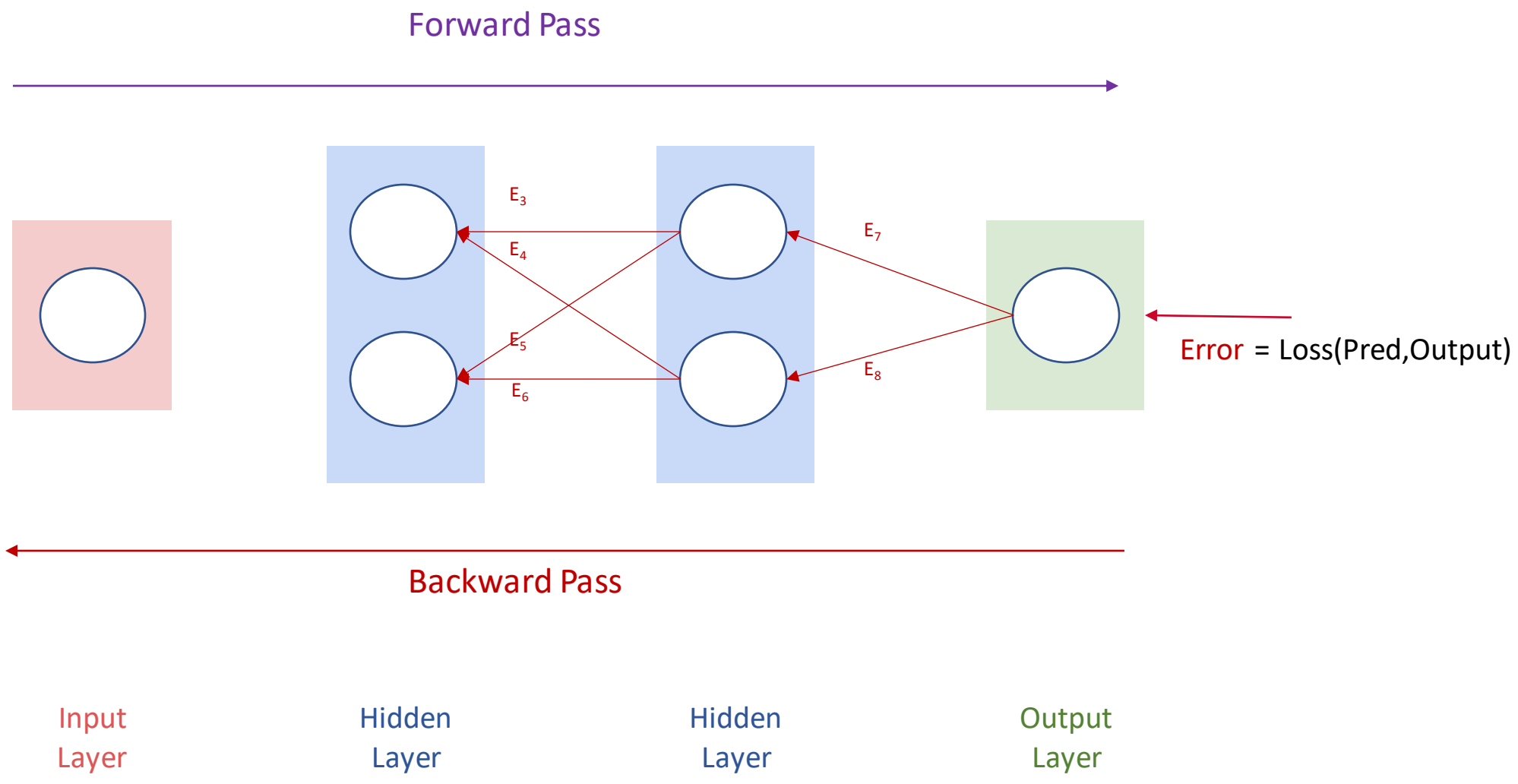
DNN Training: Forward Pass



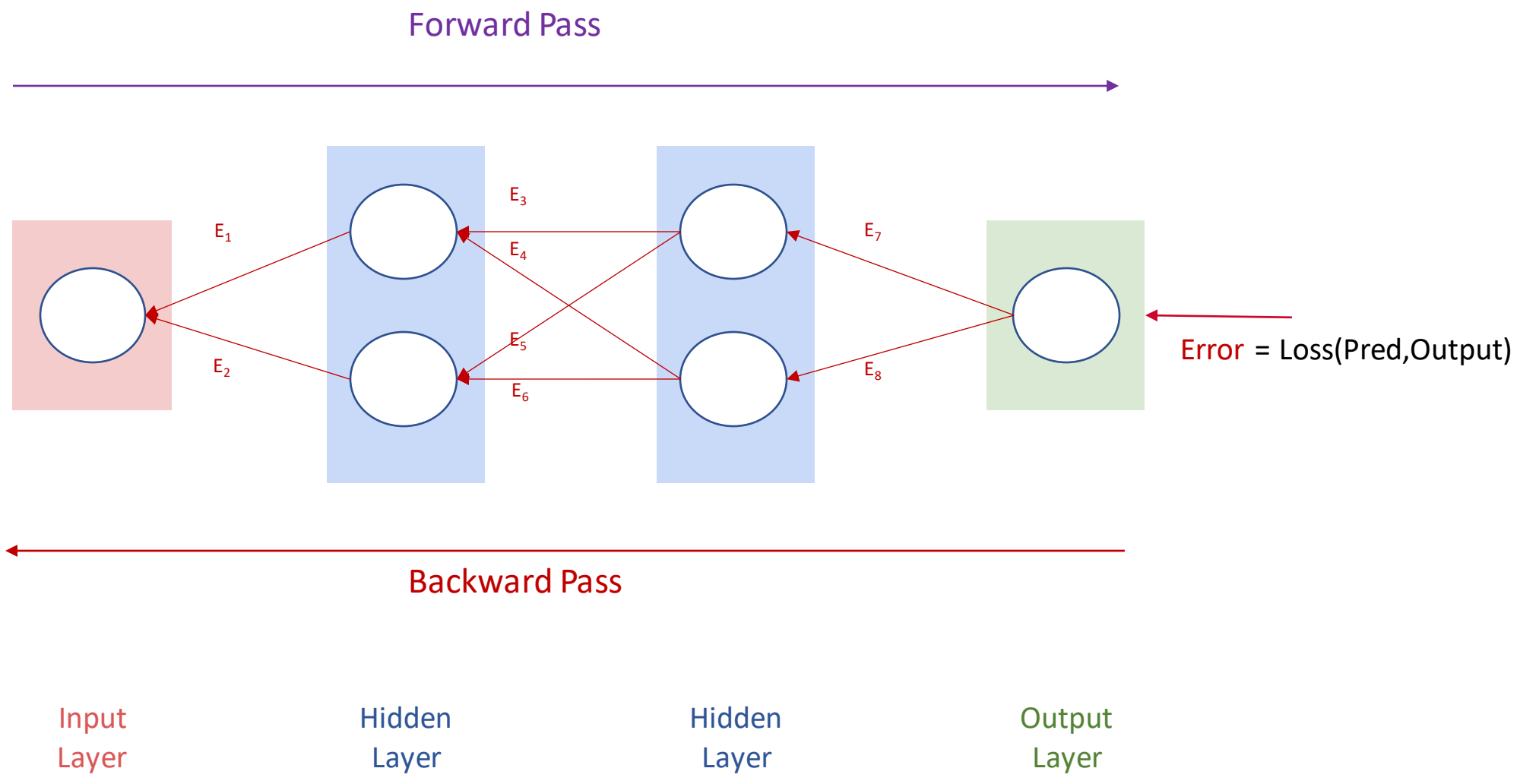
DNN Training: Backward Pass



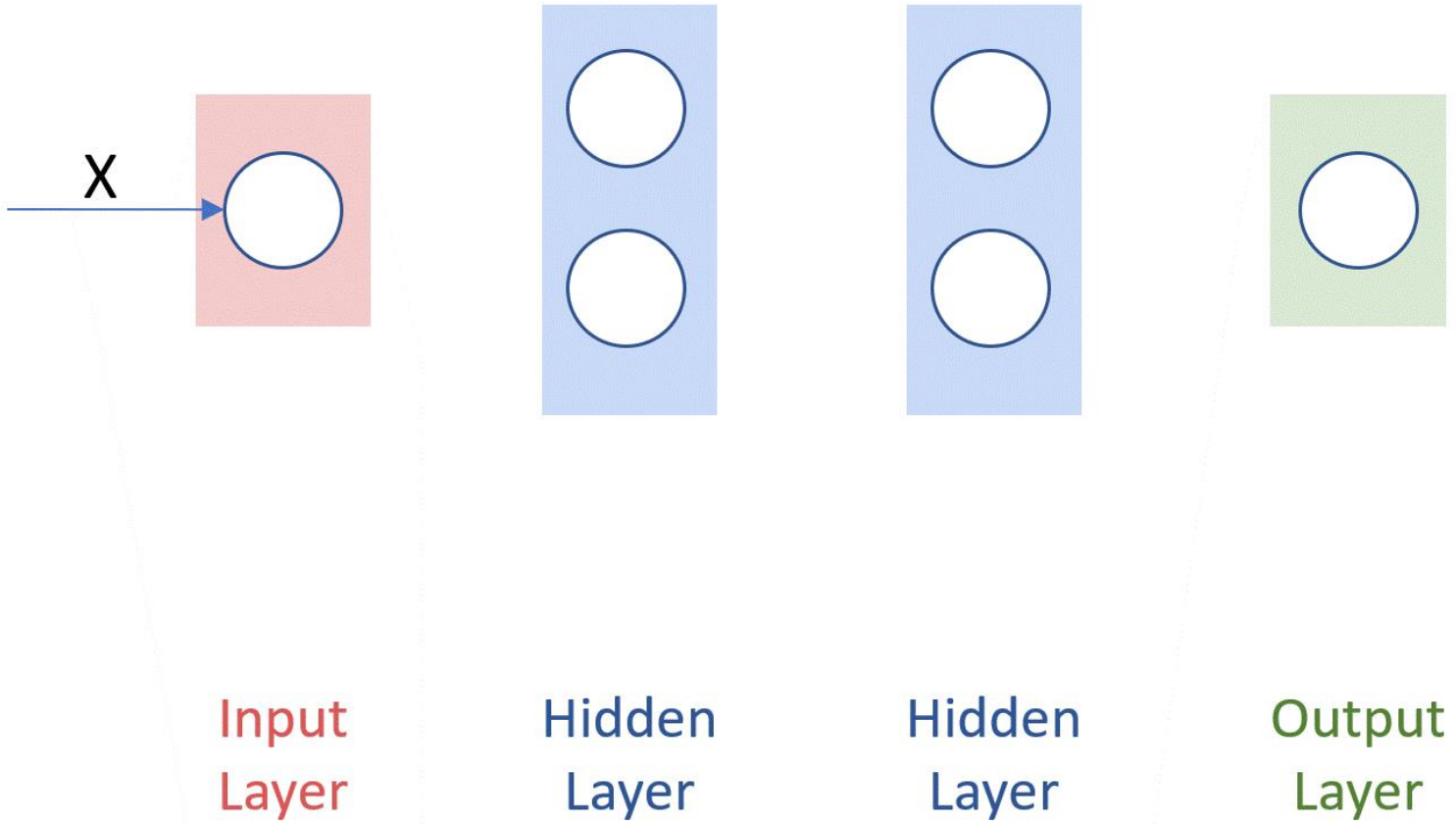
DNN Training: Backward Pass



DNN Training: Backward Pass

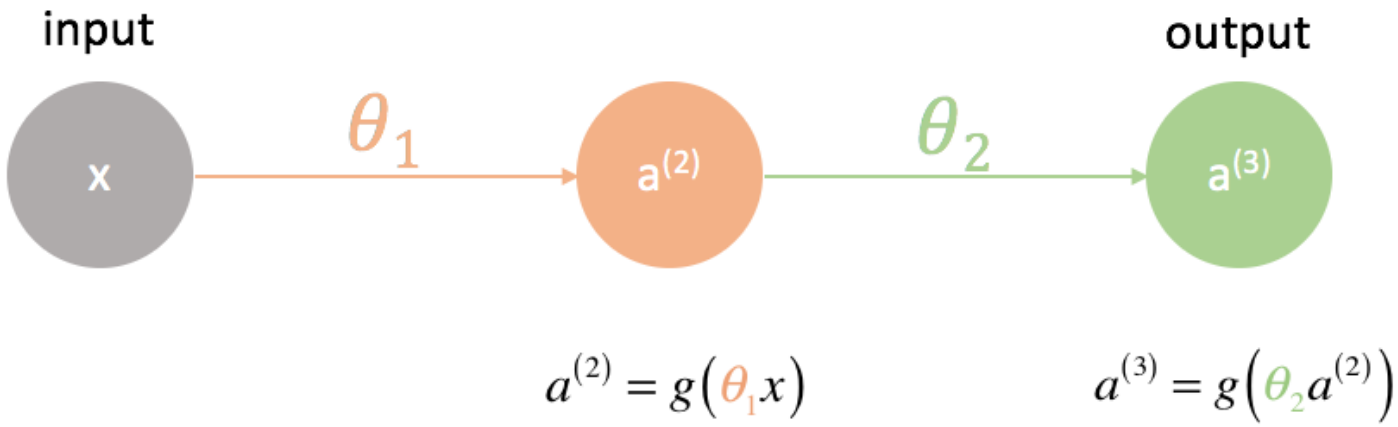


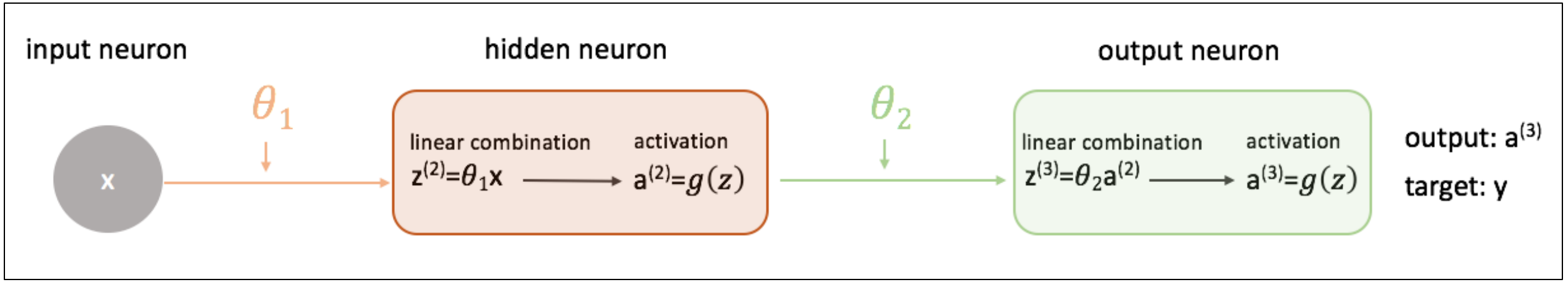
DNN Training



Essential Concepts: Activation function and Back-propagation

- Back-propagation involves complicated mathematics.
  - Luckily, most DL Frameworks give you a one line implementation -- `model.backward()`



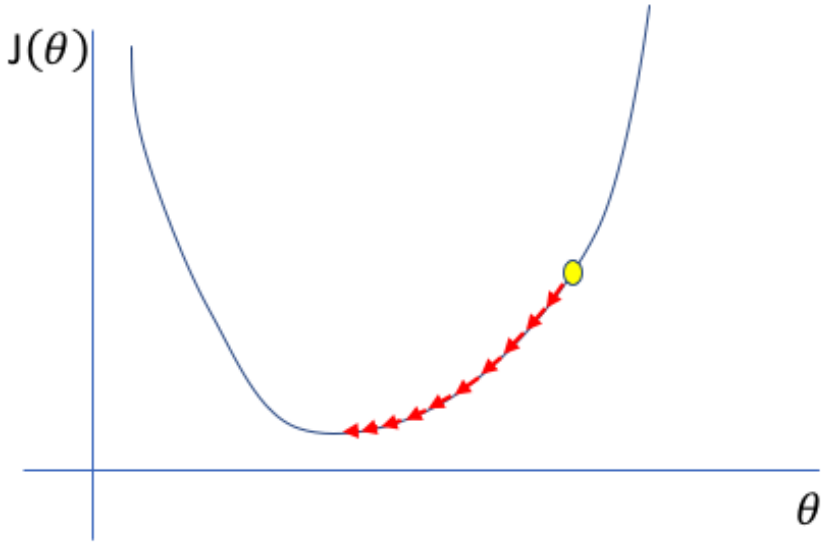


- What are Activation functions?
  - RELU (a Max fn.) is the most common activation fn.
  - Sigmoid, tanh, etc. are also used

Courtesy: https://www.jeremyjordan.me/neural-networks-training/

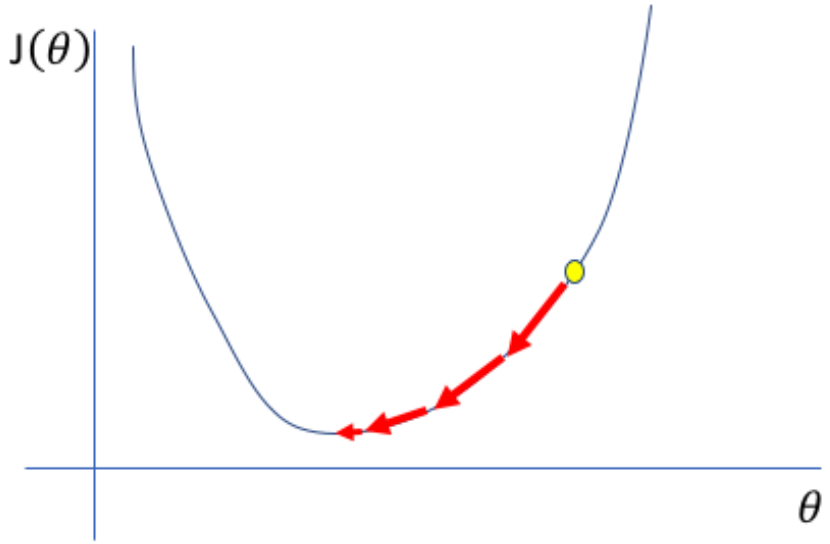
Essential Concepts: Learning Rate (α)

Too low



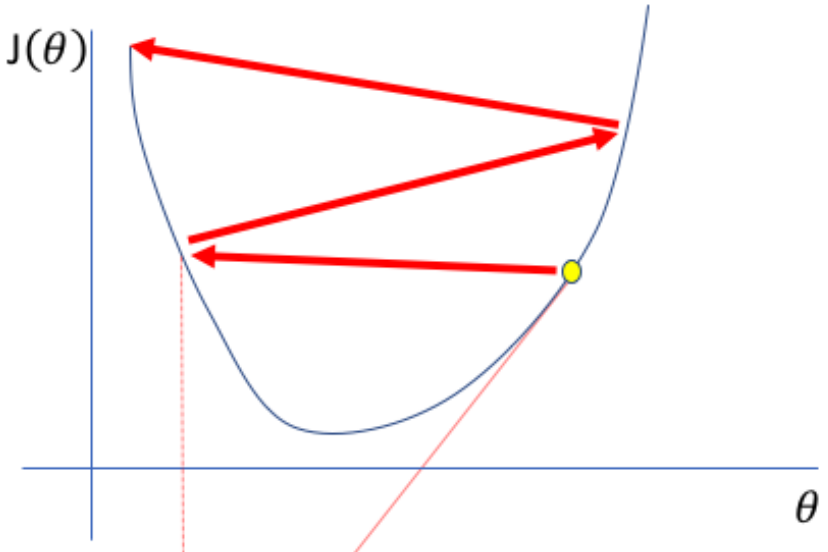
A small learning rate requires many updates before reaching the minimum point

Just right



The optimal learning rate swiftly reaches the minimum point

Too high

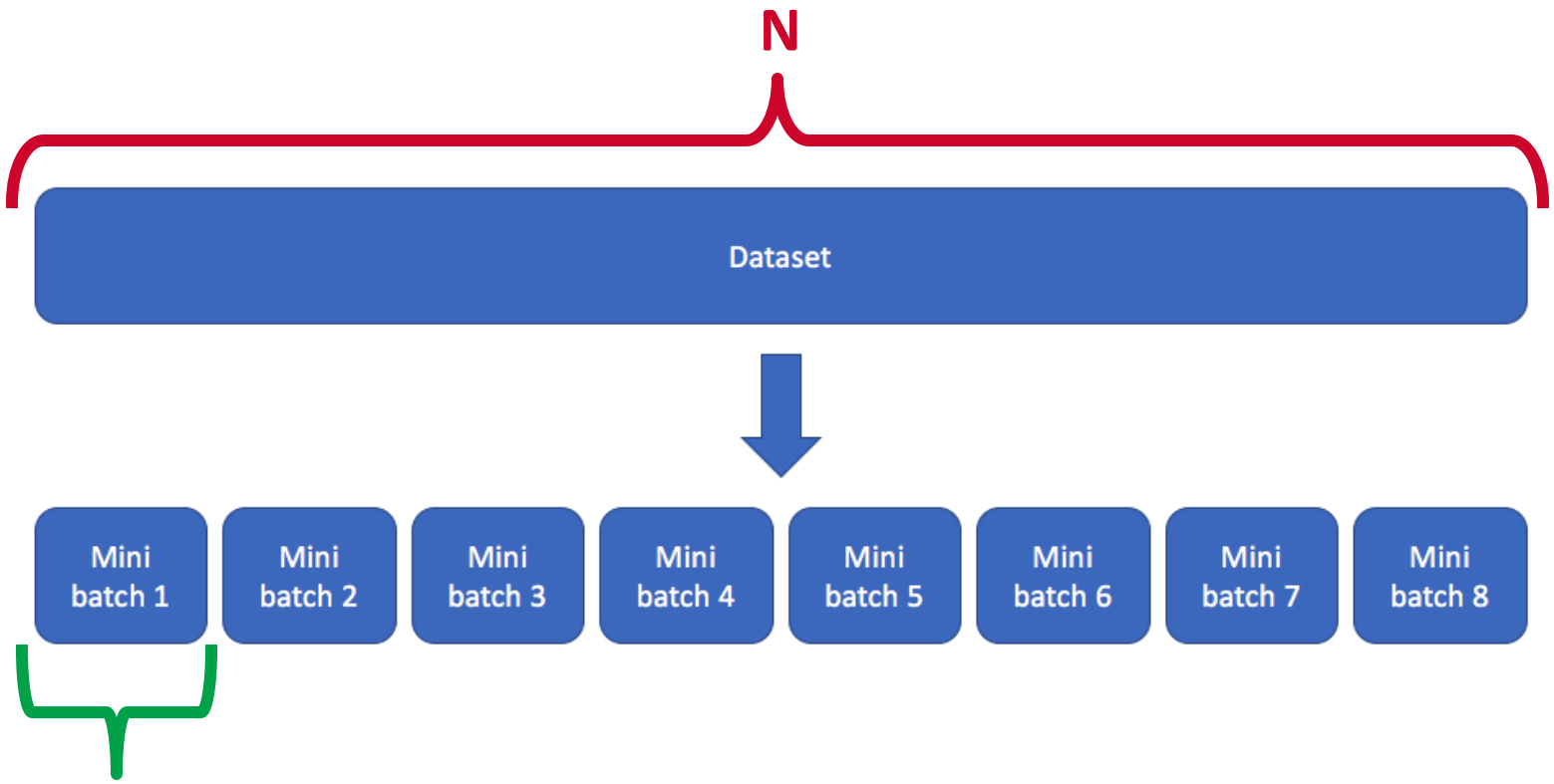


Too large of a learning rate causes drastic updates which lead to divergent behaviors

Courtesy: https://www.jeremyjordan.me/nn-learning-rate/

Essential Concepts: Batch Size

- Batched Gradient Descent
  - Batch Size = **N**
- Stochastic Gradient Descent
  - Batch Size = **1**
- Mini-batch Gradient Descent
  - Somewhere in the middle
  - Common:
    - **Batch Size** = 64, 128, 256, etc.
- Finding the optimal batch size will yield the fastest learning.

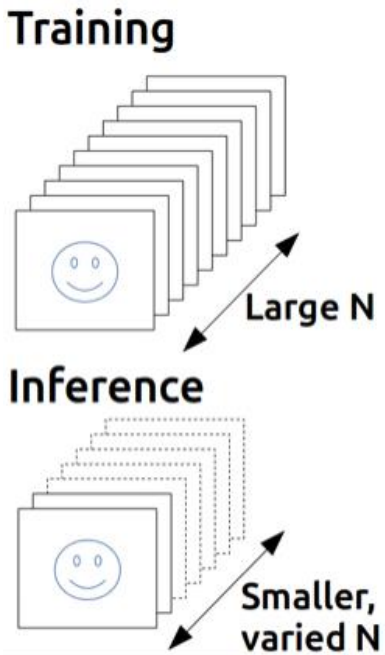


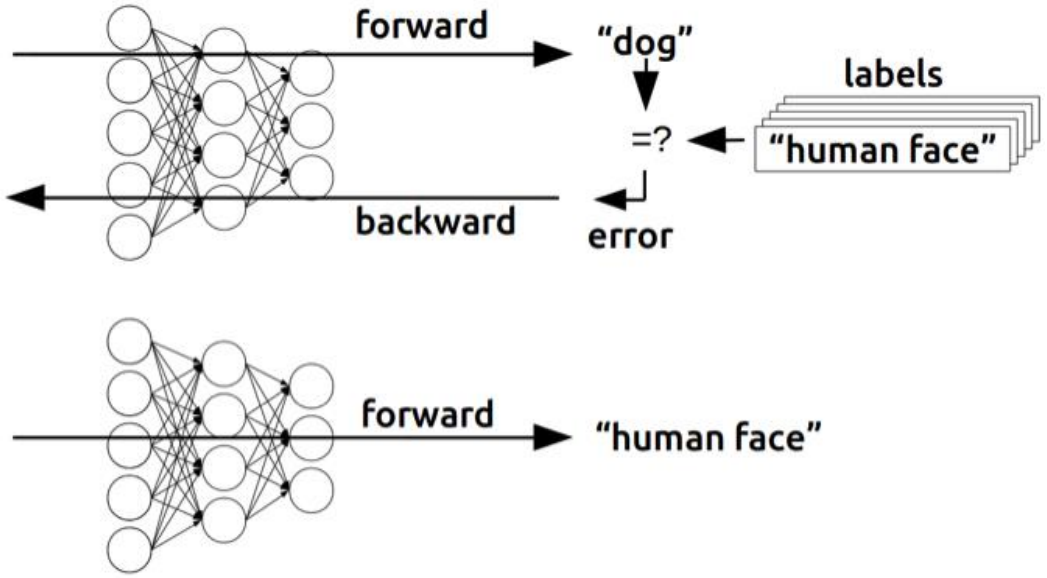
*One full pass over **N** is called an **epoch** of training*

Courtesy: https://www.jeremyjordan.me/gradient-descent/

Key Phases of Deep Learning

- Training is compute intensive
  - Many passes over data
  - Can take days to weeks
  - Model adjustment is done
- Inference
  - Single pass over the data
  - Should take seconds
  - No model adjustment
- Challenge: How to make **"Training"** faster?
  - Need Parallel and Distributed Training…





Courtesy: https://devblogs.nvidia.com/

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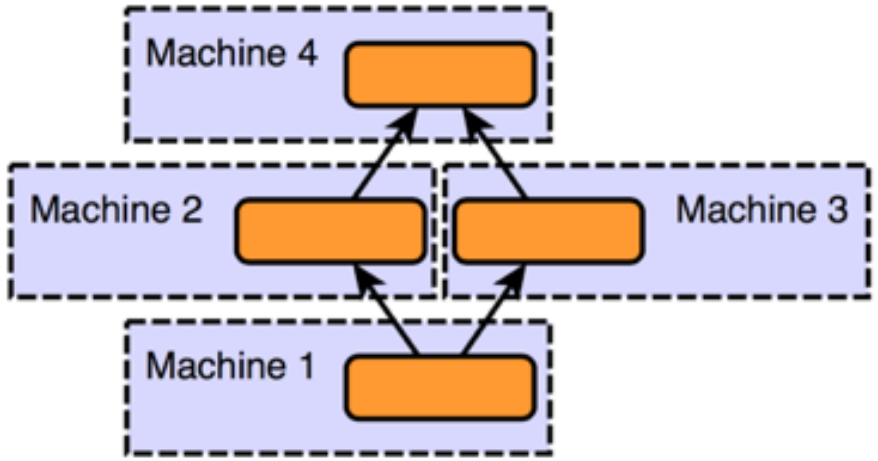
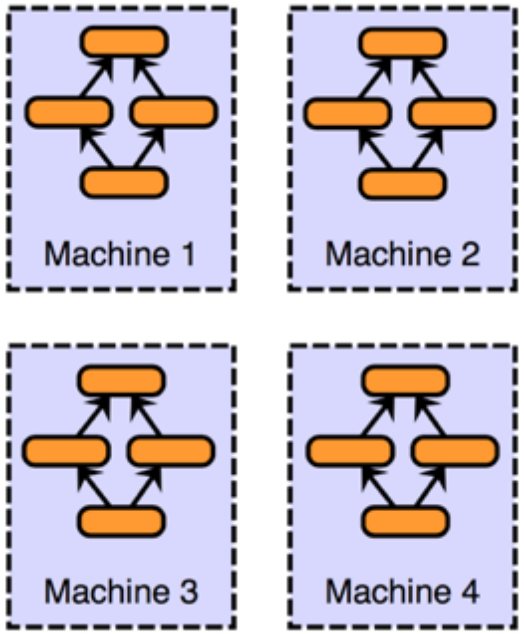
Parallelization Strategies

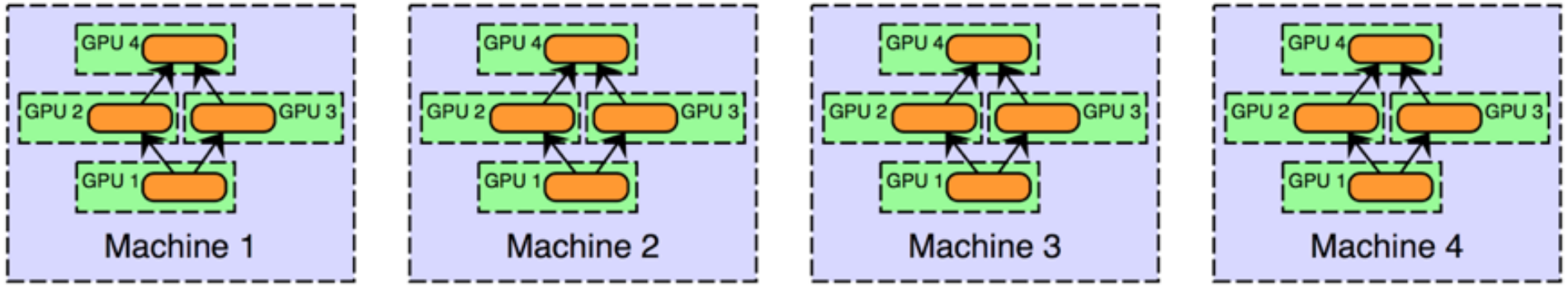
- Some parallelization strategies..
  - Data Parallelism
  - Model Parallelism
  - Hybrid Parallelism



Model Parallelism



Data Parallelism



Hybrid (Model and Data) Parallelism

Courtesy: http://engineering.skymind.io/distributed-deep-learning-part-1-an-introduction-to-distributed-training-of-neural-networks

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  - Model and Hybrid Parallelism
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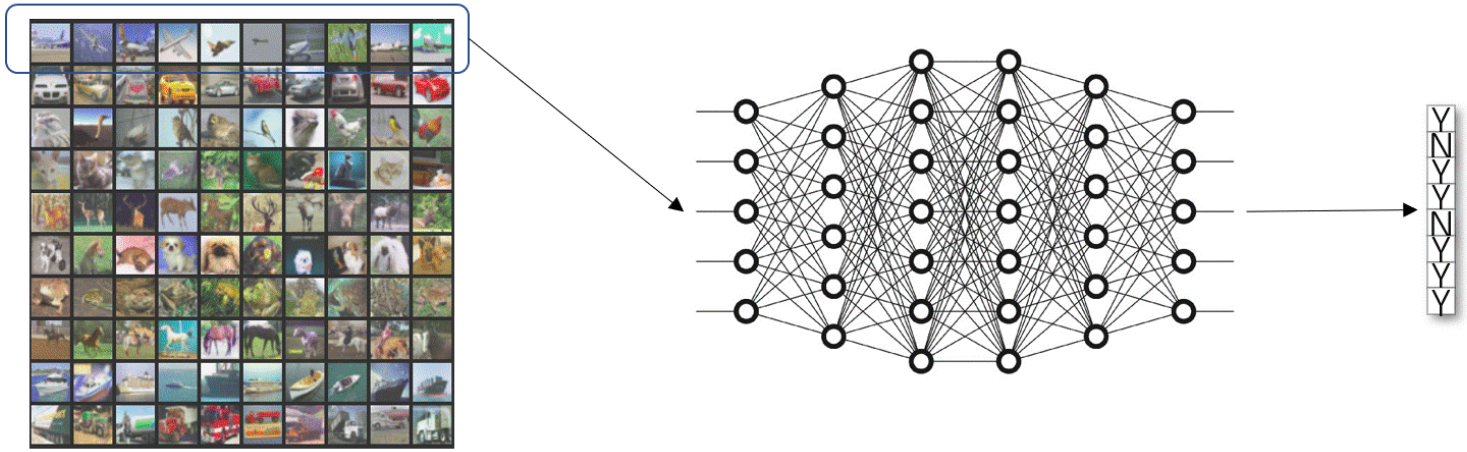
Need for Data Parallelism

Let's revisit Mini-Batch Gradient Descent

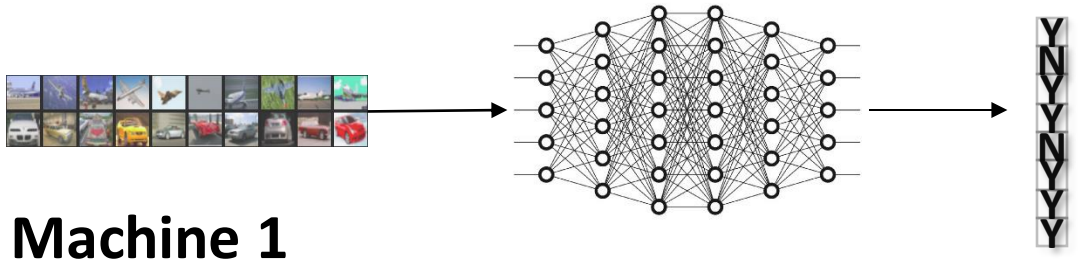


Input Dataset Machine 1 Output

Drawback: If the dataset has 1 million images, then it will take forever to run the model on such a big dataset

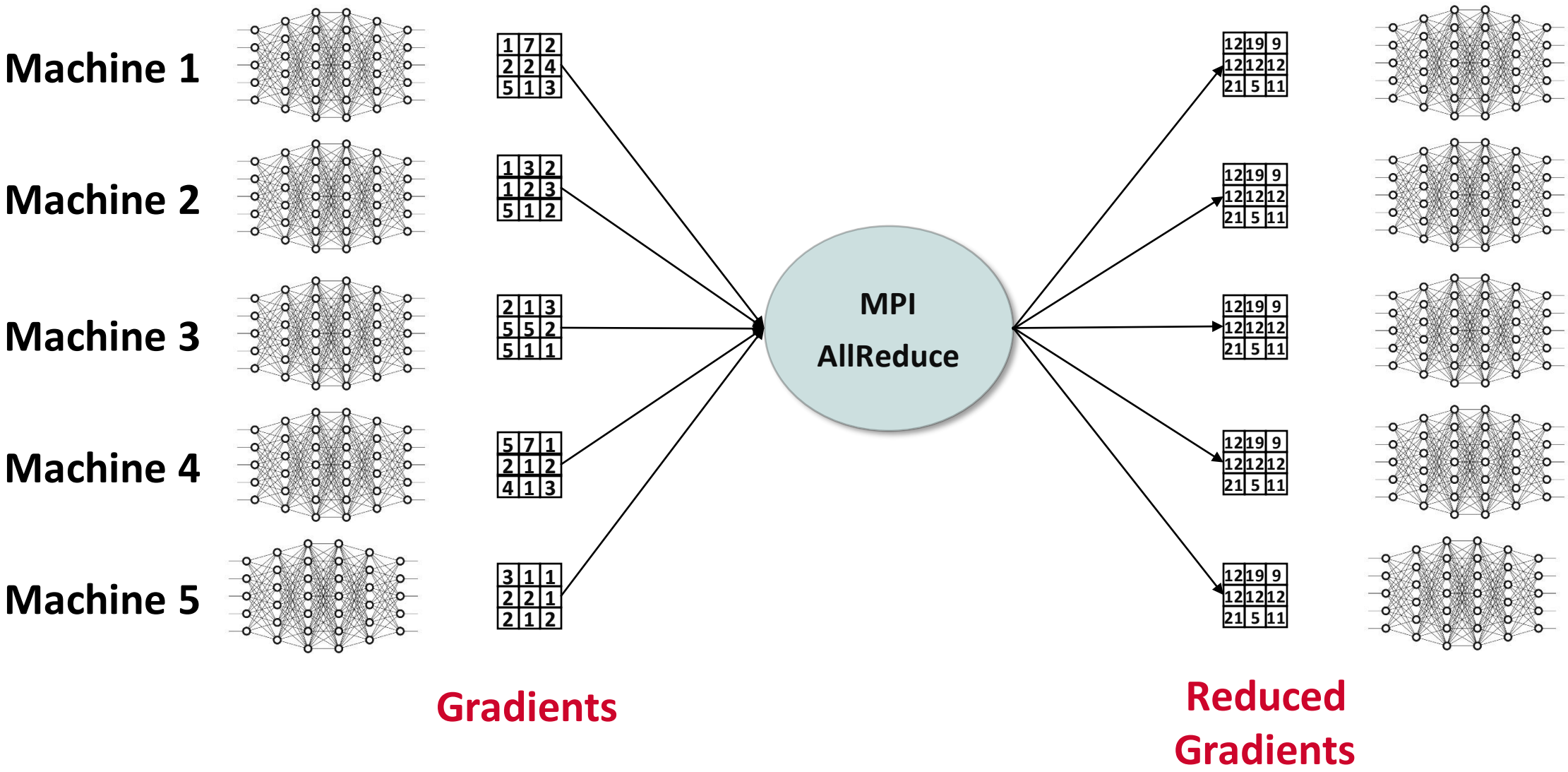
Solution: Can we use multiple machines to speedup the training of Deep learning models? **(i.e. Utilize Supercomputers to Parallelize)**

Need for Communication in Data Parallelism



Problem: Train a single model on whole dataset, not 5 models on different sets of dataset

Data Parallelism



Allreduce Collective Communication Pattern

- Element-wise Sum data from all processes and sends to all processes

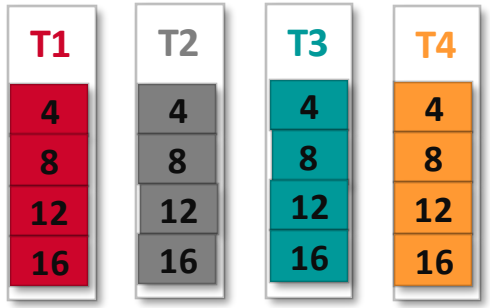
```
int MPI_Allreduce (const void *sendbuf, void * recvbuf, int count, MPI_Datatype datatype,
                   MPI_Op operation, MPI_Comm comm)
```

Input-only Parameters	
Parameter	**Description**
sendbuf	Starting address of send buffer
recvbuf	Starting address of recv buffer
type	Data type of buffer elements
count	Number of elements in the buffers
operation	Reduction operation to be performed (e.g. sum)
comm	Communicator handle

Input/Output Parameters	
Parameter	**Description**
recvbuf	Starting address of receive buffer

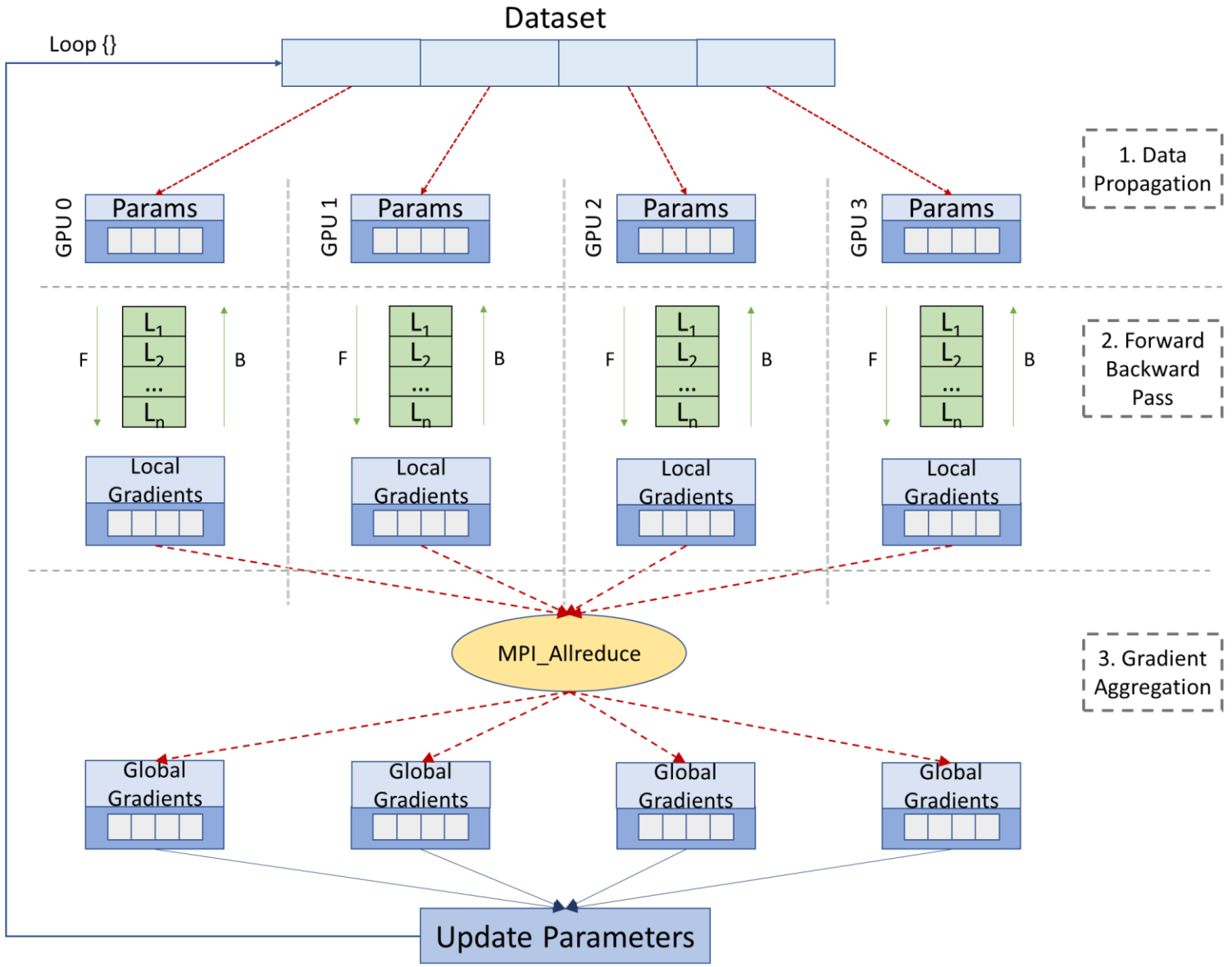
Sendbuf (Before)

Recvbuf (After)

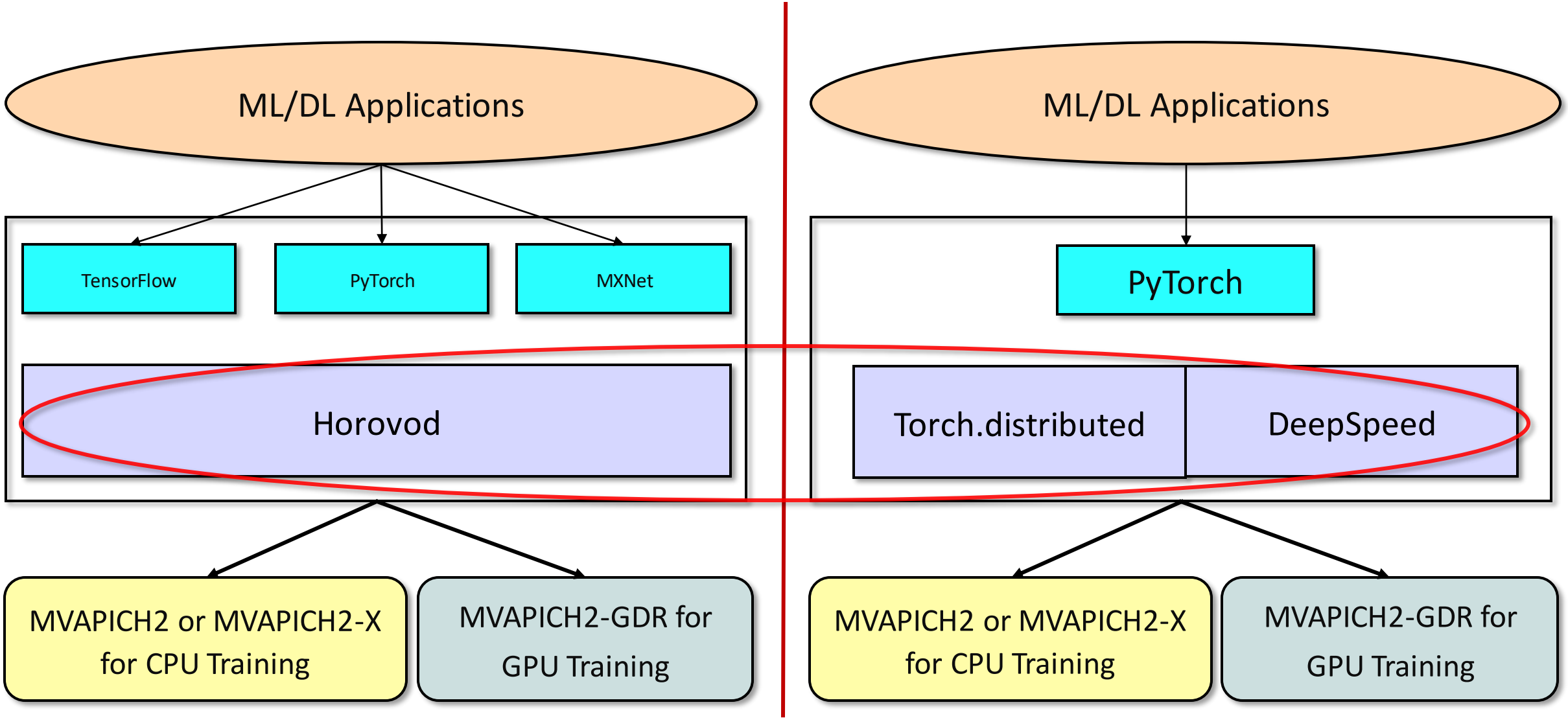


Data Parallelism and MPI Collectives

- Step1: Data Propagation
  - Distribute the Data among GPUs
- Step2: Forward Backward Pass
  - Perform forward pass and calculate the prediction
  - Calculate Error by comparing prediction with actual output
  - Perform backward pass and calculate gradients
- Step3: Gradient Aggregation
  - Call MPI_Allreduce to reduce the local gradients
  - Update parameters locally using global gradients



MVAPICH2 (MPI)-driven Infrastructure for ML/DL Training



More details available from: http://hidl.cse.ohio-state.edu

MVAPICH2 2.3.6

- **Released on 05/11/2021**
- Major Features and Enhancements
  - Support collective offload using Mellanox's SHARP for Reduce and Bcast
    - Enhanced tuning framework for Reduce and Bcast using SHARP
  - Enhanced performance for UD-Hybrid code
  - Add multi-rail support for UD-Hybrid code
  - Enhanced performance for shared-memory collectives
  - Enhanced job-startup performance for flux job launcher
  - Add support in mpirun_rsh to use srun daemons to launch jobs
  - Add support in mpirun_rsh to specify processes per node using '-ppn' option
  - Use PMI2 by default when SLURM is selected as process manager
  - Add support to use aligned memory allocations for multi-threaded applications
  - Architecture detection and enhanced point-to-point tuning for Oracle BM.HPC2 cloud shape
  - Enhanced collective tuning for Frontera@TACC and Expanse@SDSC
  - Add support for GCC compiler v11
  - Add support for Intel IFX compiler
  - Update hwloc v1 code to v1.11.14 & hwloc v2 code to v2.4.2

MVAPICH2-GDR 2.3.6

- Released on 08/12/2021
- Major Features and Enhancements
  - Based on MVAPICH2 2.3.6
  - Added support for 'on-the-fly' compression of point-to-point messages used for GPU-to-GPU communication
    - Applicable to NVIDIA GPUs
  - Added NCCL communication substrate for various MPI collectives
    - Support for hybrid communication protocols using NCCL-based, CUDA-based, and IB verbs-based primitives
    - MPI_Allreduce, MPI_Reduce, MPI_Allgather, MPI_Allgatherv, MPI_Alltoall, MPI_Alltoallv, MPI_Scatter, MPI_Scatterv, MPI_Gather, MPI_Gatherv, and MPI_Bcast
  - Full support for NVIDIA DGX, NVIDIA DGX-2 V-100, and NVIDIA DGX-2 A-100 systems
    - Enhanced architecture detection, process placement and HCA selection
    - Enhanced intra-node and inter-node point-to-point tuning
    - Enhanced collective tuning
  - Introduced architecture detection, point-to-point tuning and collective tuning for ThetaGPU @ANL
  - Enhanced point-to-point and collective tuning for NVIDIA GPUs on Frontera @TACC, Lassen @LLNL, and Sierra @LLNL
  - Enhanced point-to-point and collective tuning for Mi50 and Mi60 AMD GPUs on Corona @LLNL
  - Added several new MPI_T PVARs
  - Added support for CUDA 11.3
  - Added support for ROCm 4.1
  - Enhanced output for runtime variable MV2_SHOW_ENV_INFO
  - Tested with Horovod and common DL Frameworks
    - TensorFlow, PyTorch, and MXNet
  - Tested with MPI4Dask 0.2
    - MPI4Dask is a custom Dask Distributed package with MPI support
  - Tested with MPI4cuML 0.1
    - MPI4cuML is a custom cuML package with MPI support

Install Horovod with MVAPICH2-X and MVAPICH2-GDR

Command to install Horovod with MVAPICH2-X

```
$ HOROVOD_WITH_MPI=1 pip install --no-cache-dir horovod==0.22.1
```

Command to install Horovod with MVAPICH2-GDR

```
$ HOROVOD_GPU_ALLREDUCE=MPI HOROVOD_CUDA_HOME=/opt/cuda/10.1 HOROVOD_WITH_MPI=1 pip
install --no-cache-dir horovod
```

Run PyTorch on a single GPU

+ python pytorch_synthetic_benchmark.py --batch-size 64 --num-iters=5

.

.

V100

```
Model: resnet50
Batch size: 64
Number of GPUs: 1
Running warmup...
Running benchmark...
Iter #0: 333.9 img/sec per GPU
Iter #1: 334.2 img/sec per GPU
Iter #2: 333.9 img/sec per GPU
Iter #3: 333.8 img/sec per GPU
Iter #4: 333.9 img/sec per GPU
Img/sec per GPU: 334.0 +-0.2
----------------------------------------
Total img/sec on 1 GPU(s): 334.0 +-0.2
----------------------------------------
```

Run PyTorch on two nodes with 1 GPU/node (using MVAPICH2-GDR)

+ mpirun_rsh -np 2 gpu11 gpu12 MV2_USE_CUDA=1 MV2_CPU_BINDING_POLICY=hybrid MV2_HYBRID_BINDING_POLICY=spread MV2_USE_RDMA_CM=0 MV2_GPUDIRECT_GDRCOPY_LIB=/opt/gdrcopy2.0/lib64/libgdrapi.so LD_PRELOAD=mv2-gdr/lib/libmpi.so python pytorch_synthetic_benchmark.py --batch-size 64 --num-iters=5

.

.

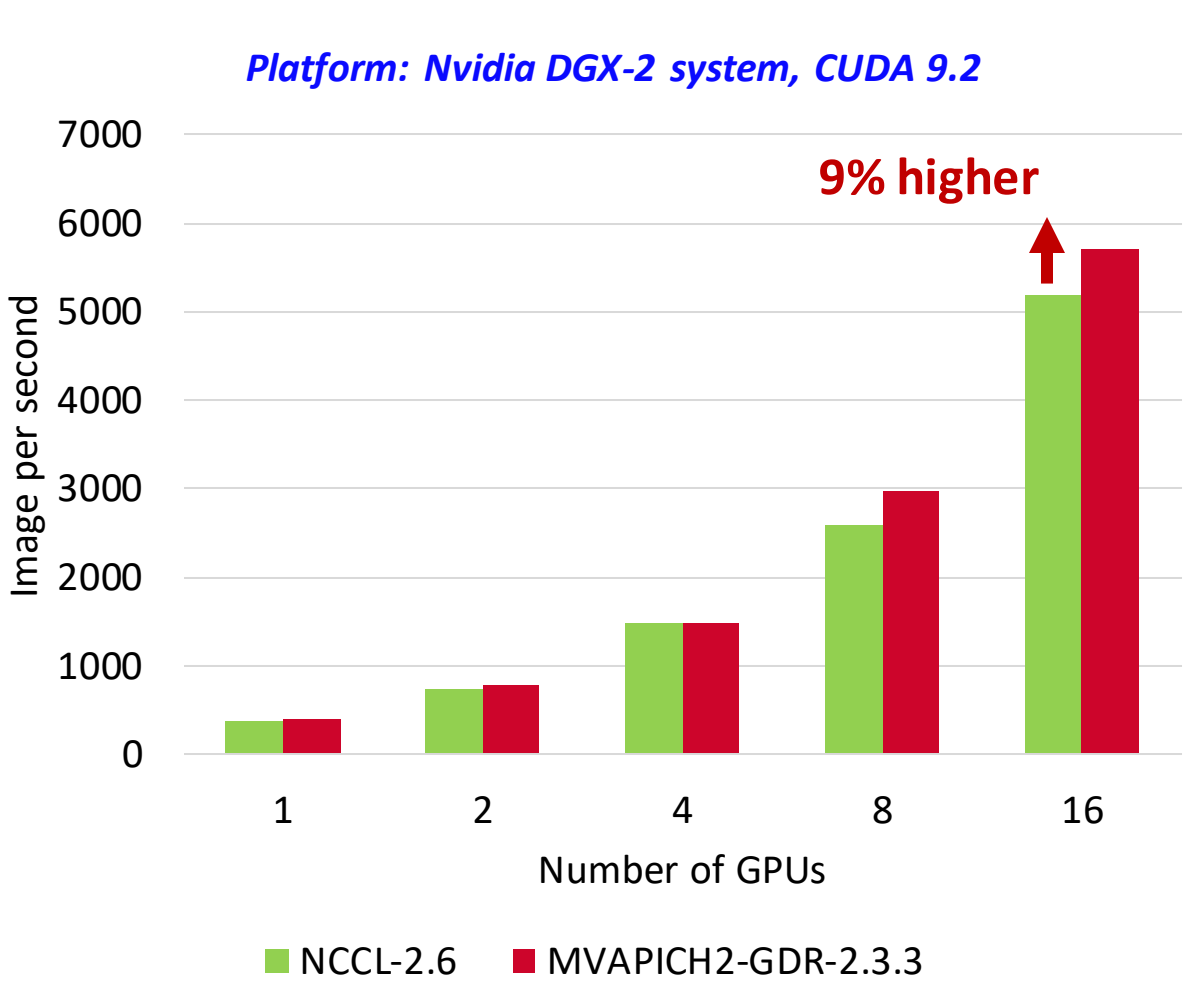
V100

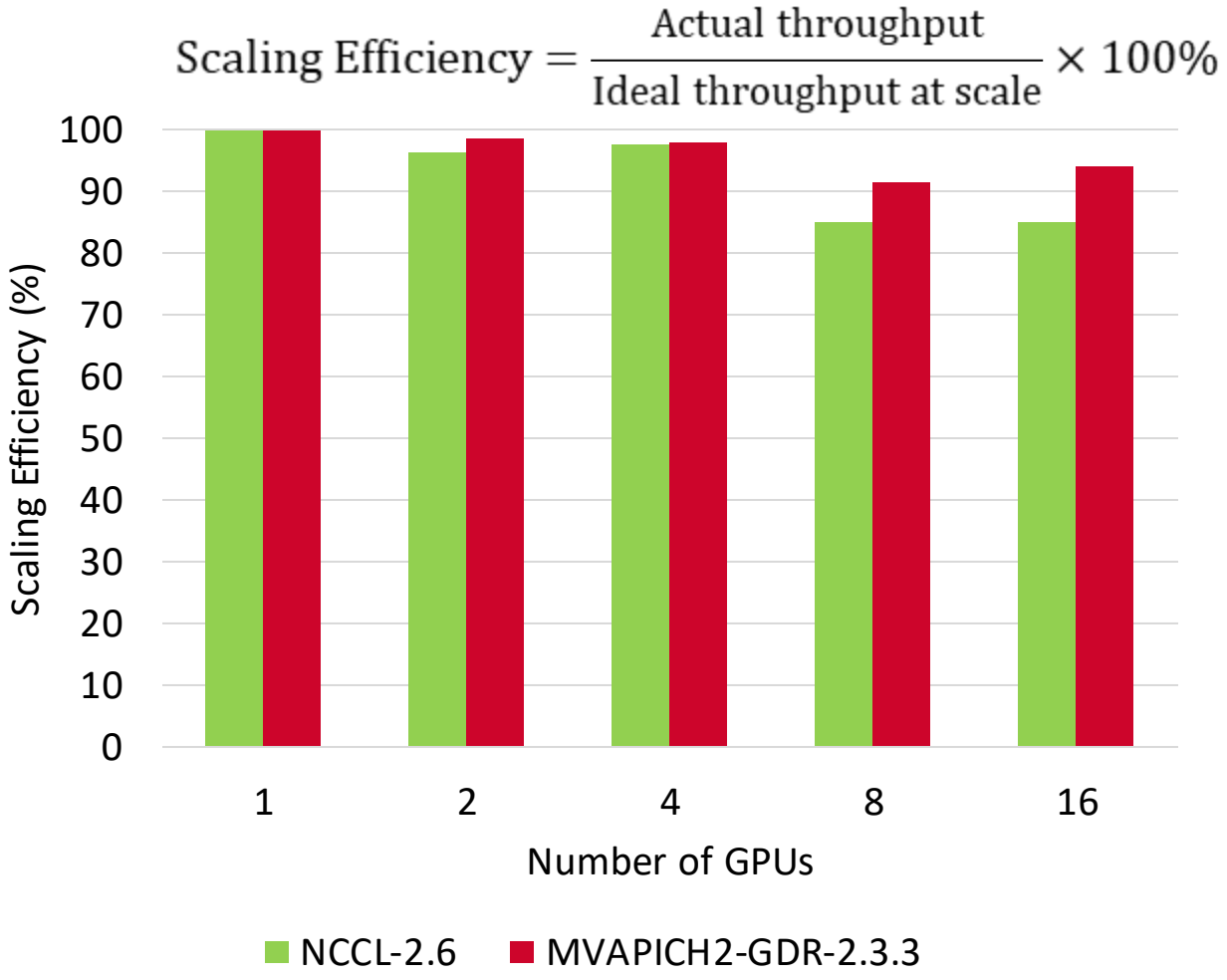
```
Model: resnet50
Batch size: 64
Number of GPUs: 2
Running warmup...
Running benchmark...
Iter #0: 317.0 img/sec per GPU
Iter #1: 314.9 img/sec per GPU
Iter #2: 315.4 img/sec per GPU
Iter #3: 318.0 img/sec per GPU
Iter #4: 316.7 img/sec per GPU
Img/sec per GPU: 316.4 +-2.2
-----------------------------------------
Total img/sec on 2 GPU(s): 632.8 +-4.3
-----------------------------------------
```

~1.89X on 2 GPUs

Scalable TensorFlow using Horovod and MVAPICH2-GDR

- **ResNet-50 Training using TensorFlow benchmark on 1 DGX-2 node (16 Volta GPUs)**

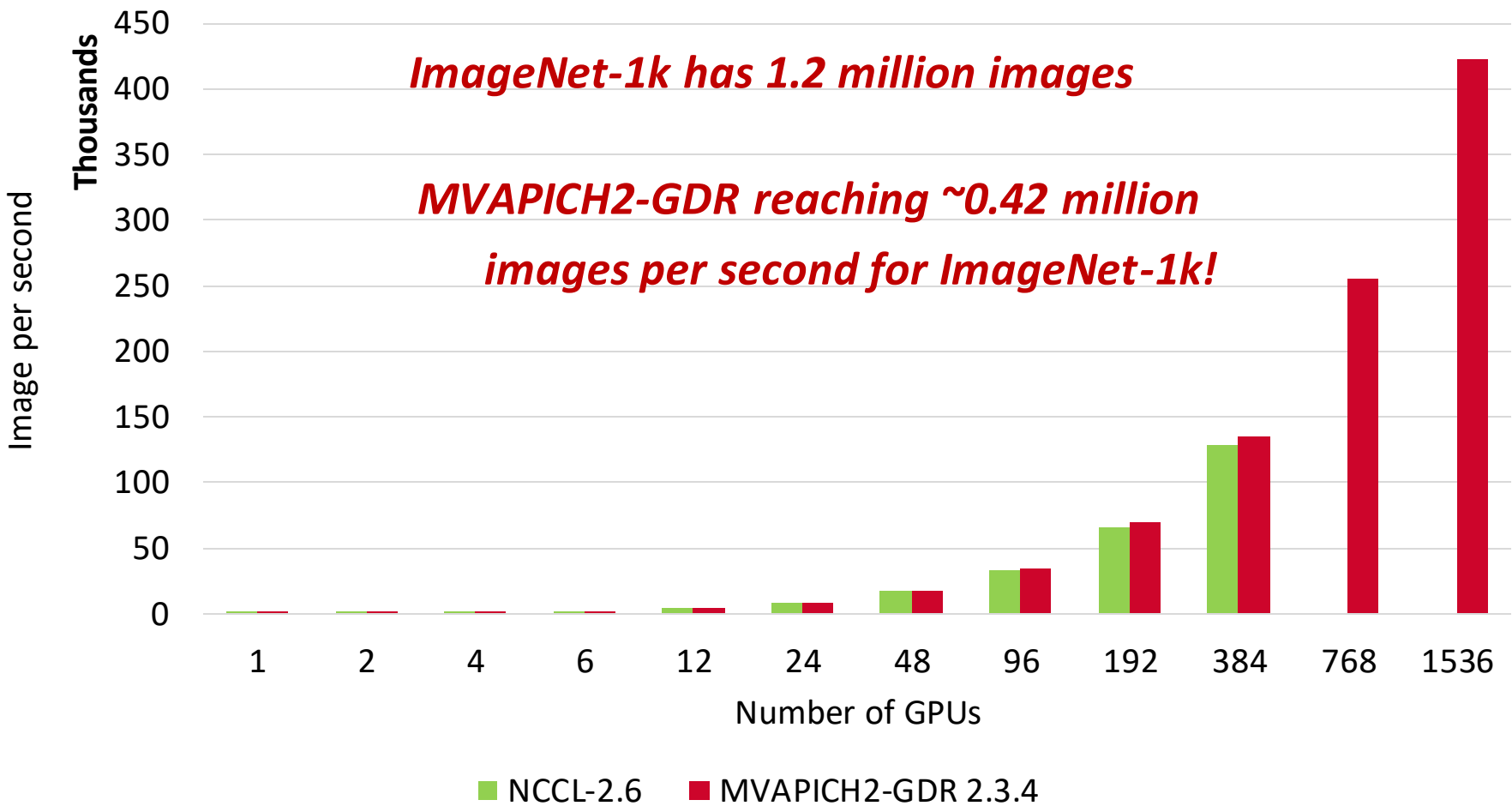




C.-H. Chu, P. Kousha, A. Awan, K. S. Khorassani, H. Subramoni and D. K. Panda, "NV-Group: Link-Efficient Reductions for Distributed Deep Learning on Modern Dense GPU Systems, " ICS-2020.

Distributed TensorFlow on ORNL Summit (1,536 GPUs)

- ResNet-50 Training using TensorFlow benchmark on SUMMIT -- 1536 Volta GPUs!
- 1,281,167 (1.2 mil.) images
- Time/epoch = 3 seconds
- Total Time (90 epochs) = 3 x 90 = 270 seconds = **4.5 minutes!**

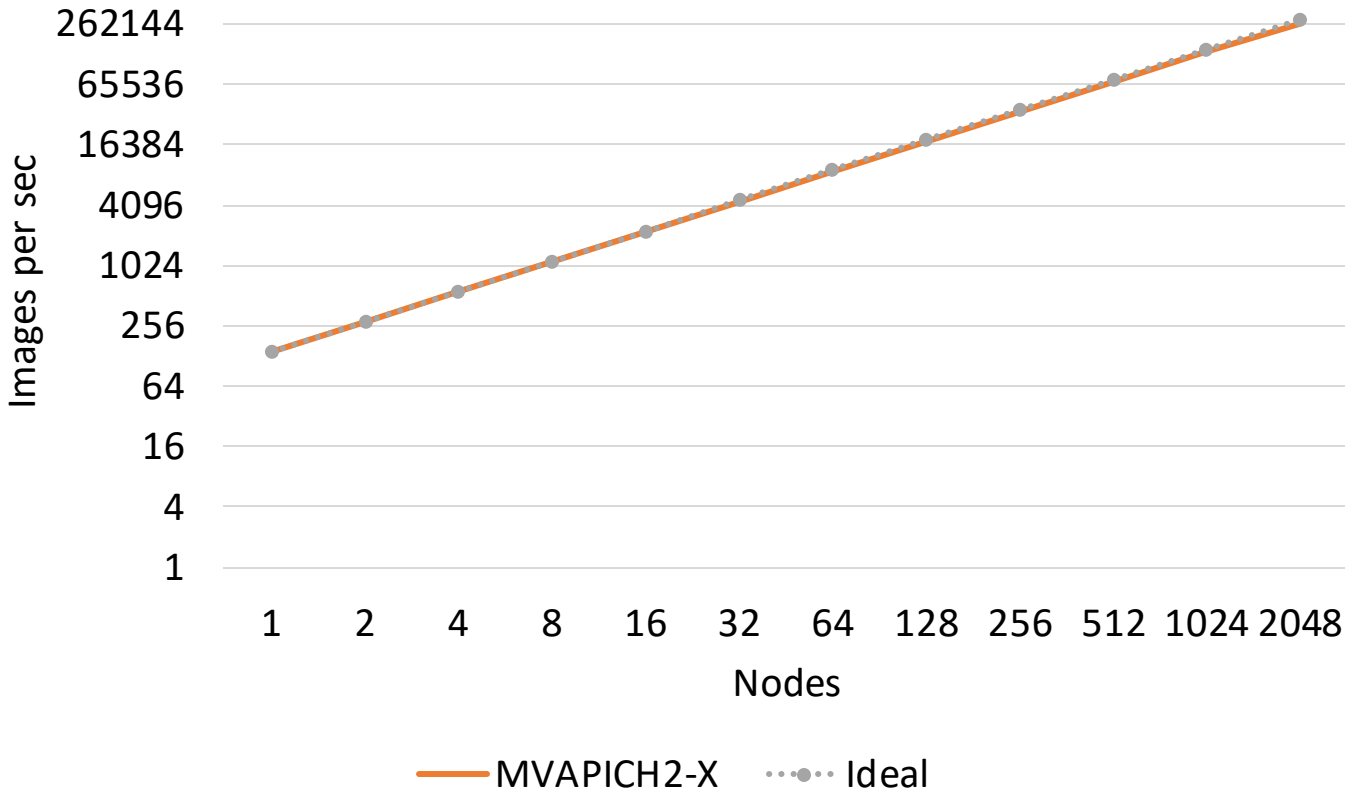


*We observed issues for NCCL2 beyond 384 GPUs

Platform: The Summit Supercomputer (#2 on Top500.org) – 6 NVIDIA Volta GPUs per node connected with NVLink, CUDA 10.1

Distributed TensorFlow on TACC Frontera (2048 CPU nodes)

- Scaled TensorFlow to 2048 nodes on Frontera using MVAPICH2 and IntelMPI
- MVAPICH2 and IntelMPI give similar performance for DNN training
- Report a peak of 260,000 images/sec on 2048 nodes
- On 2048 nodes, ResNet-50 can be trained in 7 minutes!



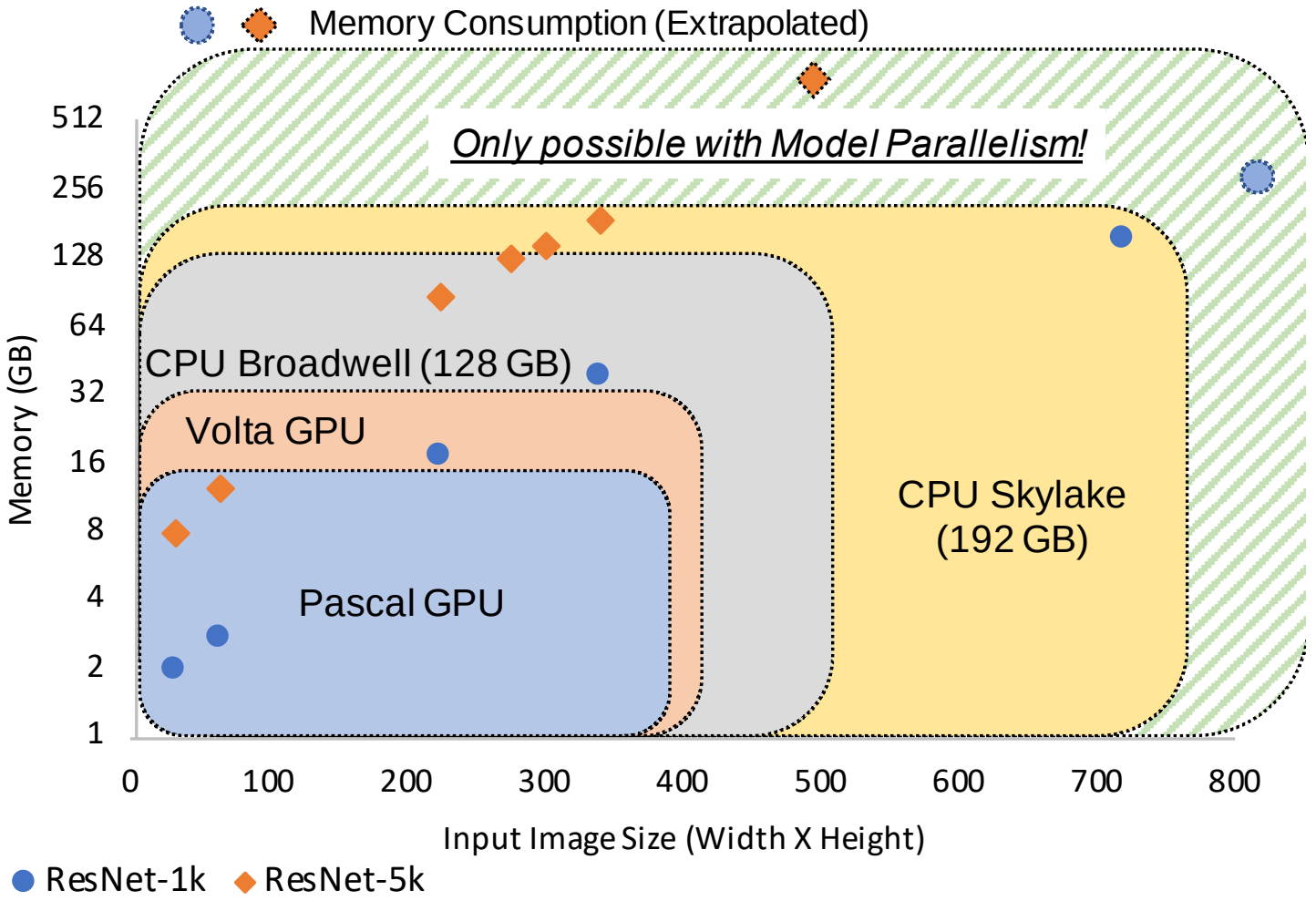
A. Jain, A. A. Awan, H. Subramoni, DK Panda, "Scaling TensorFlow, PyTorch, and MXNet using MVAPICH2 for High-Performance Deep Learning on Frontera", DLS '19 (SC '19 Workshop).

Outline

- Introduction
- Deep Neural Network Training and Essential Concepts
- **Parallelization Strategies for Distributed DNN Training**
  - Data Parallelism
  - **Model and Hybrid Parallelism**
- Machine Learning
- Data Science using Dask
- Conclusion

HyPar-Flow: Hybrid Parallelism for TensorFlow

- Why Hybrid parallelism?
  - Data Parallel training has limits! →
- We propose HyPar-Flow
  - An easy to use Hybrid parallel training framework
    - Hybrid = Data + Model
  - Supports Keras models and exploits TF 2.0 Eager Execution
  - Exploits MPI for Point-to-point and Collectives

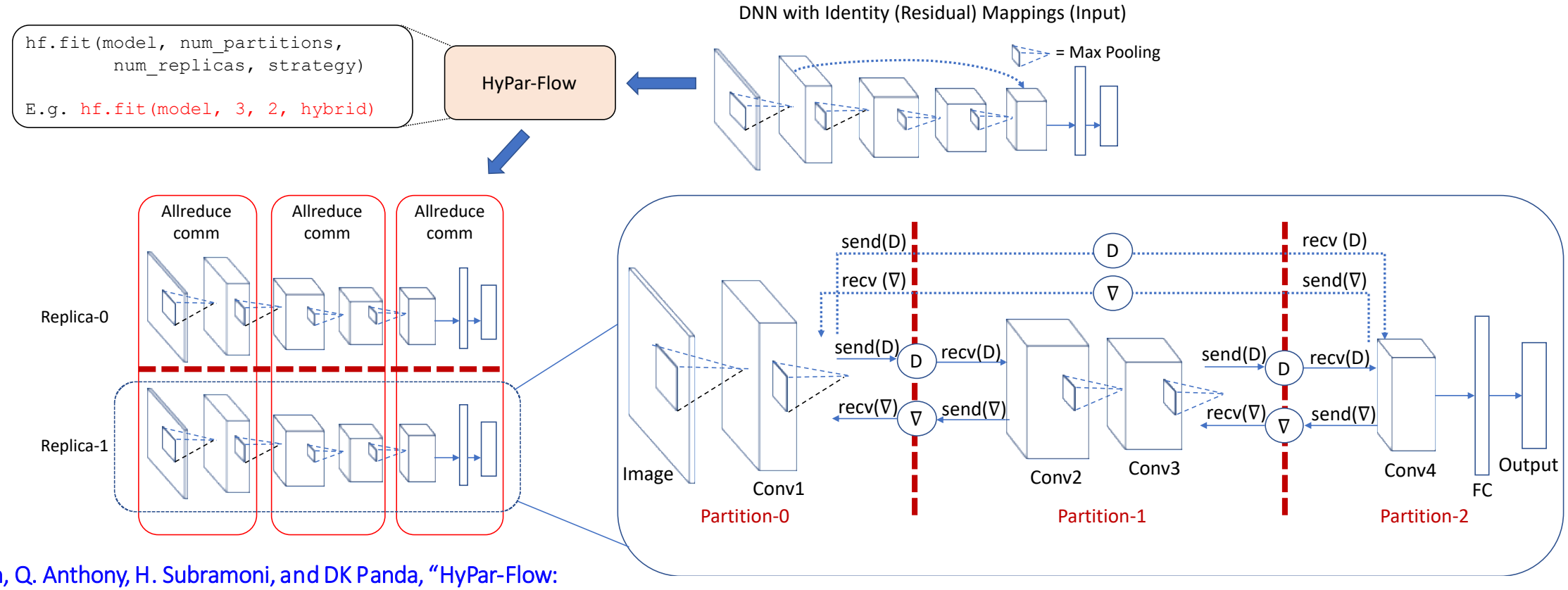


Benchmarking large-models lead to better insights and ability to develop new approaches!

A. A. Awan, A. Jain, Q. Anthony, H. Subramoni, and DK Panda, "HyPar-Flow: Exploiting MPI and Keras for Hybrid Parallel Training of TensorFlow models", ISC '20, https://arxiv.org/pdf/1911.05146.pdf

Model/Hybrid Parallelism and MPI Collectives

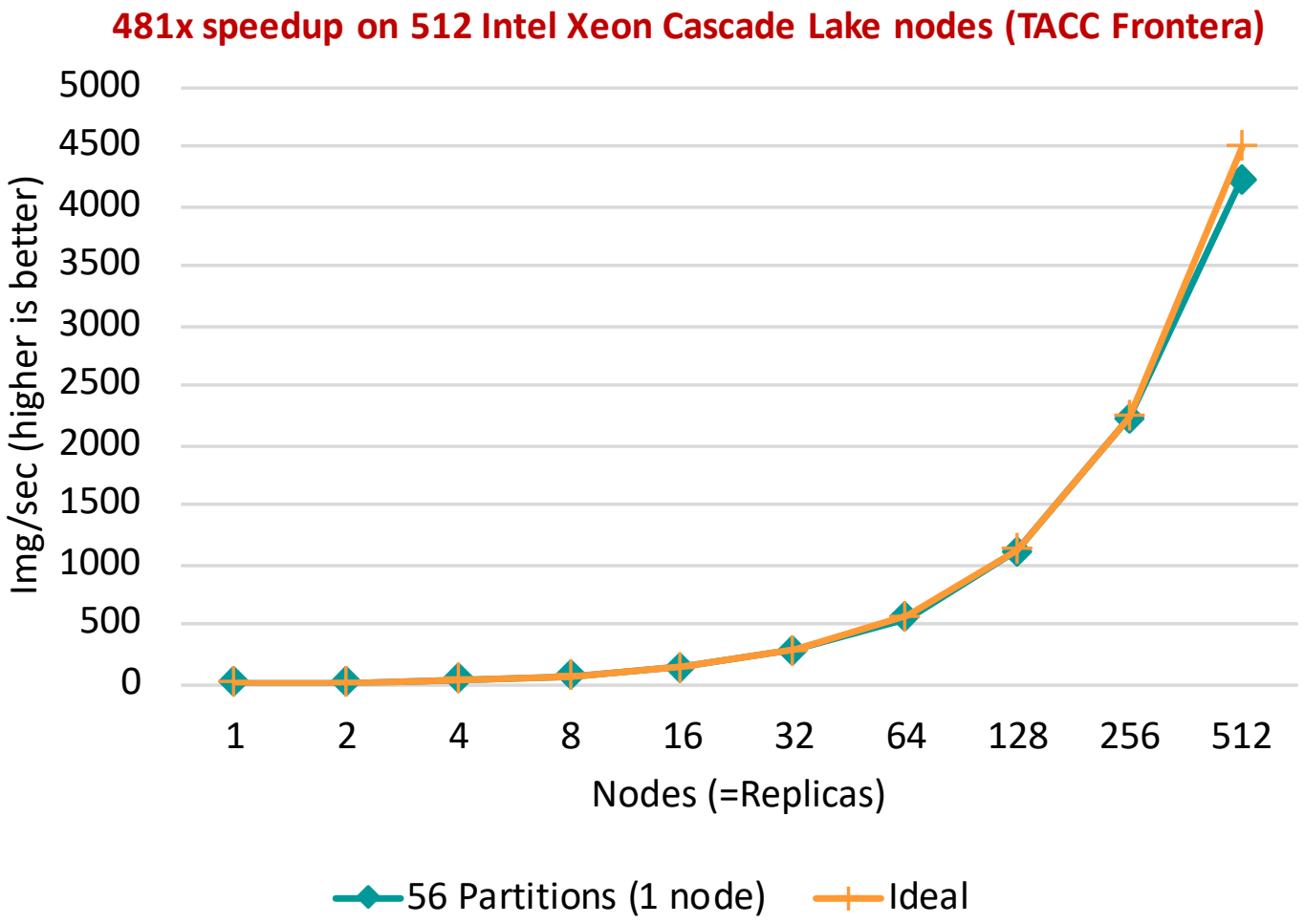
- HyPar-Flow is practical (easy-to-use) and high-performance (uses MPI)
  - Based on Keras models and exploits TF 2.0 Eager Execution
  - Leverages MPI Pt-to-pt. and Collectives for communication



A. A. Awan, A. Jain, Q. Anthony, H. Subramoni, and DK Panda, "HyPar-Flow: Exploiting MPI and Keras for Hybrid Parallel Training of TensorFlow models", ISC'20, https://arxiv.org/pdf/1911.05146.pdf

HyPar-Flow at Scale (512 nodes on TACC Frontera)

- ResNet-1001 with variable batch size
- Approach:
  - 48 model-partitions for 56 cores
  - 512 model-replicas for 512 nodes
  - Total cores: 48 x 512 = 24,576
- Speedup
  - **253X** on 256 nodes
  - **481X** on 512 nodes
- Scaling Efficiency
  - **98%** up to 256 nodes
  - **93.9%** for 512 nodes

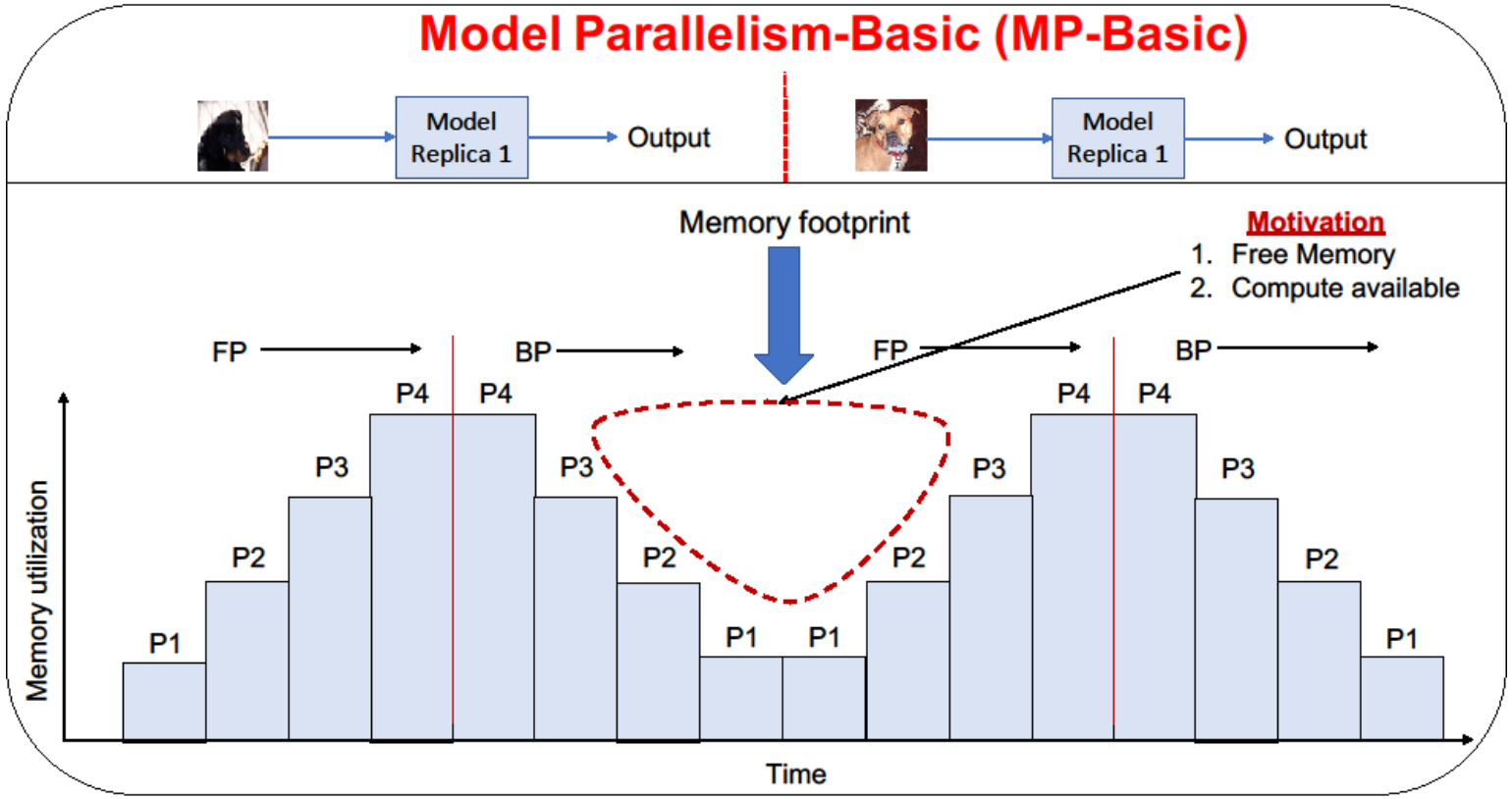


A. A. Awan, A. Jain, Q. Anthony, H. Subramoni, and DK Panda, "HyPar-Flow: Exploiting MPI and Keras for Hybrid Parallel Training of TensorFlow models", ISC '20, https://arxiv.org/pdf/1911.05146.pdf

GEMS: GPU Enabled Memory Aware Model Parallelism Systems

Why do we need Memory aware designs?

- Data and Model Parallel training has limitation!
- Maximum Batch Size depends on the memory.
- Basic Model Parallelism suffers from underutilization of memory and compute →

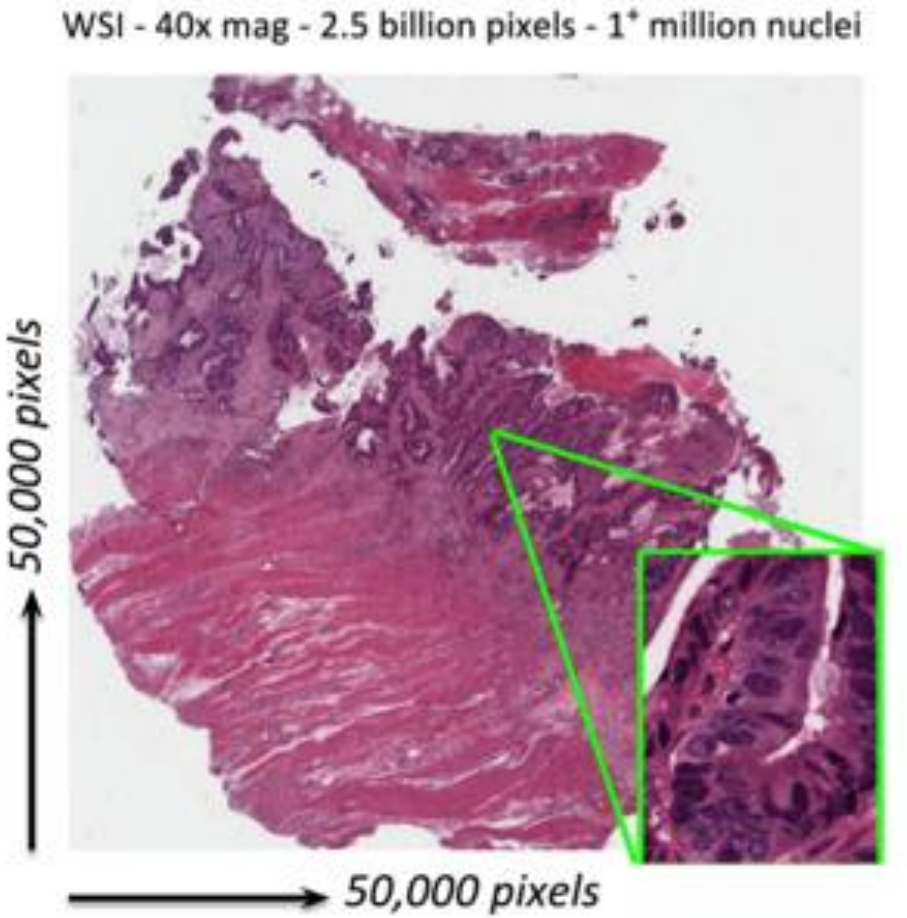


Memory requirement increases with the increase in image size!

A. Jain, A. Awan, A. Aljuhani, J. Hashmi, Q. Anthony, H. Subramoni, D. Panda, R. Machiraju, A. Parwani, "GEMS: GPU Enabled Memory Aware Model Parallelism System for Distributed DNN", SC'20.

Exploiting Model Parallelism in AI-Driven Digital Pathology

- Pathology whole slide image (WSI)
  - Each WSI = 100,000 x 100,000 pixels
  - Can not fit in a single GPU memory
  - Tiles are extracted to make training possible
- Two main problems with tiles
  - Restricted tile size because of GPU memory limitation
  - Smaller tiles loose structural information
- Can we use Model Parallelism to train on larger tiles to get better accuracy and diagnosis?
- Reduced training time significantly
  - **7.25 hours (1 node, 4 GPUs) -> 27 mins (32 nodes, 128 GPUs)**



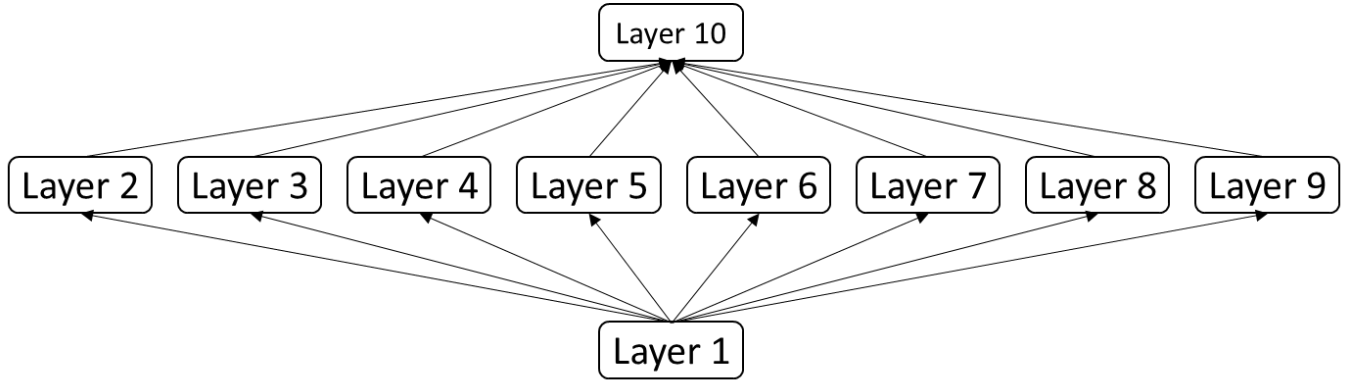
Courtesy: https://blog.kitware.com/digital-slide-archive-large-image-and-histomicstk-open-source-informatics-tools-for-management-visualization-and-analysis-of-digital-histopathology-data/

A. Jain, A. Awan, A. Aljuhani, J. Hashmi, Q. Anthony, H. Subramoni, D. Panda, R. Machiraju, A. Parwani, "GEMS: GPU Enabled Memory Aware Model Parallelism System for Distributed DNN", SC'20.

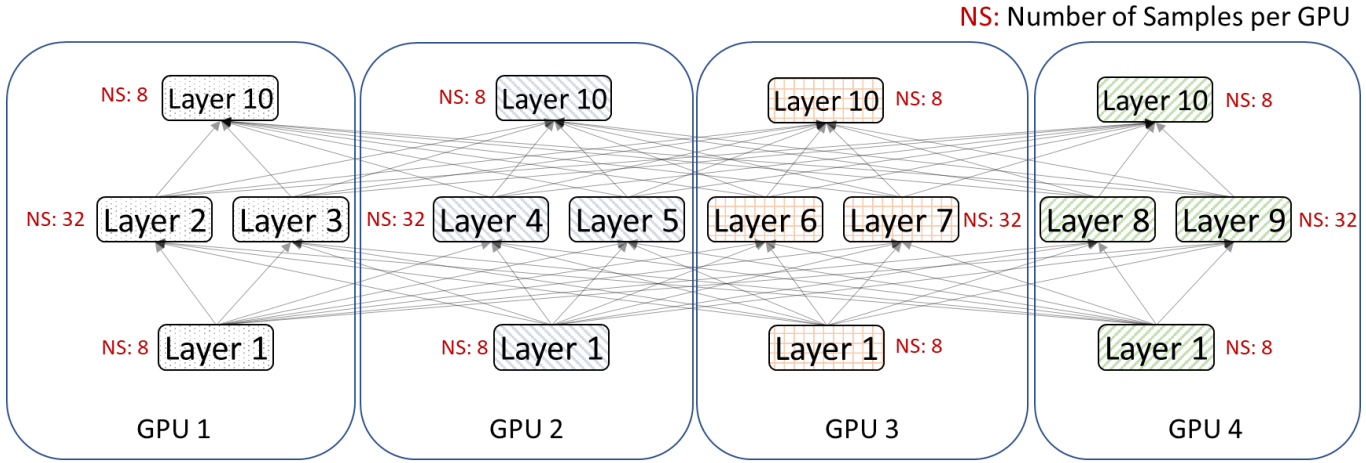
SUPER: SUb-Graph Parallelism for TransformERs

Sub-Graph Parallelism

- Exploits inherent parallelism in modern DNN architectures
- Improves the Performance of multi-branch DNN architectures →
- Can be used to accelerate the training of state-of-the-art Transformer models
- Provides better than Data-Parallelism for in-core models



Simple example of a multi-branch DNN architecture



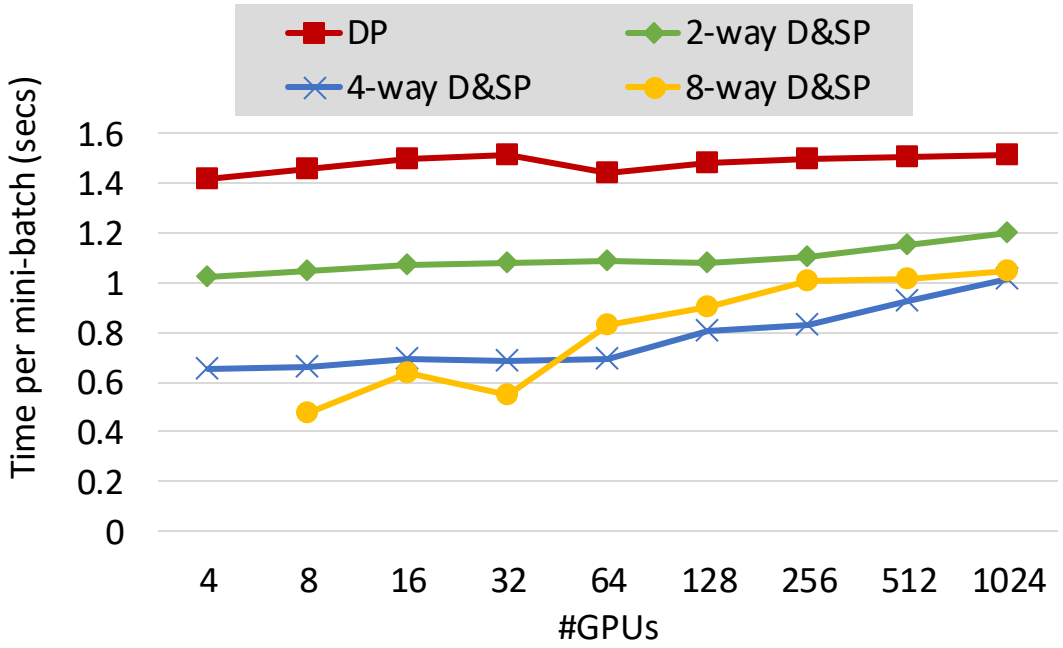
4-way Sub-Graph Parallelism combined with Data-Parallelism (D&SP)

A. Jain, T. moon, T. Benson, H. Subramoni, S. Jacobs, D. Panda, B. Essen, "SUPER: SUb-Graph Parallelism for TransformERs", IPDPS '21

Accelerating Transformers using SUPER

- We propose sub-graph parallelism integrated with data parallelism to accelerate the training of Transformers.
- Approach
  - Data and Sub-Graph Parallelism (D&SP)
    - #-way D&SP (#: number of sub-graphs)
- Setup
  - T5-Large-Mod on WMT Dataset
  - 1024 NVIDIA V100 GPUs
- Speedup
  - Up to **3.05X** over Data Parallelism (DP)

Up to 3.05X speedup over Data Parallel designs (LLNL Lassen)



A. Jain, T. moon, T. Benson, H. Subramoni, S. Jacobs, D. Panda, B. Essen, "SUPER: SUb-Graph Parallelism for TransformERs", IPDPS '21

Outline

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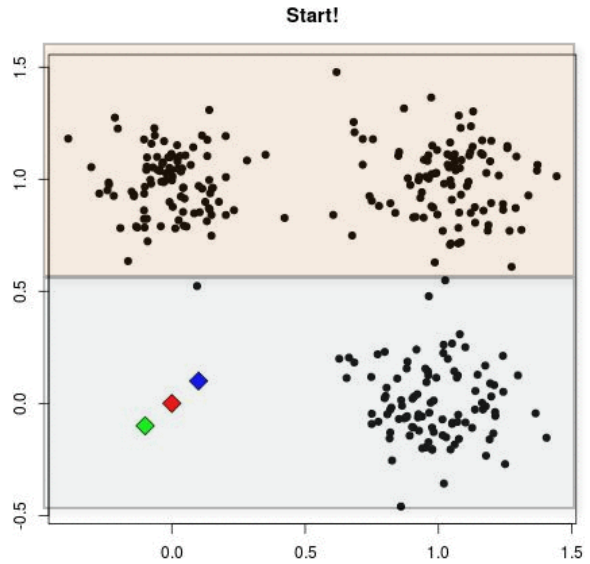
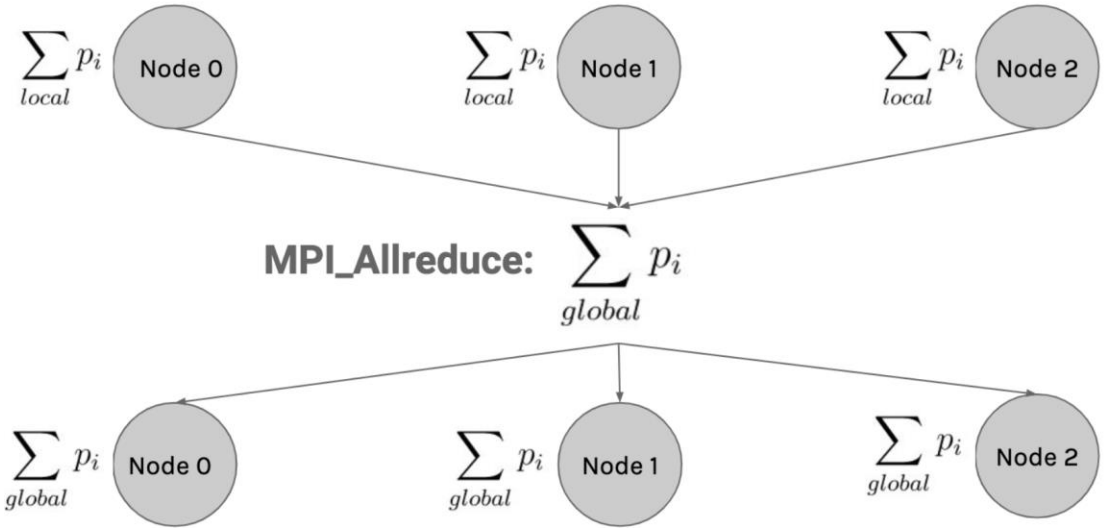
Parallelizing K-Means Clustering



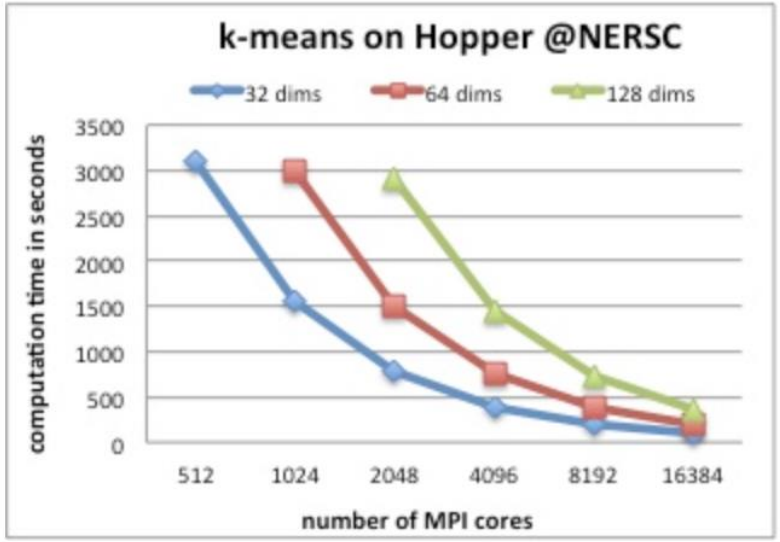
Proc 0

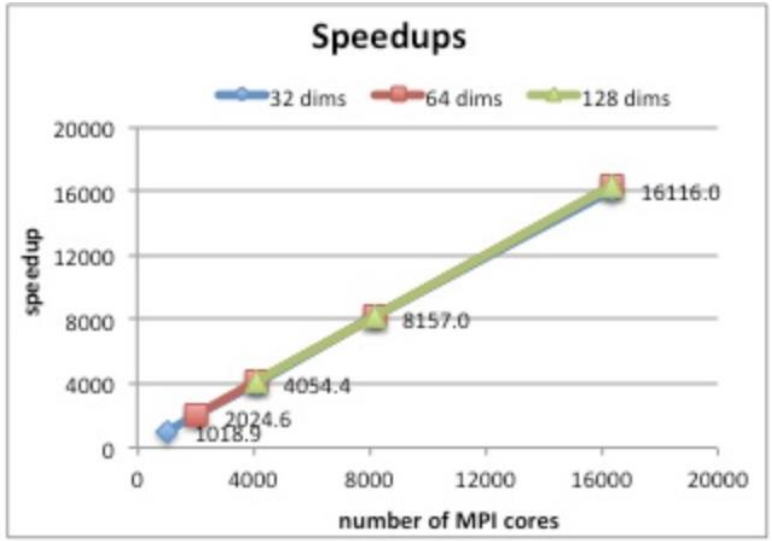
Proc 1

Domain Decomposition – Divide data objects amongst P processors



Recompute centroids after MPI_Allreduce





Courtesy: https://github.com/tmscarla/k-means-parallel http://users.eecs.northwestern.edu/~wkliao/Kmeans/

Support for Parallel and Distributed Execution

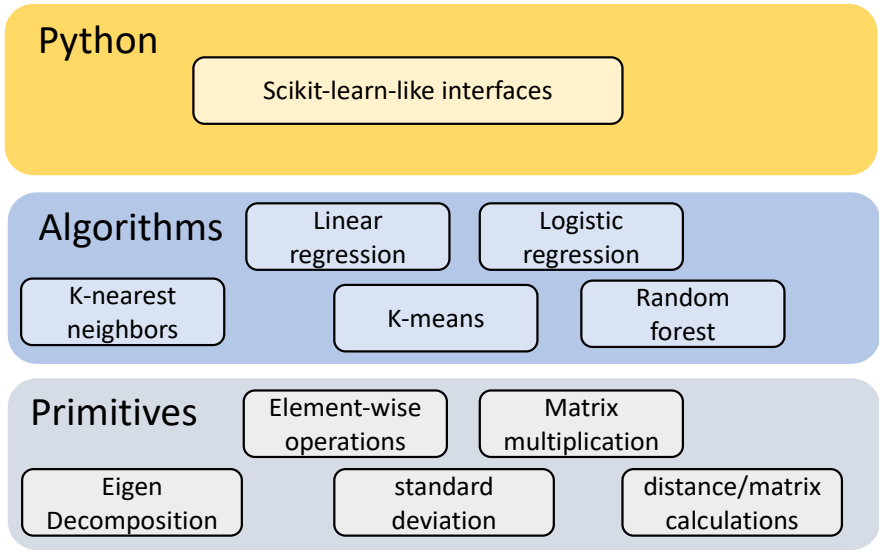
- Scikit-learn:
  - Supports execution via Joblib (https://joblib.readthedocs.io/en/latest/)
  - Joblib supports multi-threaded and multi-process execution (on multiple nodes)
- XGBoost:
  - Multiple ways to run on cluster of nodes:
    - Dask (http://dask.org)
    - Ray (https://ray.io/)
    - AWS YARN
    - Apache Spark (https://spark.apache.org/) using XGBoost4J-Spark
- cuML:
  - Execution is supported on multiple nodes using Dask (http://dask.org) and NVIDIA's NCCL

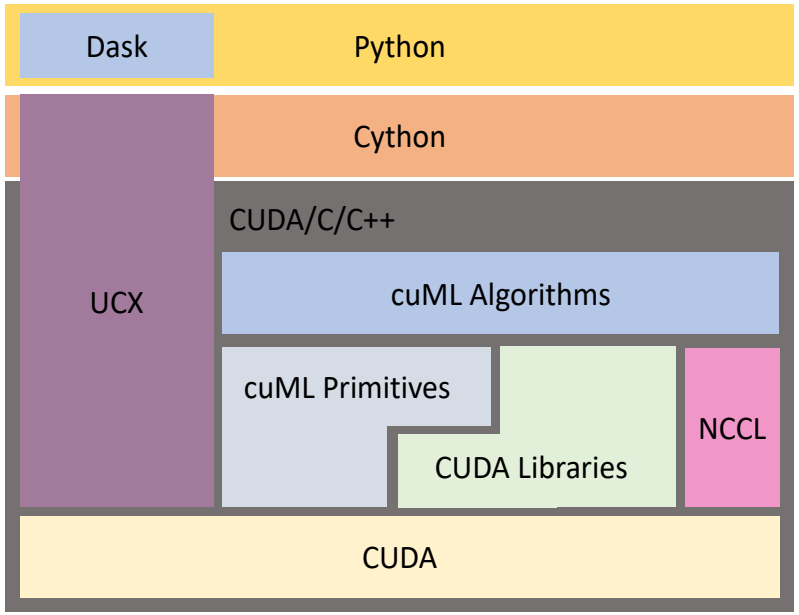
The cuML Library: Accelerating ML on GPUs

- The NVIDIA RAPIDS project aims to build end-to-end data science analytic pipelines on GPUs
- An important component is the cuML library:
  - GPU-accelerated ML library
  - GPU-counterpart of Scikit-learn
  - Supports the execution of ML workloads on Multi-Node Multi-GPUs (MNMG) systems
- Most existing ML libraries, including Scikit-learn and Apache Spark's MLlib, only support CPU execution of ML algorithms
  - Conventional wisdom has been that only DNNs are a good match for GPUs because of high computational requirements

Main components of the cuML library

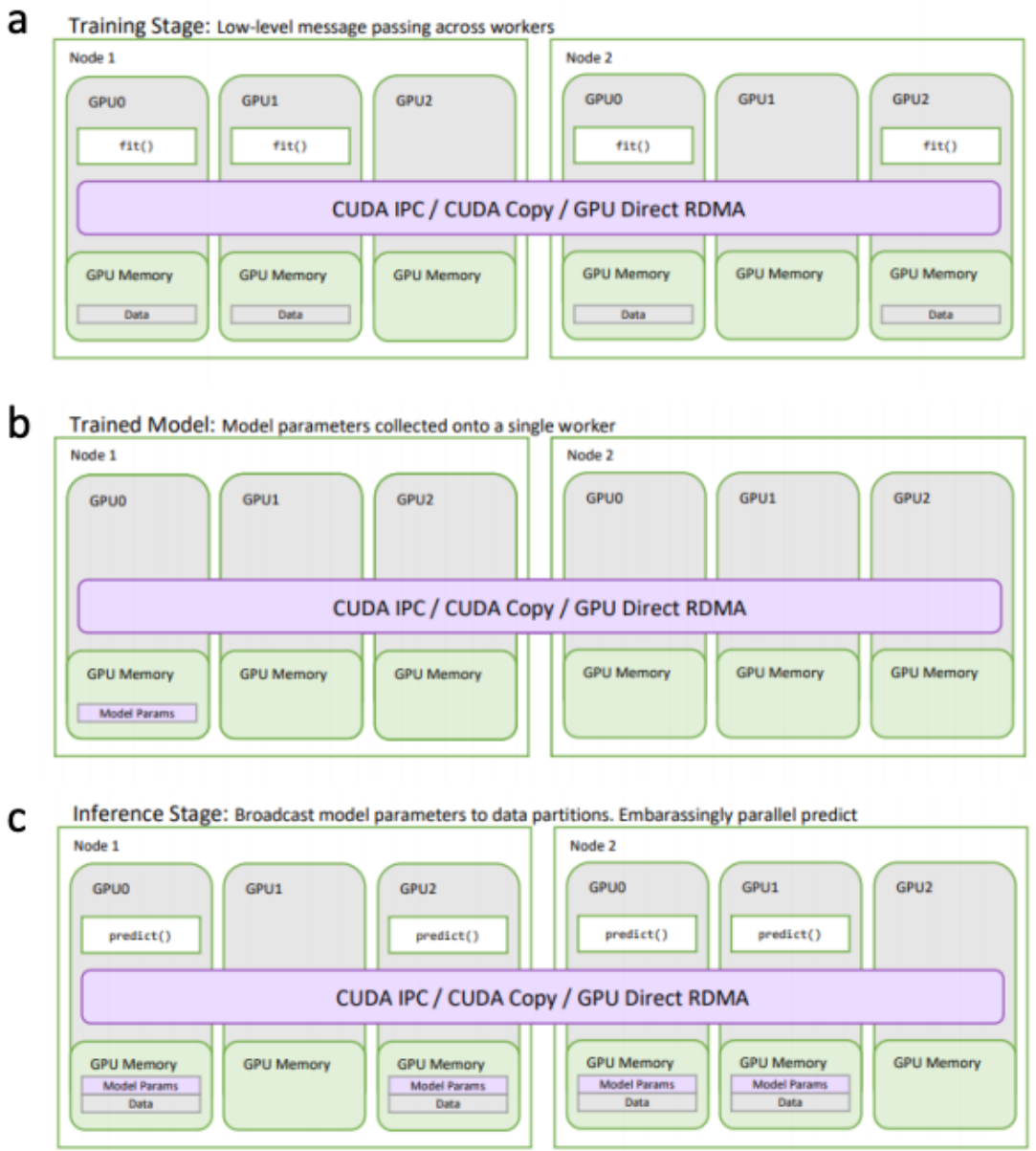
- Main components
  - Python layer
    - Provides a Scikit-learn like interface
    - Hides the complexities of the CUDA/C/C++ layer
  - Primitives and cuML algorithms built on top of CUDA
    - ML Algorithms
    - Primitives
      - Reusable building blocks for building machine learning algorithms
      - Common for different machine learning algorithms
      - Used to build different machine learning algorithms
  - Communication Support in cuML:
    - Point-to-point communication: Dask
    - Collective communication: NVIDIA Collective Communications Library (NCCL)





Parallel and Distributed Training in cuML

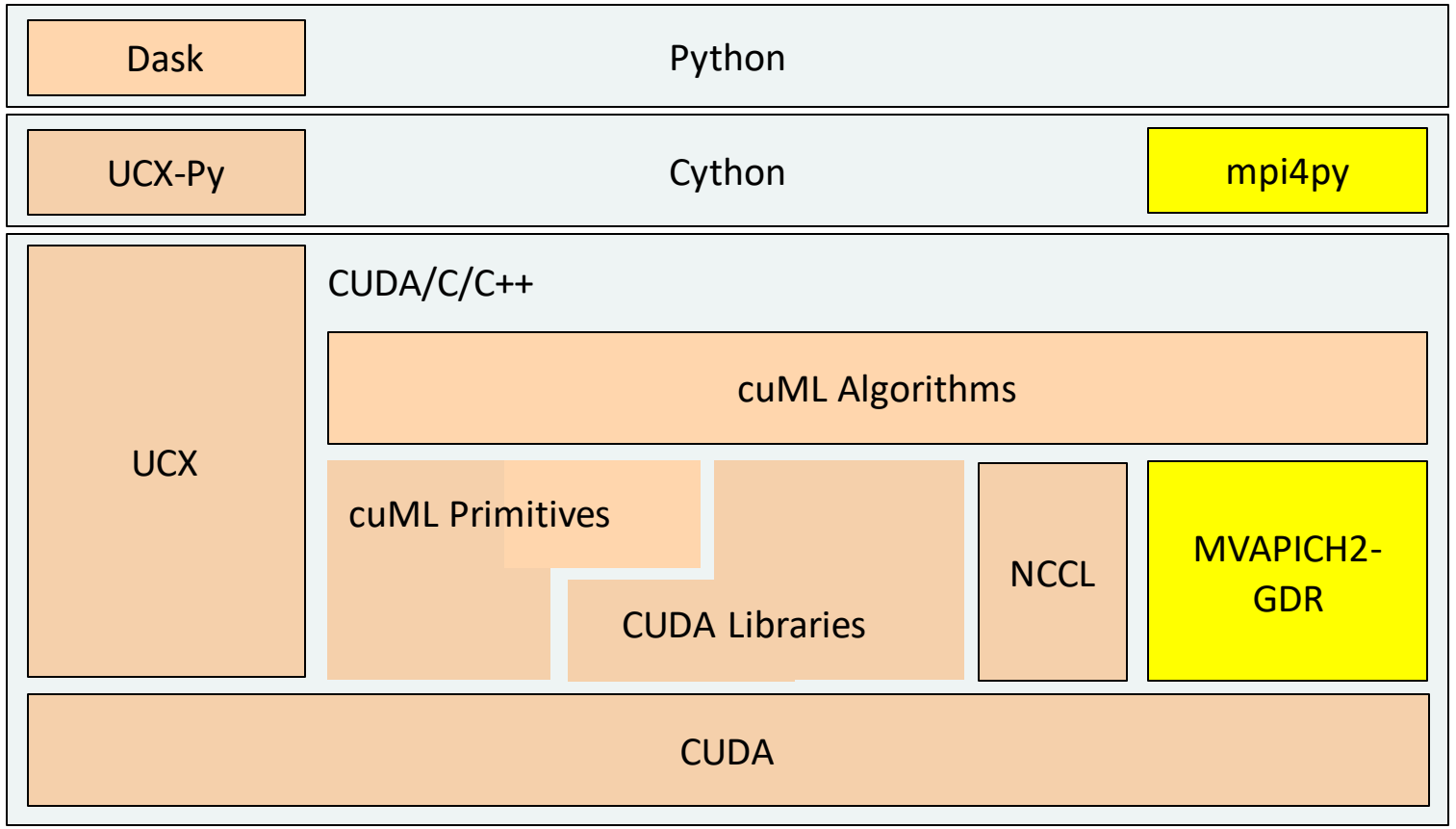
- Distributed training
  - Using data parallelism, the fit() function is executed on all workers containing a partition of the training dataset
- Trained Model:
  - The trained parameters are brought to a single worker using MPI_Reduce()
- Inference Stage:
  - The trained parameters are broadcasted to all workers with prediction partitions



Courtesy: https://arxiv.org/pdf/2002.04803.pdf

Accelerating cuML with MVAPICH2-GDR

- Utilize MVAPICH2-GDR (with mpi4py) as communication backend during the training phase (the fit() function) in the Multi-node Multi-GPU (MNMG) setting over cluster of GPUs
- Communication primitives:
  - Allreduce
  - Reduce
  - Broadcast
- Exploit optimized collectives



MPI4cuML Release

- MPI4cuML 0.1 was released in Feb ‘21 adding support for MPI to cuML:
  - Can be downloaded from: http://hidl.cse.ohio-state.edu
- Features:
  - Based on cuML 0.15
  - MVAPICH2 support for C++ and Python APIs
    - Included use of cuML C++ CUDA-Aware MPI example for KMeans clustering
    - Enabled cuML handles to use MVAPICH2-GDR backend for Python cuML applications
      - KMeans, PCA, tSVD, RF, LinearModels
    - Added switch between available communication backends (MVAPICH2 and NCCL)
  - Built on top of mpi4py over the MVAPICH2-GDR library
  - Tested with
    - Mellanox InfiniBand adapters (FDR and HDR)
    - Various x86-based multi-core platforms (AMD and Intel)
    - NVIDIA V100 and P100 GPUs

MPI4cuML Installation

- MPI4cuML is available to download from: http://hidl.cse.ohio-state.edu/
  - The userguide is available at: http://hidl.cse.ohio-state.edu/download/hidl/mpi4cuml/mpi4cuml-userguide.pdf

- Setup Instructions
  - Installation Pre-requisites:
    - Install the MVAPICH2-GDR Library
    - Install the mpi4py Library
  - Install MPI4cuML

- Running GPU-based cuML Applications
  - Writing the host file
  - KMeans on real and synthetic data

Setup Instructions: Pre-requisites

Install the MVAPICH2-GDR Library

Install the mpi4py Library

```
$ git clone https://github.com/mpi4py/mpi4py.git
$ cd mpi4py
$ edit mpi.cfg file
# MVAPICH2
# ------------
[MVAPICH2]
mpi_dir = /path/to/MVAPICH2-GDR/install/directory
mpicc = %(mpi_dir)s/bin/mpicc
mpicxx = %(mpi_dir)s/bin/mpicxx
include_dirs = %(mpi_dir)s/include
library_dirs = %(mpi_dir)s/lib64
runtime_library_dirs = %(library_dirs)s

$ python setup.py build --mpi=MVAPICH2-GDR
$ pip install .
```

Setup Instructions: Install MPI4cuML

Install MPI4cuML

```
$ wget http://hidl.cse.ohio-state.edu/download/hidl/cuml/mpi4cuml-0.1.tar.gz
$ tar -xzvf mpi4cuml-0.1.tar.gz
$ cd mpi4cuml-0.1/
$ conda env update -n mpi4cuml --file=conda/environments/cuml_dev_cuda10.2.yml
$ export LIBRARY_PATH=/path/to/miniconda3/envs/mpi4cuml/lib:$LIBRARY_PATH
$ export LD_LIBRARY_PATH=/path/to/miniconda3/envs/mpi4cuml/lib:$LIBRARY_PATH
$ ./build.sh cpp-mgtests

$ conda list
$ conda list | grep cuml
```

Build KMeans

```
$ cmake .. -DCUML_LIBRARY_DIR=/path/to/directory/with/libcuml.so
  -DCUML_INCLUDE_DIR=/path/to/directory/with/kmeans/kmeans_c.h
$ make
$  LD_PRELOAD=$MPILIB/lib64/libmpi.so:$CUML_HOME/cpp/build/libcuml++.so
```

Running MPI4cuML Applications

Writing the host file

```
$ cd mpi4cuml/cpp/examples/mg_kmeans
$ vim hosts
.. write name of the compute nodes ..
```

Run KMeans with synthetic data

```
$ MPILIB/bin/mpirun_rsh  -export-all  -np 4 -hostfile hosts MV2_USE_CUDA=1
  MV2_USE_GDRCOPY=1  MV2_GPUDIRECT_GDRCOPY_LIB=/opt/gdrcopy2.0/lib64/libgdrapi.so
  ./kmeans_mg_example
```

Run KMeans with real dataset

```
.. Download data from https://www.kaggle.com/c/homesite-quote-conversion/data ..
$ unzip all.zip
$ ./prepare_input.py  [train_file=train.csv]  [test_file=test.csv]  [output=output.txt]
$  LD_PRELOAD=$MV2_HOME/lib/libmpi.so:$CUML_HOME/cpp/build/libcuml++.so
$ MV2_HOME/bin/mpirun_rsh  --export-all  -np 4 -hostfile=hosts  MV2_USE_CUDA=1
  MV2_USE_GDRCOPY=1  MV2_GPUDIRECT_GDRCOPY_LIB=/opt/gdrcopy2.0/lib64/libgdrapi.so
  ./kmeans_mg_example  -num_rows  260753 -num_cols  298 -input output.txt
```

Run K-Means at C++ Layer on one node with 1 GPU/node (using MVAPICH2-GDR)

$ sbatch -N 1 run_cuml_kmeans_single.sh

+ time /opt/tutorials/dl-tutorial-21/mv2-gdr/bin/mpirun_rsh -np 1 gpu04 MV2_USE_CUDA=1 MV2_SUPPORT_DL=1 /opt/tutorials/dl-tutorial-21/cuML/mpi4cuml-0.1/cpp/examples/mg_kmeans/kmeans_mg_example -num_rows 260753 -num_cols 298 -input data.txt -k 100 -max_iterations=3000

Running on **1** GPU(s)

Reading input with 260753 rows and 298 columns from ../data.txt.

Run KMeans with k=100, **max_iterations=3000**

	num_pts	inertia
0	2466	1.096572e+11
1	2638	1.245608e+11
2	2739	1.362806e+11
3	2659	1.267454e+11
…		
98	2343	1.048909e+11
99	2687	1.310442e+11

Global inertia = 1.246384e+13

real 0m31.455s

user 0m0.019s

sys 0m0.008s

Run K-Means at C++ Layer on two nodes with 1 GPU/node (using MVAPICH2-GDR)

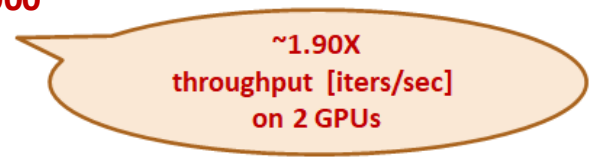
$ sbatch -N 1 run_cuml_kmeans_single.sh

+ time /opt/tutorials/dl-tutorial-21/mv2-gdr/bin/mpirun_rsh -np 2 gpu05 gpu04 MV2_USE_CUDA=1 MV2_SUPPORT_DL=1 /opt/tutorials/dl-tutorial-21/cuML/mpi4cuml-0.1/cpp/examples/mg_kmeans/kmeans_mg_example -num_rows 260753 -num_cols 298 -input data.txt -k 100 -max_iterations=3000

Running on **2** GPU(s)

Reading input with 260753 rows and 298 columns from ../data.txt.

Run KMeans with k=100, **max_iterations=6000**



	num_pts	inertia
0	2466	1.096572e+11
1	2638	1.245608e+11
2	2739	1.362806e+11
3	2659	1.267454e+11
…		
98	2343	1.048909e+11
99	2687	1.310442e+11

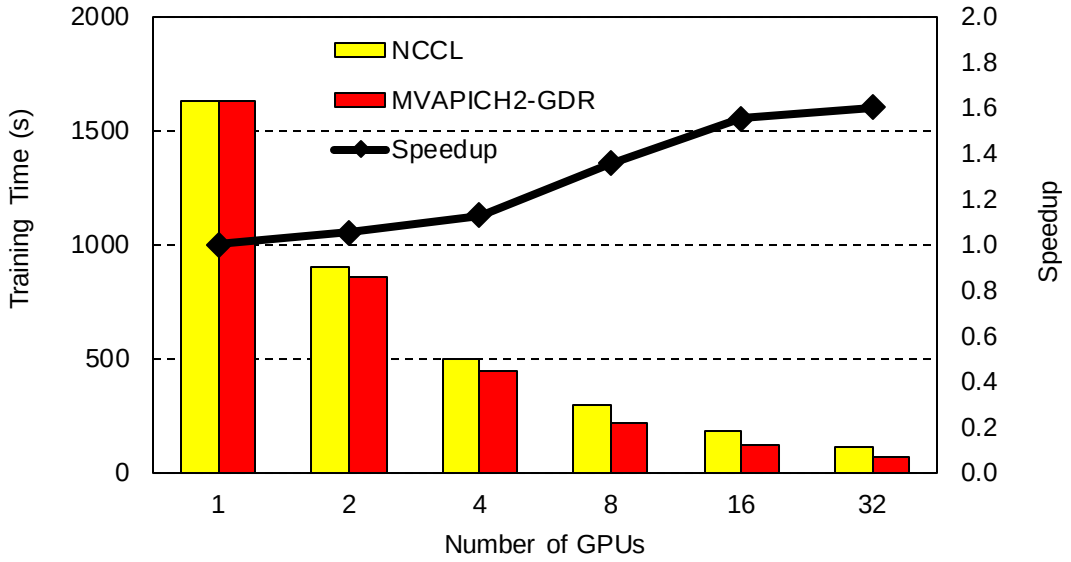
Global inertia = 1.246384e+13

real 0m33.078s

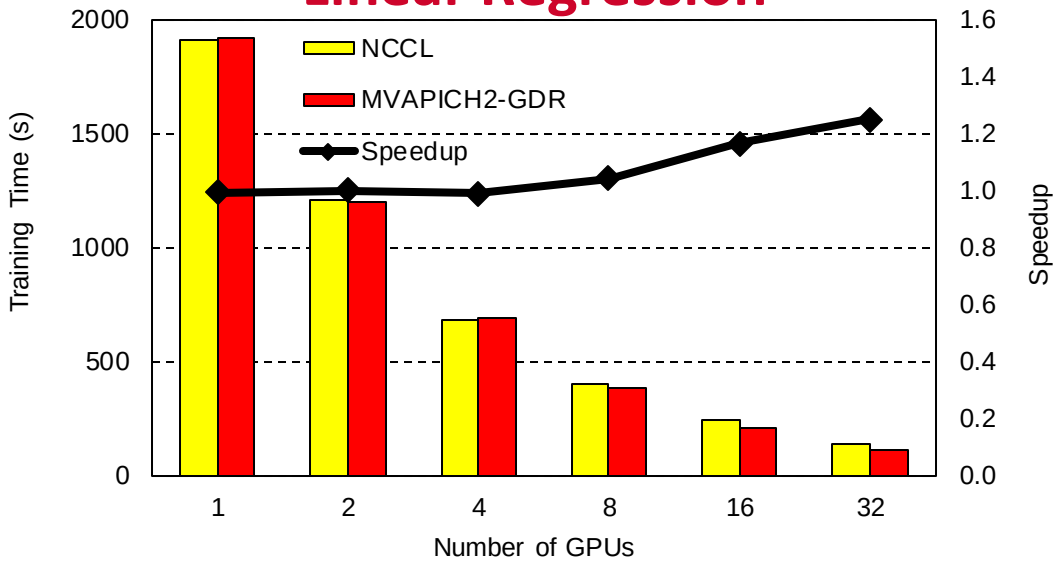
user 0m0.035s

sys 0m0.017s

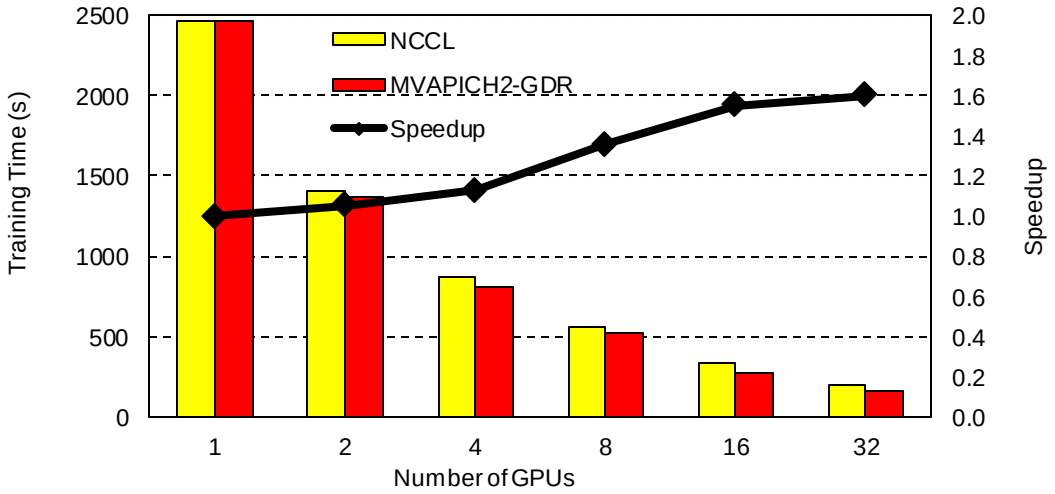
K-Means



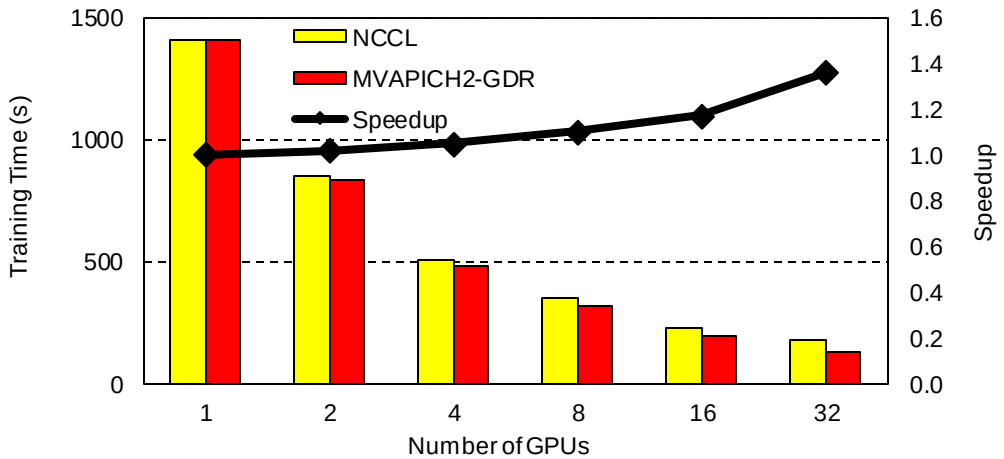
Linear Regression



Nearest Neighbors



Truncated SVD



M. Ghazimirsaeed , Q. Anthony , A. Shafi , H. Subramoni , and D. K. Panda, Accelerating GPU-based Machine Learning in Python using MPI Library: A Case Study with MVAPICH2-GDR, MLHPC Workshop, Nov 2020

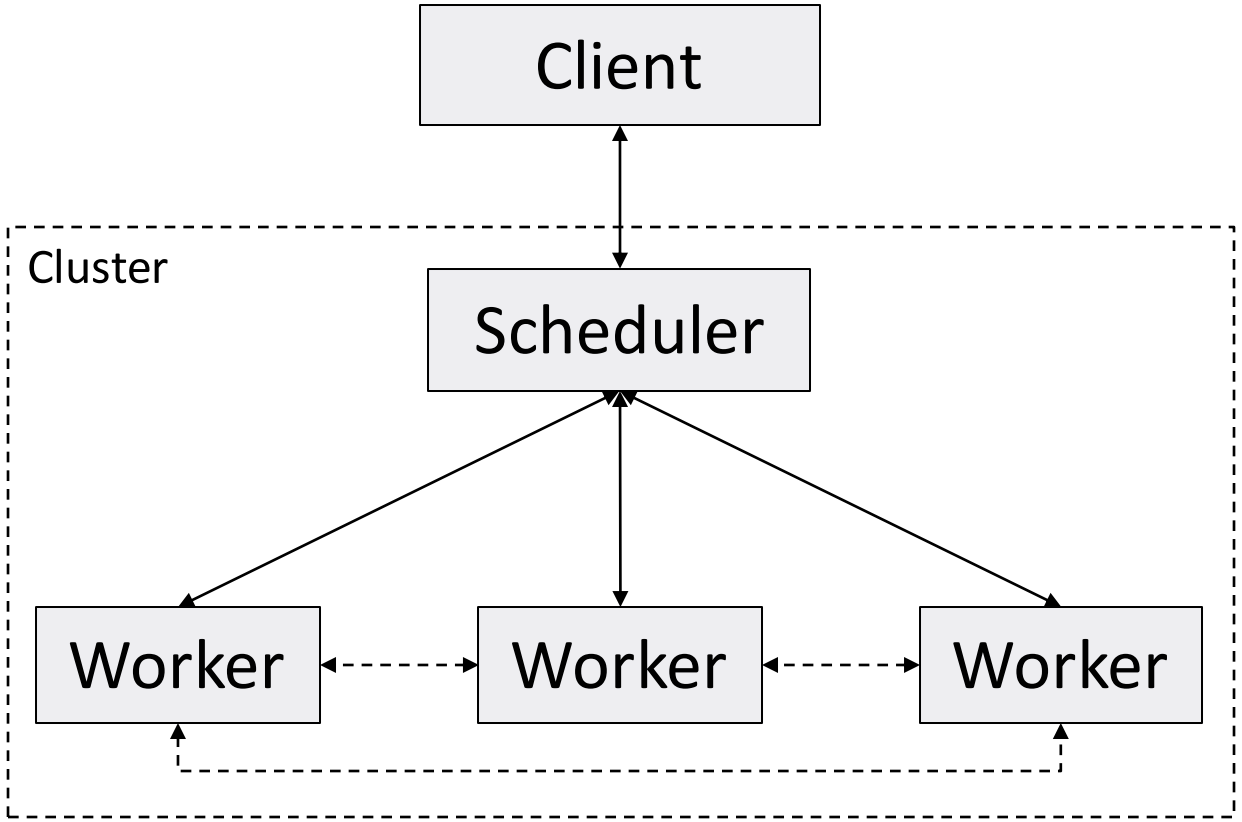
Outline

- Introduction
- Deep Neural Network Training and Essential Concepts
- Parallelization Strategies for Distributed DNN Training
- Machine Learning
- **Data Science using Dask**
- Conclusion

Introduction to Dask

- Dask is a popular task-based distributed computing framework:
  - Scales Python applications from laptops to high-end systems
  - Builds a task-graph that is executed lazily on parallel hardware
  - Natively extends popular data processing libraries like numPy, Pandas
- Dask Distributed library supports parallel and distributed execution:
  - Built using the asyncio package that allows execution of asynchronous/non-blocking/concurrent operations called *coroutines:*
    - These are defined using async and invoked using await
  - Dask Distributed library currently has two communication backends:
    - TCP: Tornado-based
    - UCX: Built using a Cython wrapper called UCX-Py
    - MPI4Dask: MVAPICH2-based MPI communication device
- Other Data Science frameworks include Apache Spark and Ray

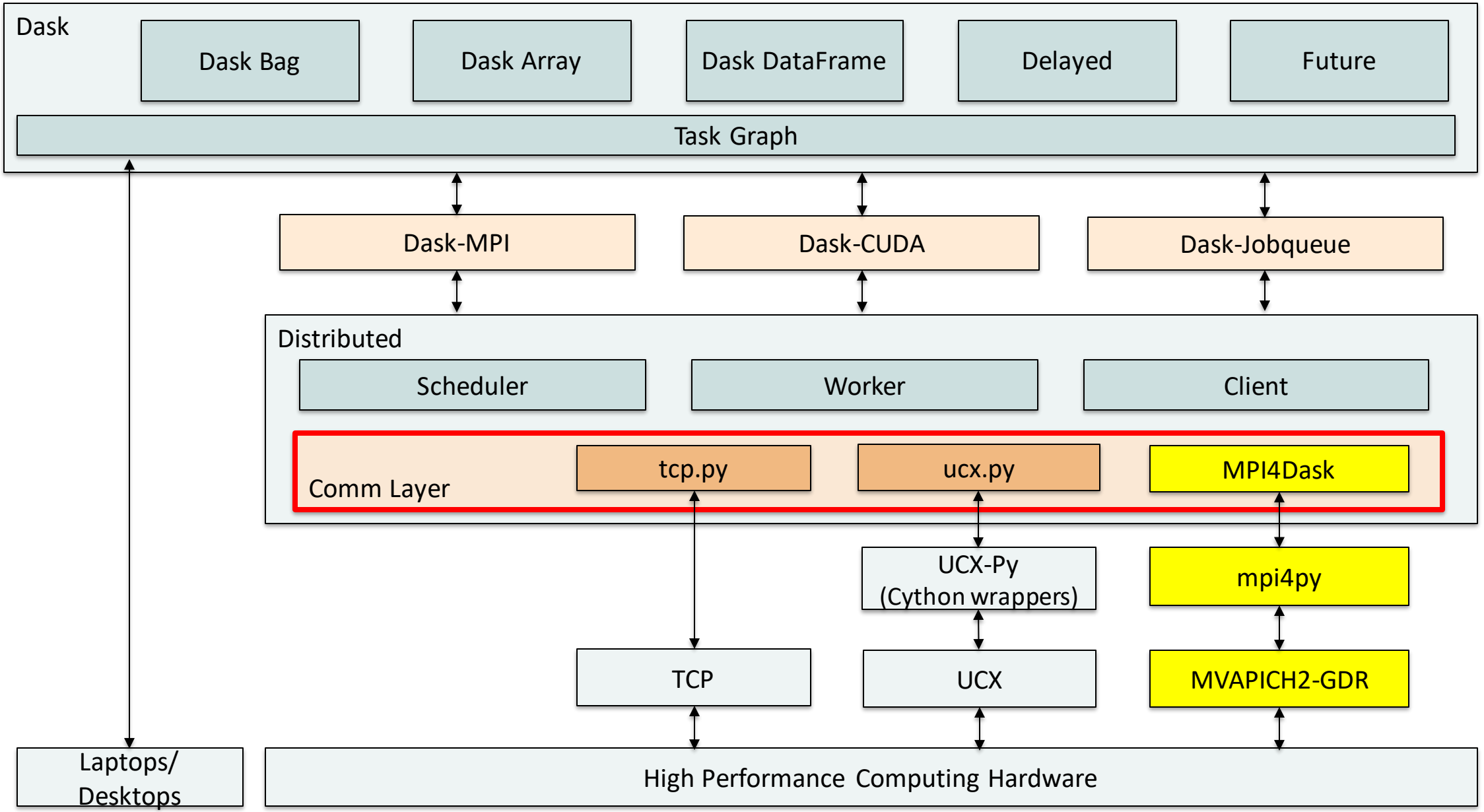
Dask Distributed Execution Model



MPI4Dask: MPI-based Communication Backend for Dask

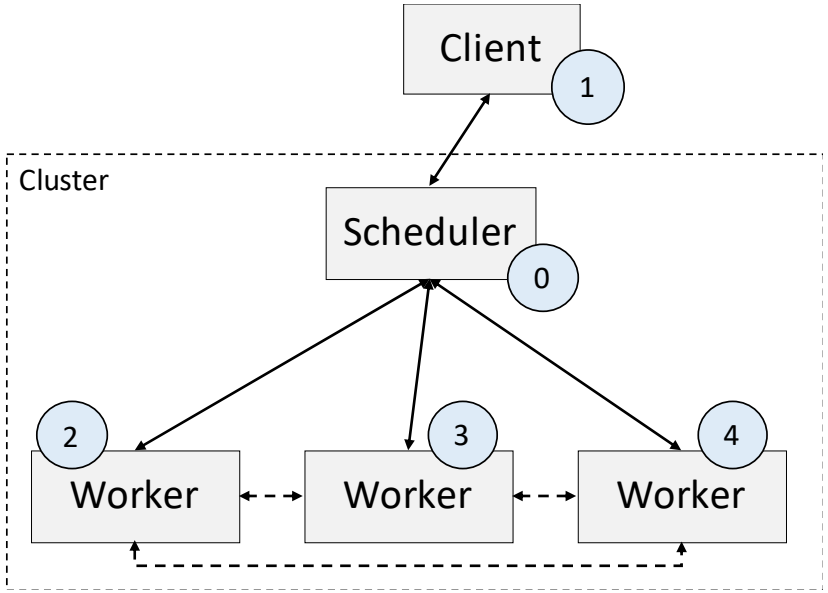
- Dask currently has two communication backends:
  - TCP: Tornado-based
  - UCX: Built using a GPU-aware Cython wrapper called UCX-Py
- MPI4Dask is an MVAPICH2-based communication backend for Dask:
  - First MPI-based communication device for Dask
  - Optimizes CPU and GPU communication in the Dask framework on modern HPC clusters

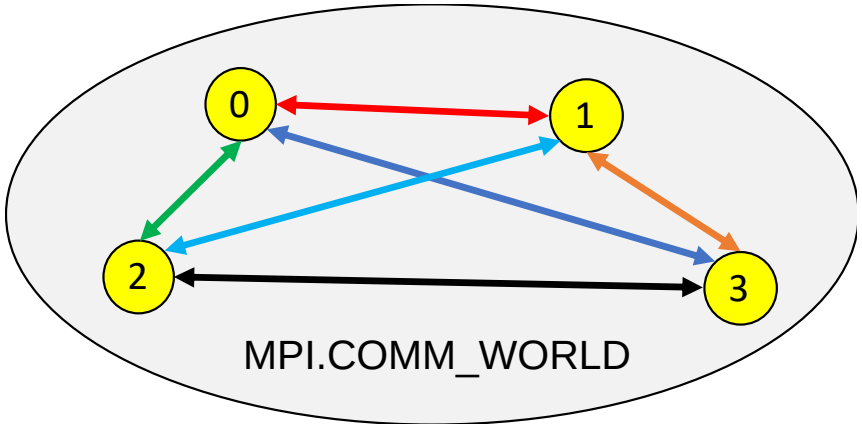
Dask Architecture



MPI4Dask: Bootstrapping and Dynamic Connectivity

- Several ways to start Dask programs:
  - Manual
  - Utility classes:
    - LocalCUDACluster, SLURMCluster, SGECluster, PBCCluster, and others
- MPI4Dask uses the Dask-MPI to bootstrap execution of Das programs
- Dynamic connectivity is established using the asyncio package in MPI4Dask:
  - Scheduler and workers listen for incoming connections by calling asyncio.start_server()
  - Workers and client connect using asyncio.open_connection()





MPI4Dask: Point-to-point Communication Coroutines

- Implements communication coroutines for point-to-point MPI functions:
  - Using mpi4py (Cython wrappers) and MVAPICH2-GDR
- mpi4py provides two flavors of point-to-point communication functions:
  - Send()/Recv() – for exchanging data in buffers (faster and used in MPI4Dask)
  - send()/recv() – for communicating Python objects (pickle/unpickle)
  - GPU buffers implement the __cuda_array_interface__
- Implemented chunking mechanism for large messages
- The send and receive communication coroutines are as follows:

```
request = comm.Isend([buf, size], dest, tag)
status = request.Test()

while status is False:
   await asyncio.sleep(0)
   status = request.Test()
```

```
request = comm.Irecv([buf, size], src, tag)
status = request.Test()

while status is False:
   await asyncio.sleep(0)
   status = request.Test()
```

MPI4Dask Release

- MPI4Dask 0.2 was released in Mar '21 adding support for MPI to Dask:
  - Can be downloaded from: http://hibd.cse.ohio-state.edu
- Features:
  - Based on Dask Distributed 2021.01.0
  - Compliant with user-level Dask APIs and packages
  - Support for MPI-based communication in Dask for cluster of GPUs
  - Implements point-to-point communication co-routines
  - Efficient chunking mechanism implemented for large messages
  - (NEW) Built on top of mpi4py over the MVAPICH2, MVAPICH2-X, and MVAPICH2-GDR libraries
  - (NEW) Support for MPI-based communication for CPU-based Dask applications
  - Supports starting execution of Dask programs using Dask-MPI
  - Tested with
    - (NEW) CPU-based Dask applications using numPy and Pandas data frames
    - (NEW) GPU-based Dask applications using cuPy and cuDF
    - Mellanox InfiniBand adapters (FDR and EDR)
    - Various multi-core platforms
    - NVIDIA V100 and Quadro RTX 5000 GPUs

MPI4Dask Installation

- MPI4Dask is available to download from: http://hibd.cse.ohio-state.edu/
  - The userguide is available at: http://hibd.cse.ohio-state.edu/static/media/hibd/dask/mpi4dask-0.2-userguide.pdf
- Section 3: Setup Instructions
  - 3.1 Installation Pre-requisites:
    - 3.1.1 Install Miniconda
    - 3.1.2 Modules/Libraries for GPU-based Dask Applications:
    - 3.1.3 Modules/Libraries for CPU-based Dask Applications:
    - 3.1.4 Install the MVAPICH2 Library (MVAPICH2-X, MVAPICH2, or MVAPICH2-GDR)
    - 3.1.5 Install the mpi4py Library
    - 3.1.6 Install Dask-MPI package
  - 3.2 Install MPI4Dask
- Section 4. Running GPU-based Dask Applications
  - 4.1 Writing the host file
  - 4.2 Sum of cuPy Array and its Transpose
  - 4.3 cuDF Merge
- Section 5. Running GPU-based Dask Applications
  - 5.1 Writing the host file
  - 5.2 Sum of numPy Array and its Transpose
  - 5.3 Sum of Pandas Data Frame
  - 5.4 SVD

Installation Pre-requisites

Modules/Libraries for GPU-based Dask Applications:

$ conda install -c conda-forge -c rapidsai -c nvidia automake make libtool pkg-config libhwloc psutil python=3.8 setuptools cython cudatoolkit=10.2 cupy dask-cudf dask==2021.1.1 distributed numpy rmm

Modules/Libraries for CPU-based Dask Applications:

$ conda install -c conda-forge -c rapidsai -c nvidia automake make libtool pkg-config libhwloc psutil python=3.8 setuptools cython dask==2021.1.1 distributed=2021.1.1 numpy

Install the MVAPICH2 Library (MVAPICH2-X, MVAPICH2, or MVAPICH2-GDR)

Install the mpi4py Library

$ git clone https://github.com/mpi4py/mpi4py.git

$ edit mpi.cfg file

[MVAPICH2]

mpi_dir = /path/to/MVAPICH2-GDR/install/directory

mpicc = %(mpi_dir)s/bin/mpicc

mpicxx = %(mpi_dir)s/bin/mpicxx

include_dirs = %(mpi_dir)s/include

library_dirs = %(mpi_dir)s/lib64

runtime_library_dirs = %(library_dirs)s

$ python setup.py build --mpi=MVAPICH2-GDR; $ pip install .

Install Dask-MPI and MPI4Dask

Install Dask-MPI package

```
$ git clone https://github.com/dask/dask-mpi.git
$ cd dask-mpi
$ python setup.py build
$ pip install .
```

Install MPI4Dask

```
$ wget http://hibd.cse.ohio-state.edu/download/hibd/dask/mpi4dask-0.2.tar.gz
$ tar -xzvf mpi4dask-0.2.tar.gz
$ cd mpi4dask-0.2/distributed
$ python setup.py build
$ pip install .

$ conda list
$ conda list | grep distributed
$ conda list |grep dask
```

Running GPU and CPU Dask Applications

Sum of cuPy Array and its Transpose [GPU]

```
$ cd mpi4dask-0.2/dask-apps/gpu
$ LD_PRELOAD=$MPILIB/lib64/libmpi.so $MPILIB/bin/mpirun_rsh -export-all -np 4 -hostfile hosts MV2_USE_CUDA=1
MV2_USE_GDRCOPY=1 MV2_GPUDIRECT_GDRCOPY_LIB=/opt/gdrcopy2.0/lib64/libgdrapi.so MV2_CPU_BINDING_LEVEL=SOCKET
MV2_CPU_BINDING_POLICY=SCATTER python cupy_sum_mpi.py
```

cuDF Merge [GPU]

```
$ cd mpi4dask-0.2/dask-apps/gpu
$ LD_PRELOAD=$MPILIB/lib/libmpi.so $MPILIB/bin/mpirun_rsh -export-all -np 4 -hostfile hosts MV2_USE_CUDA=1
MV2_USE_GDRCOPY=1 MV2_GPUDIRECT_GDRCOPY_LIB=/opt/gdrcopy2.0/lib64/libgdrapi.so MV2_CPU_BINDING_LEVEL=SOCKET
MV2_CPU_BINDING_POLICY=SCATTER python cudf_merge_mpi.py --type gpu --protocol mpi --runs 20 --chunk-size 1_000_000_00
```

Sum of numPy Array and its Transpose [CPU]

```
$ cd mpi4dask-0.2/dask-apps/cpu
$ LD_PRELOAD=$MPILIB/lib/libmpi.so $MPILIB/bin/mpirun_rsh -export-all -np 4 -hostfile hosts MV2_CPU_BINDING_LEVEL=SOCKET
MV2_CPU_BINDING_POLICY=SCATTER python numpy_sum_mpi.py
```

Sum of Pandas DataFrame [CPU]

```
$ cd mpi4dask-0.2/dask-apps/cpu
$ LD_PRELOAD=$MPILIB/lib/libmpi.so $MPILIB/bin/mpirun_rsh -export-all -np 4 -hostfile hosts MV2_CPU_BINDING_LEVEL=SOCKET
MV2_CPU_BINDING_POLICY=SCATTER python dask-cudf_sum_mpi.py
```

Sum of cuPy Array and its Transpose (with TCP device)

```
$ srun -N 4 --reservation=dltutorial run_cupy_sum_tcp.sh
```

Sample Output:

```
+ /opt/tutorials/dl-tutorial-21/dask/mvapich2/install/bin/mpirun_rsh -np 4 -hostfile
   /tmp/shafi.16/hosts LD_PRELOAD=/opt/tutorials/dl-tutorial-
   21/dask/mvapich2/install/lib/libmpi.so MV2_USE_CUDA=1 MV2_CPU_BINDING_LEVEL=SOCKET
   MV2_CPU_BINDING_POLICY=SCATTER MV2_USE_GDRCOPY=1
   MV2_GPUDIRECT_GDRCOPY_LIB=/opt/gdrcopy2.0/lib64/libgdrapi.so
   MV2_SUPPRESS_JOB_STARTUP_PERFORMANCE_WARNING=1 /opt/tutorials/dl-tutorial-
   21/dask/miniconda3/envs/mpi4dask_tutorial/bin/python /opt/tutorials/dl-tutorial-
   21/labs/lab1/cupy_sum_tcp.py
<Client: 'tcp://10.3.1.1:46566' processes=2 threads=56, memory=269.79 GB>
Time for iteration 0 : 15.613967895507812
Time for iteration 1 : 12.97205138206482
Time for iteration 2 : 13.211132526397705
Time for iteration 3 : 12.941233396530151
Time for iteration 4 : 13.074704647064209
Median Wall-clock Time: 13.07 s
+ set +x
```

Sum of cuPy Array and its Transpose (with MPI device)

```
$ srun -N 4 --reservation=dltutorial run_cupy_sum_mpi.sh
```

Sample Output:

```
+ /opt/tutorials/dl-tutorial-21/dask/mvapich2/install/bin/mpirun_rsh -np 4 -hostfile
   /tmp/shafi.16/hosts LD_PRELOAD=/opt/tutorials/dl-tutorial-
   21/dask/mvapich2/install/lib/libmpi.so MV2_USE_CUDA=1 MV2_CPU_BINDING_LEVEL=SOCKET
   MV2_CPU_BINDING_POLICY=SCATTER MV2_USE_GDRCOPY=1
   MV2_GPUDIRECT_GDRCOPY_LIB=/opt/gdrcopy2.0/lib64/libgdrapi.so
   MV2_SUPPRESS_JOB_STARTUP_PERFORMANCE_WARNING=1 /opt/tutorials/dl-tutorial-
   21/dask/miniconda3/envs/mpi4dask_tutorial/bin/python /opt/tutorials/dl-tutorial-
   21/labs/lab1/cupy_sum_mpi.py
<Client: 'mpi://10.3.1.1:31549' processes=2 threads=56, memory=269.79 GB>
Time for iteration 0 : 9.499887466430664
Time for iteration 1 : 5.288544416427612
Time for iteration 2 : 4.123088598251343
Time for iteration 3 : 4.088623523712158
Time for iteration 4 : 4.115798234939575
Median Wall-clock Time: 4.12 s
+ set +x
```

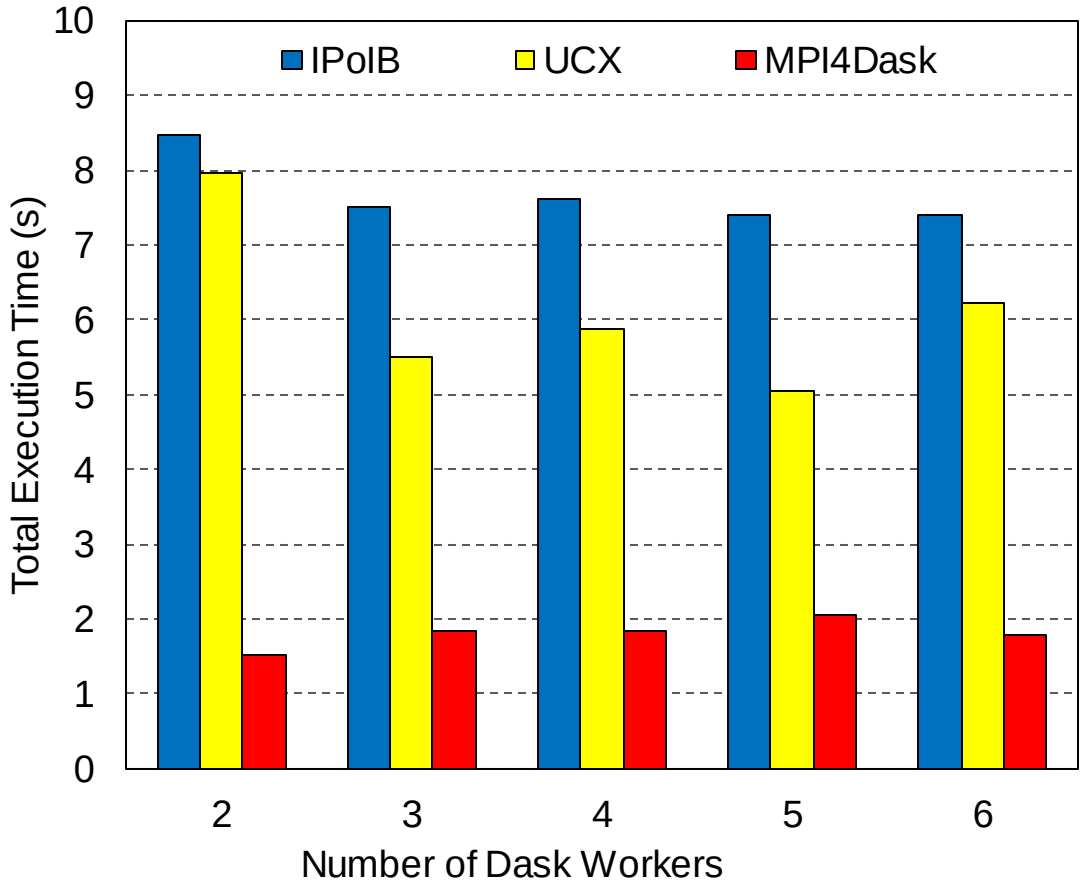
MVAPICH2-GDR: 3.17x faster

Configurable options in the script (cupy_sum_mpi.py)

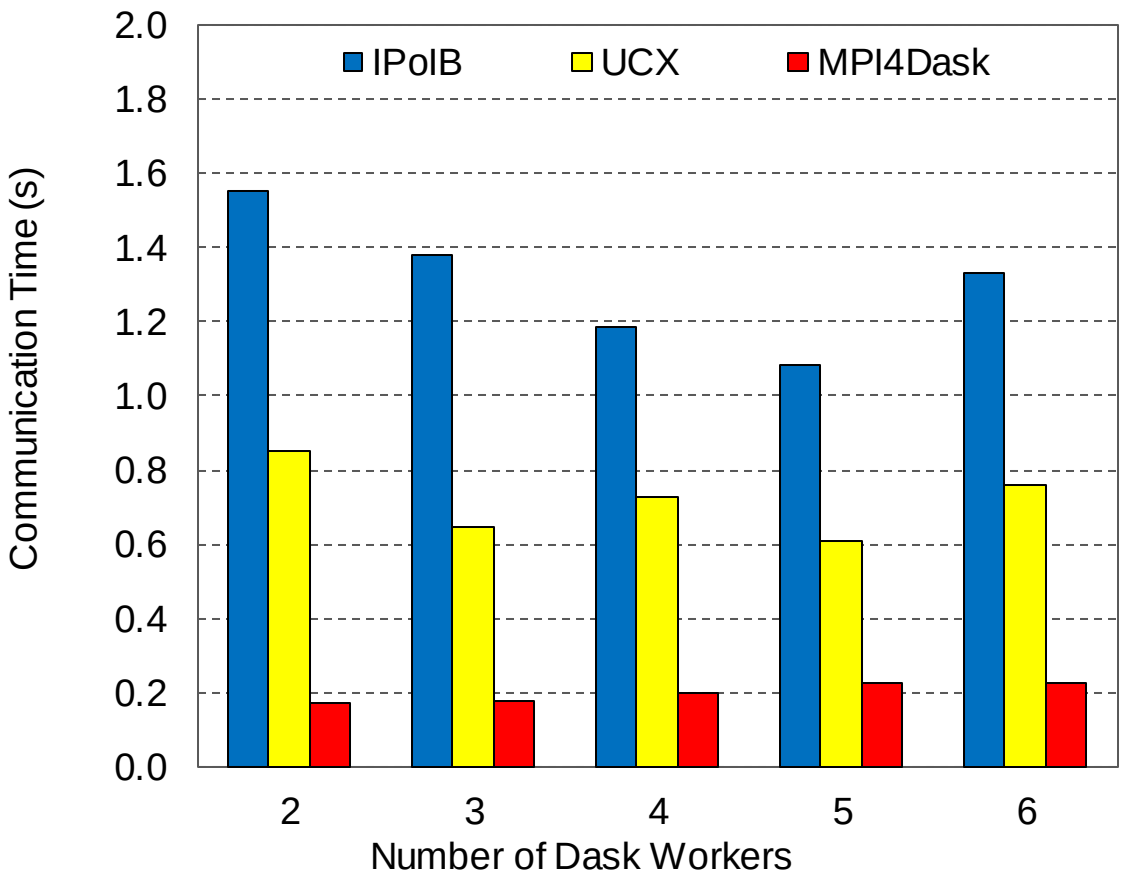
```
DASK_PROTOCOL      = 'mpi'   # Options are ['mpi', 'tcp']
GPUS_PER_NODE      = 1       # number of GPUs in the system
RUNS               = 5       # repetitions for the benchmark
DASK_INTERFACE     = 'ib0'   # interface to use for communication
THREADS_PER_NODE   = 28      # number of threads per node.
```

Benchmark #1: Sum of cuPy Array and its Transpose (RI2)

3.47x better on average



6.92x better on average



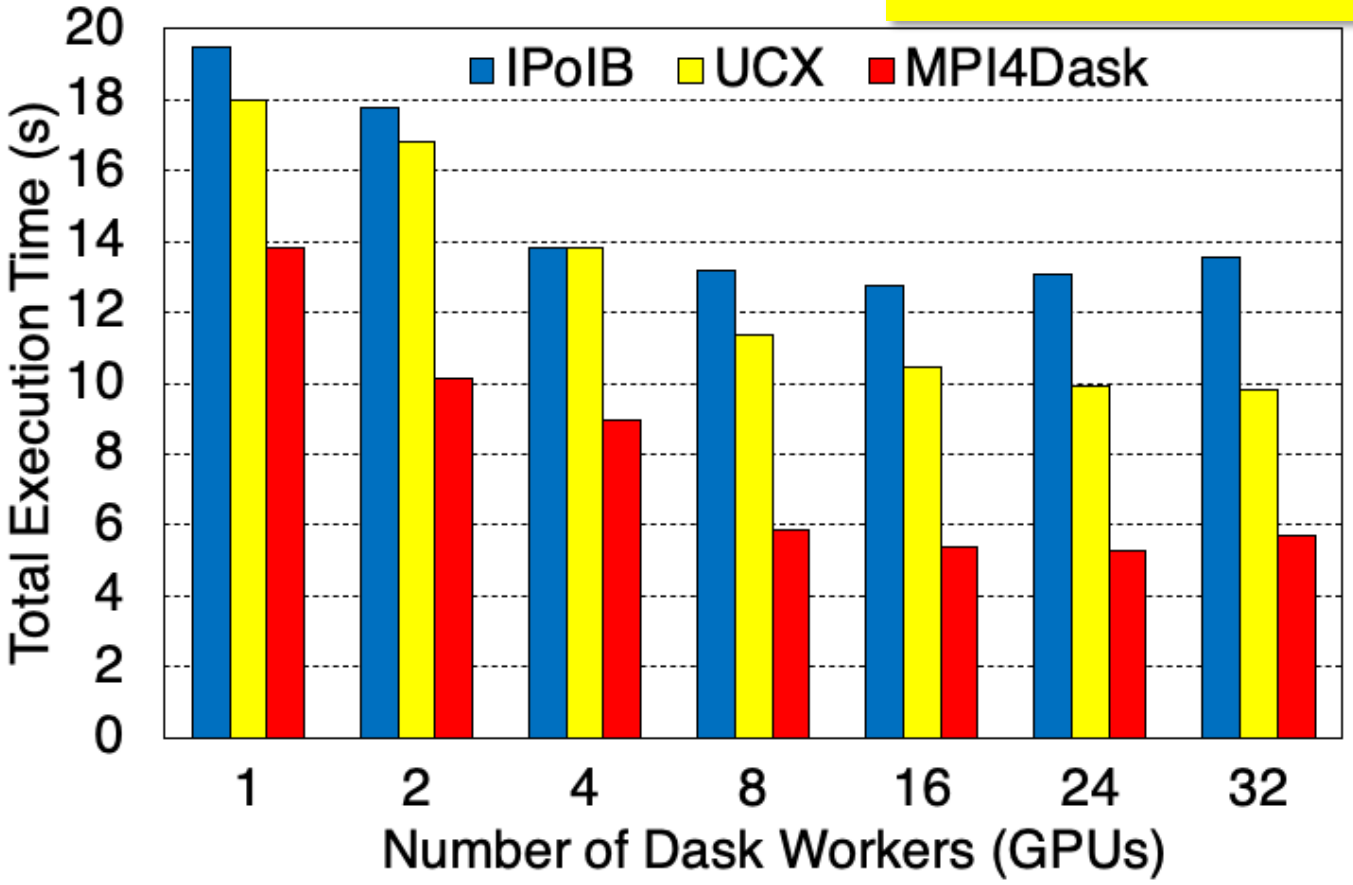
A. Shafi , J. Hashmi , H. Subramoni , and D. K. Panda, Efficient MPI-based Communication for GPU-Accelerated Dask Applications, CCGrid '21, https://arxiv.org/abs/2101.08878

MPI4Dask 0.2 release

(http://hibd.cse.ohio-state.edu)

Benchmark #1: Sum of cuPy Array and its Transpose (TACC Frontera GPU Subsystem)

1.71x better on average



A. Shafi , J. Hashmi , H. Subramoni , and D. K. Panda, Efficient MPI-based Communication for GPU-Accelerated Dask Applications, CCGrid '21
https://arxiv.org/abs/2101.08878

MPI4Dask 0.2 release

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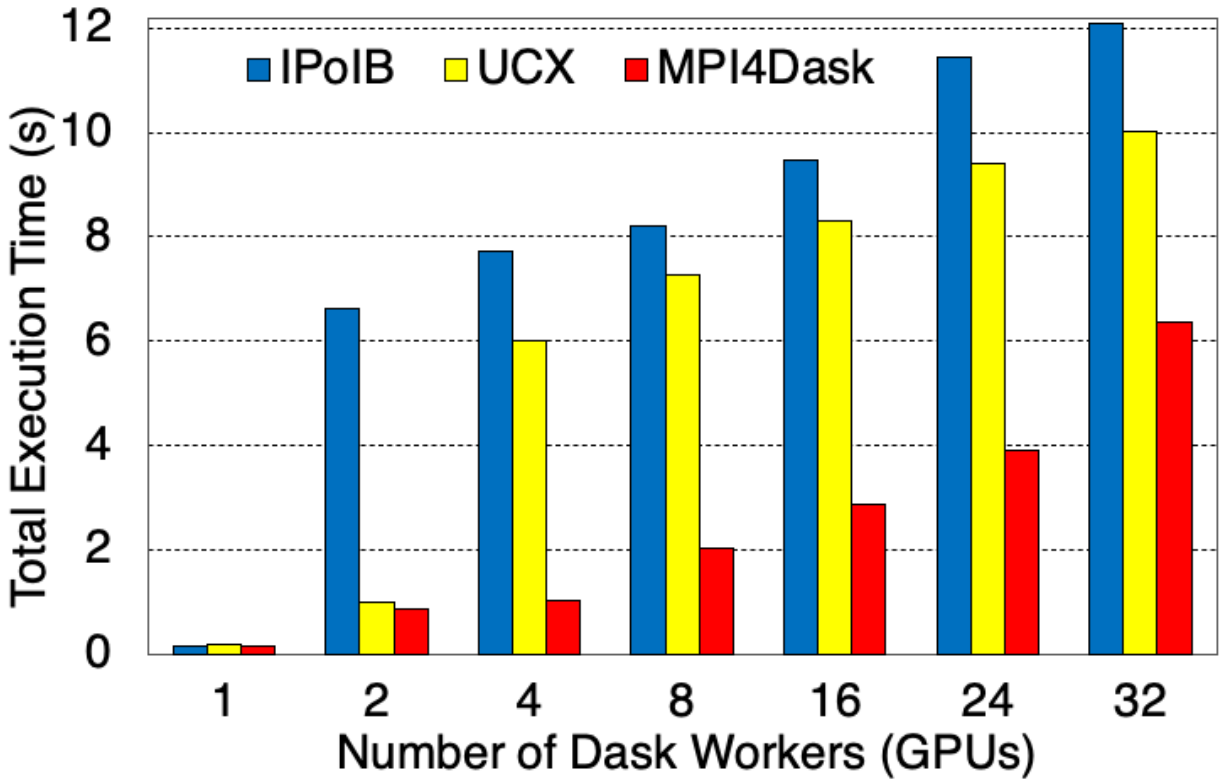
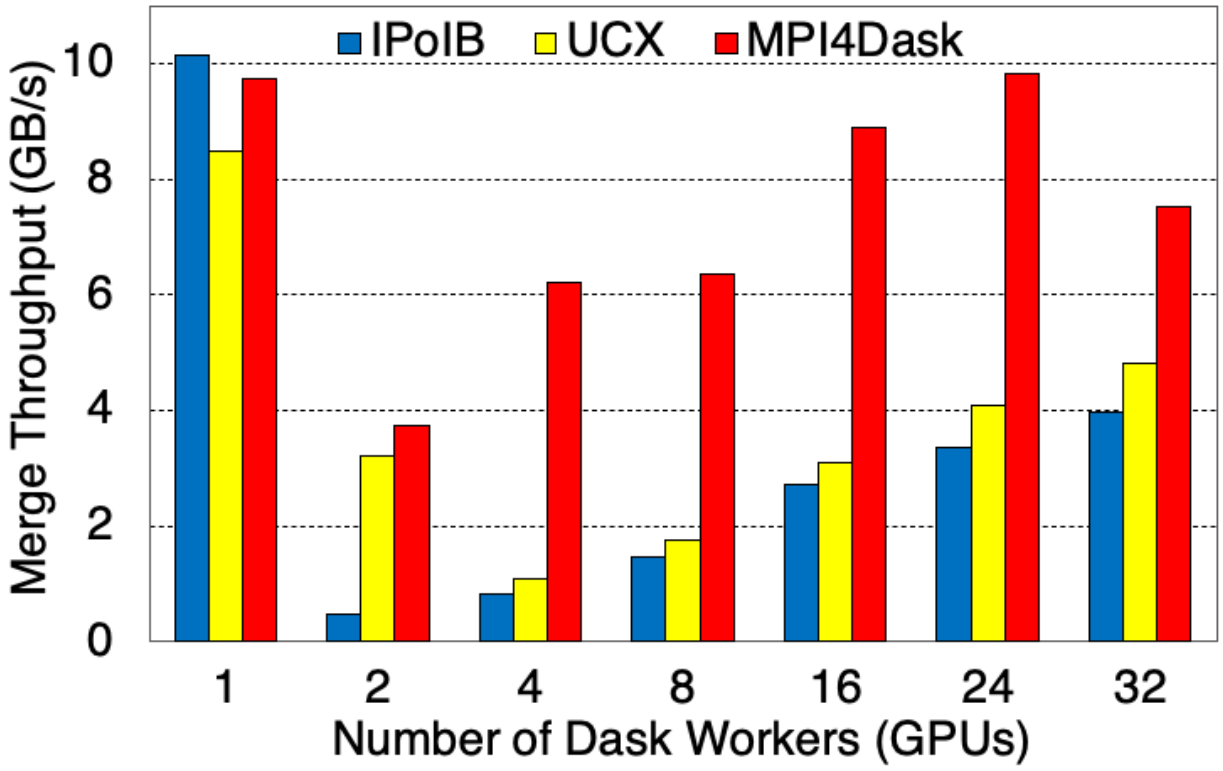
Benchmark #2: cuDF Merge (TACC Frontera GPU Subsystem)

2.91x better on average



2.90x better on average



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- Introduction
- Deep Neural Network Training and Essential Concepts
- Parallelization Strategies for Distributed DNN Training
- Machine Learning
- Data Science using Dask
- **Conclusion**

Convergence of ML/DL, Data Science, and HPC

- Is Machine Learning/Deep Learning and Data Science an HPC Problem?
  - Distributed Model/DNN Training is definitely an HPC problem
  - Inference – not yet an HPC problem
  - Support for Data Science frameworks on HPC systems is improving (yet lagging)
- Why HPC can help?
  - Decades of research for communication models and performance optimizations
  - MPI, PGAS, and other communication runtimes can help for “data-parallel” training
- Some of the needs for ML/DL and Data Science frameworks are an exact match
  - Compute intensive problem
- Some needs are new for distributed/parallel communication runtimes
  - Large Message Communication
  - CUDA-Aware Communication

Exploiting GPUs and Unified Communication Layer for Data Science Frameworks

- The support for GPUs has been added to Dask as part of the NVIDIA RAPIDS project
- The RAPIDS Accelerator for Apache Spark is currently adding support for GPU processing for the Apache Spark Framework
  - SQL Plugin for executing SQL queries entirely on GPUs
  - Shuffle Plugin based on the UCX communication library (GPU-to-GPU)
  - https://nvidia.github.io/spark-rapids/
- Opportunity to utilize GPU-to-GPU communication provided by MPI libraries like MVAPICH2-GDR
- Is it possible to have an MPI-based communication layer for Data Science frameworks?

Conclusion

- Exponential growth in Machine Learning/Deep Learning/Data Science frameworks
- Provided an overview of issues, challenges, and opportunities for designing efficient communication runtimes
  - Efficient, scalable, and hierarchical designs are crucial for ML/DL/Data Science frameworks
  - Co-design of communication runtimes and ML/DL/Data Science frameworks will be essential
- Presented use-cases to demonstrate the complex interaction between DL/ML/Dask middleware with the underling HPC technologies and middleware
- Need collaborative efforts to achieve the full potential

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- Q. Zhou (Ph.D.)
- K. Al Attar (M.S.)
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Past Students

- A. Awan (Ph.D.)
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- A. Singh (Ph.D.)
- J. Sridhar (M.S.)
- S. Srivastava (M.S.)
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Thank You!

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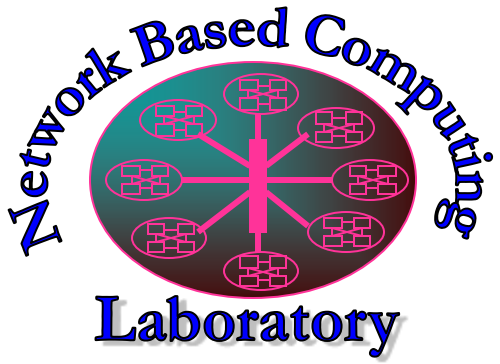

Network-Based Computing Laboratory

http://nowlab.cse.ohio-state.edu/

MVAPICH

MPI, PGAS and Hybrid MPI+PGAS Library

The MVAPICH2 Project

http://mvapich.cse.ohio-state.edu/

The High-Performance Deep Learning Project

http://hidl.cse.ohio-state.edu/