Using Multiple GPUs for Distributed Deep Learning on Neuron

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Korea Institute of Science and Technology Information

Some Motivational thoughts on large-scale DL/LM on top of national supercomputing facilities

- **KISTI-6 /w ~600PF is coming in 2 years**
  - ✓ It is expected that several thousands of GPUs(?) are available
- **Is large-scale LM (Language Model) training a exclusive task that can be conducted by big tech companies (e.g., Google, Meta, MS) running data center facilities?**
- **Why is it that large-scale LM R&D is so hard in Korea?**
  - ✓ Lack of computing resources
  - ✓ Lack of datasets
  - ✓ Lack of skills??
- **What can KISTI do in contributing to large-scale LM R&D in Korea?**
  - ✓ KISTI is uniquely positioned to running a genenal-purpose national supercomputing facilitiy in Korea
- **Is KISTI's supercomputing facility easy to access for users to do large-scal distributed deep learning R&D?**
- **What are the most significant barriers that prevent users from having access to KISTI supercomputing facilities in conducting large-scale distributed training?**
  - ✓ Is it because of the tranditional batch-scheduling based service?
  - ✓ ??

Objectives

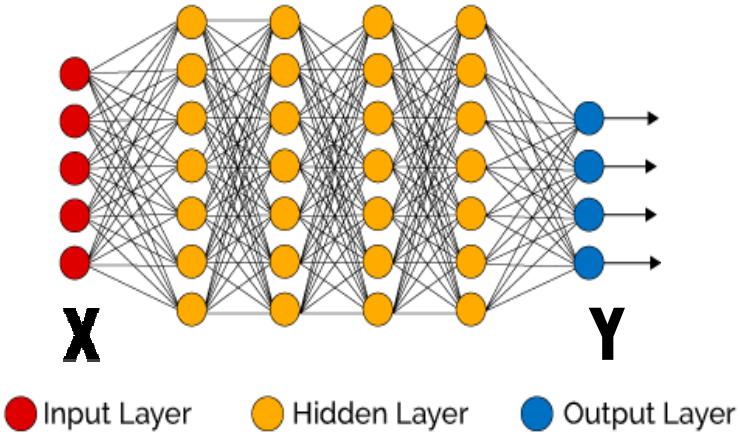
- **Guide users to run his/her DL codes using multiple GPU nodes on Neuron (KISTI GPU Cluster)**
- **Introduce how to set up a virtual environment**
  - install Conda and create/set up his/her virtual environment
  - run his/her codes interactively on Neuron
- **Introduce how to run Distributed DL training on Neuron**
  - Horovod
  - Singularity Container
  - …

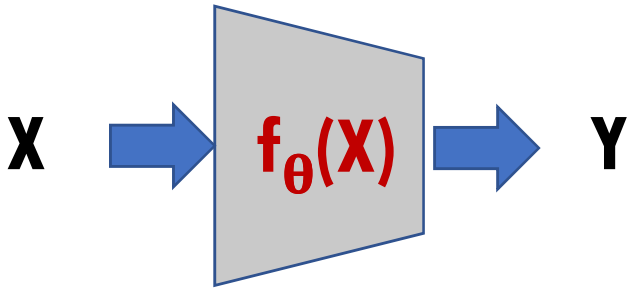
Agenda

- **Why distributed training?**
- **Distributed DL Approaches**
  - Data Parallel
    - Parameter Server(s)
    - Ring AllReduce
  - Model Parallel
    - Pipeline parallel
    - Tensor parallel
  - Multi-dimensional (3D) Parallel
- **KISTI GPU Cluster: Neuron**
- **Hands-on Exercises**
  - Conda Virtual Environment
  - Distributed Data Parallel(DDP) using Horovod
  - DDP using Singularity Container

Deep Learning in a slide

Courtesy of Prof. Sanjeev Arora





θ : parameters

(X, Y) : (Input, Label) pair of Training data

$\ell(\theta, x, y)$ Loss function (how well net output matched true label y on point x) Can be l_2, cross-entropy….

Objective $\operatorname{argmin}_\theta E_i[\ell(\theta, x_i, y_i)]$

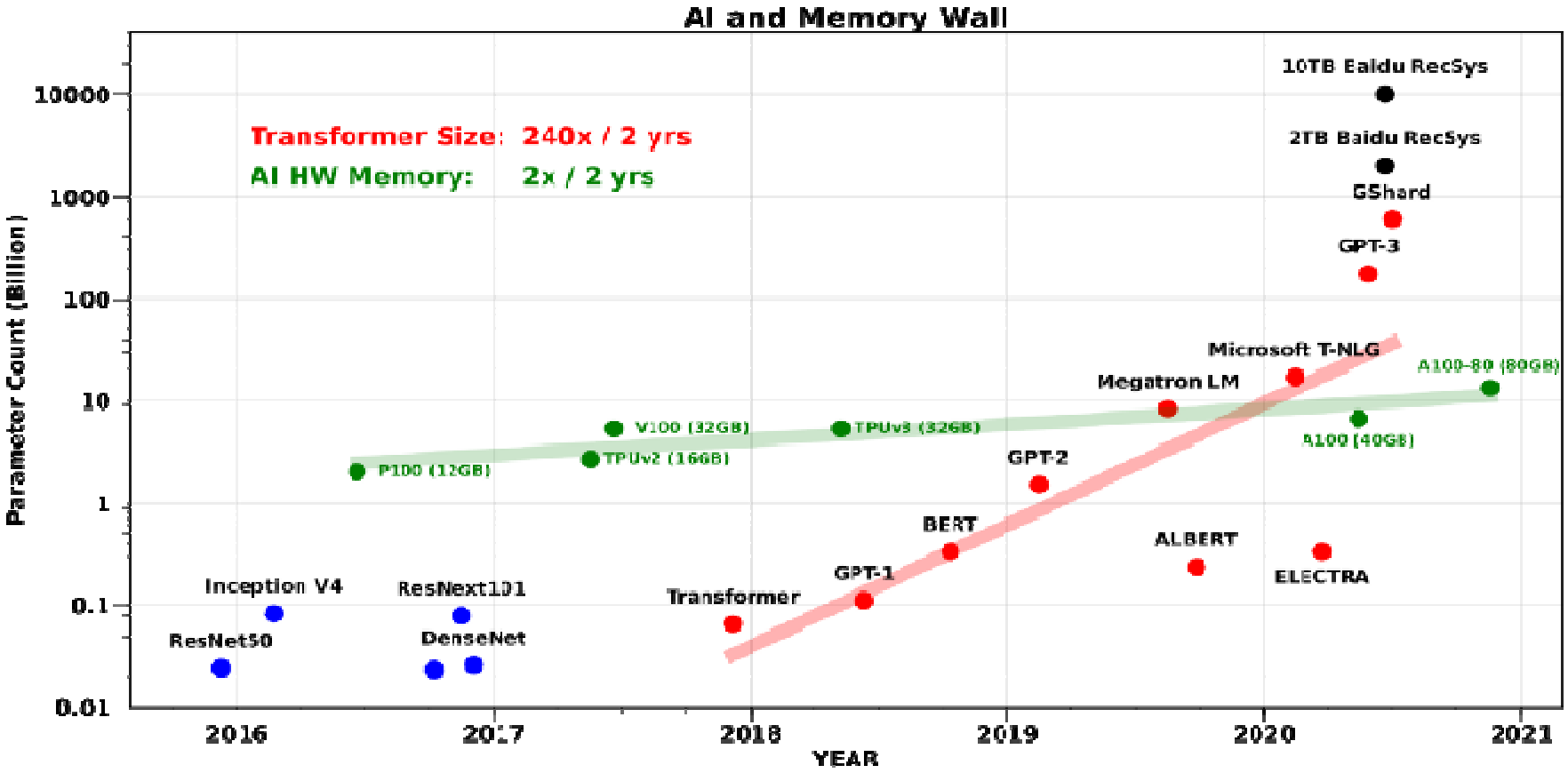
Gradient Descent $\theta^{(t+1)} \leftarrow \theta^{(t)} - \eta \nabla_\theta (E_i[\ell(\theta^{(t)}, x_i, y_i)])$

Stochastic GD: Estimate ∇ via small sample of training data.

Why Distributed Training?

Why Distributed Training

- **Model size is growing too big to fit**
  - Transformer('17): 465M, GPT-3('20):175B



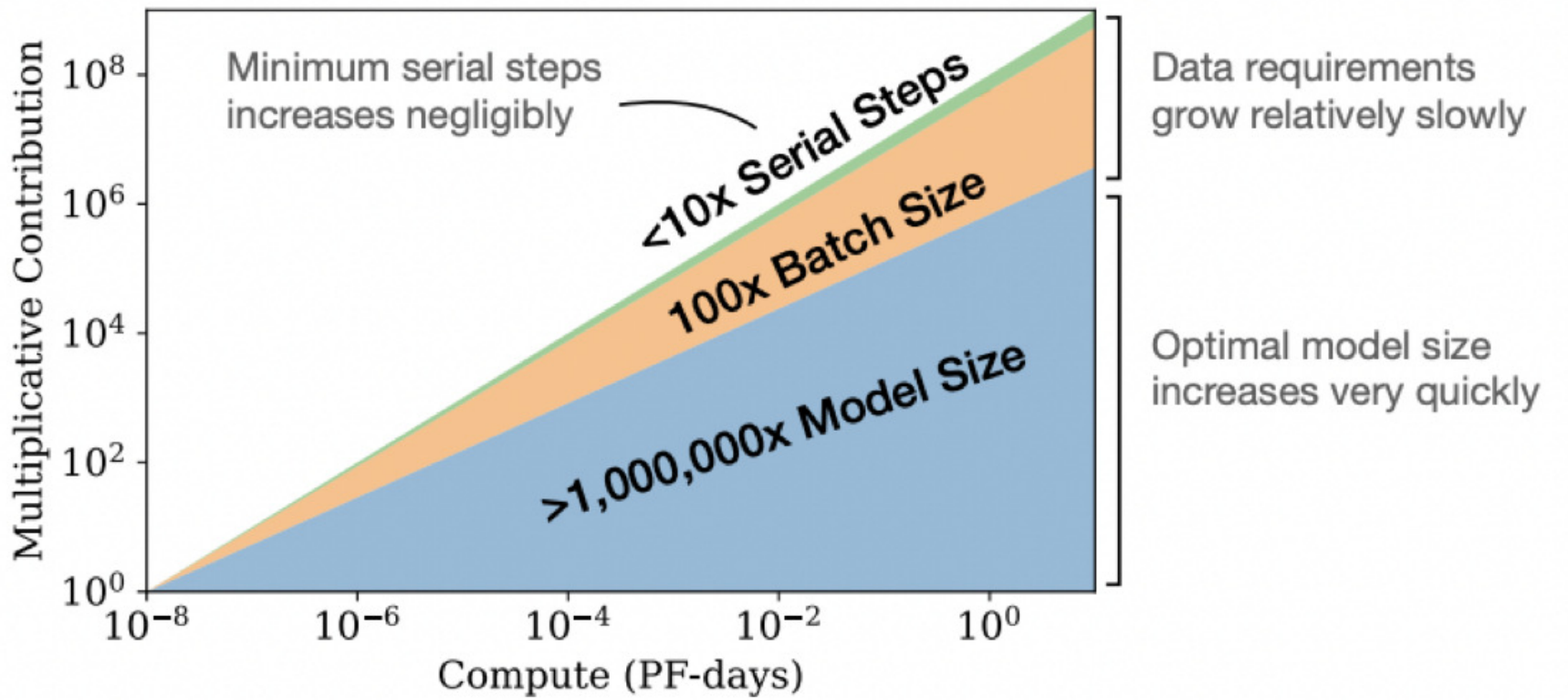
https://medium.com/riselab/ai-and-memory-wall-2cb4265cb0b8

Why Distributed Training

- **With More compute power and memory using multiple devices (GPU/TPU/CPU)**
  - Enable training large model
  - Speed up model training and shorten training time
  - Shorter training time allows you to do more experiments to reach your modeling goal

Scaling Laws

- **Larger models are significantly more sample-efficient**
  - ✓ optimally compute-efficient training involves training very large models on a relatively modest amount of data and stopping significantly before convergence.

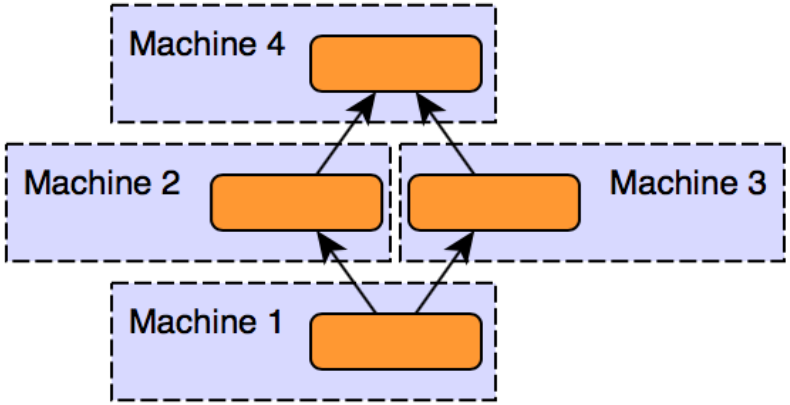


Scaling Laws for Neurral Language Models
https://arxiv.org/pdf/2001.08361.pdf

Distributed DL Approaches

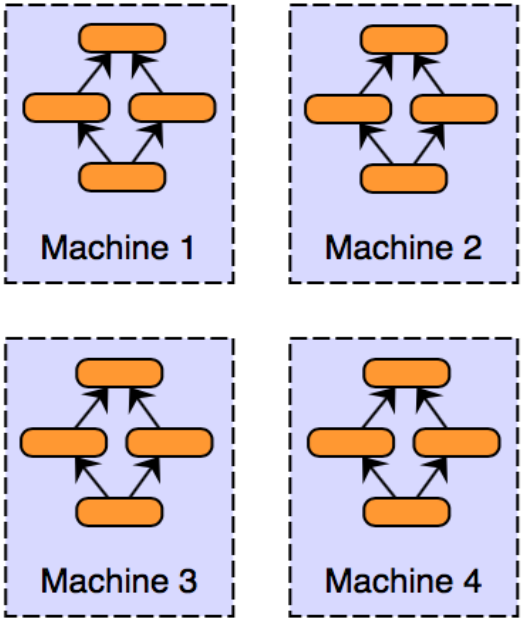
Distributed DL approaches

Model Parallelism



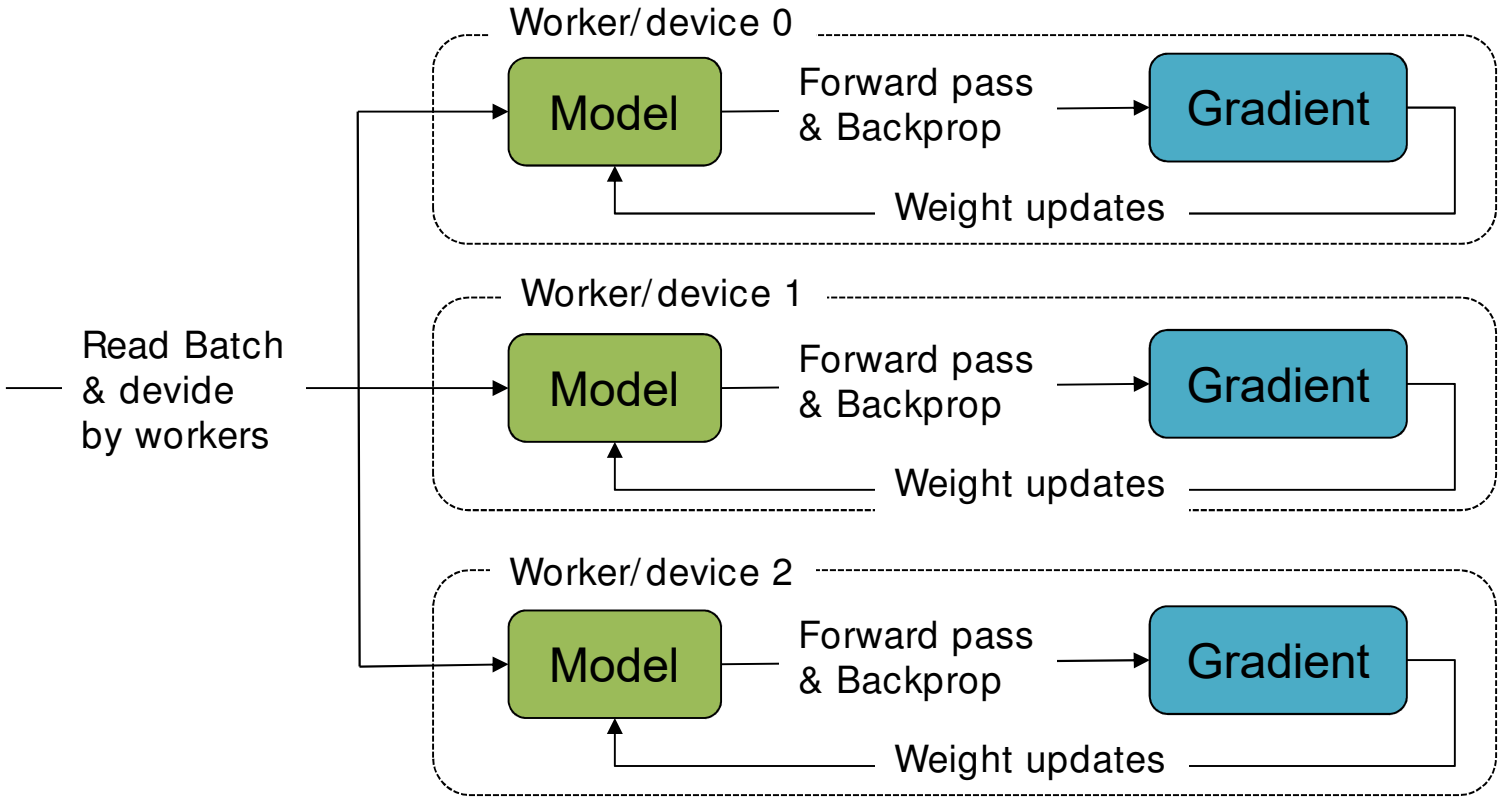
- Different parts of **model** running on multiple GPUs
- Model is too large, which cannot fit in a single device

Data Parallelism



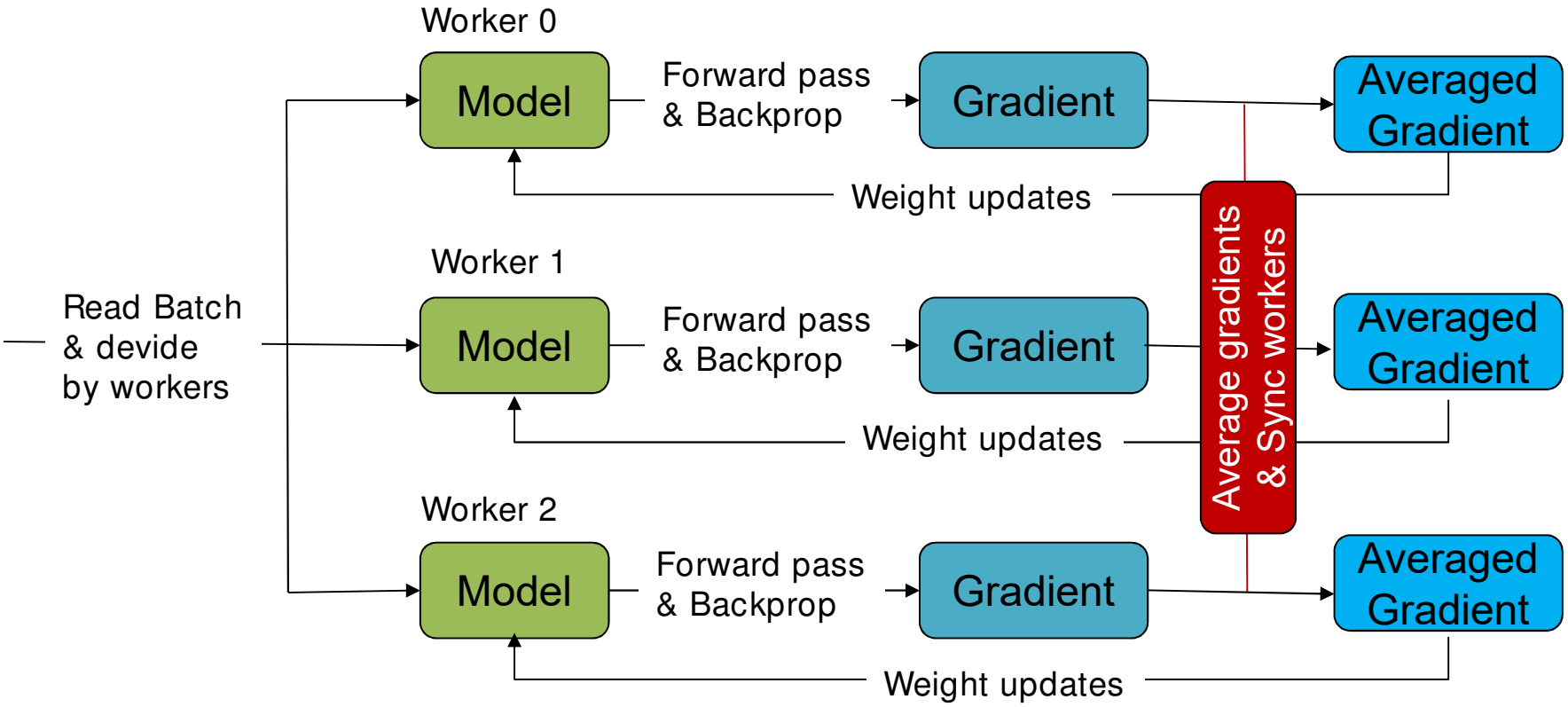
- Different parts of **data** running on multiple GPUs
- Data is too large, which need to be processed in parallel

Data Parallel

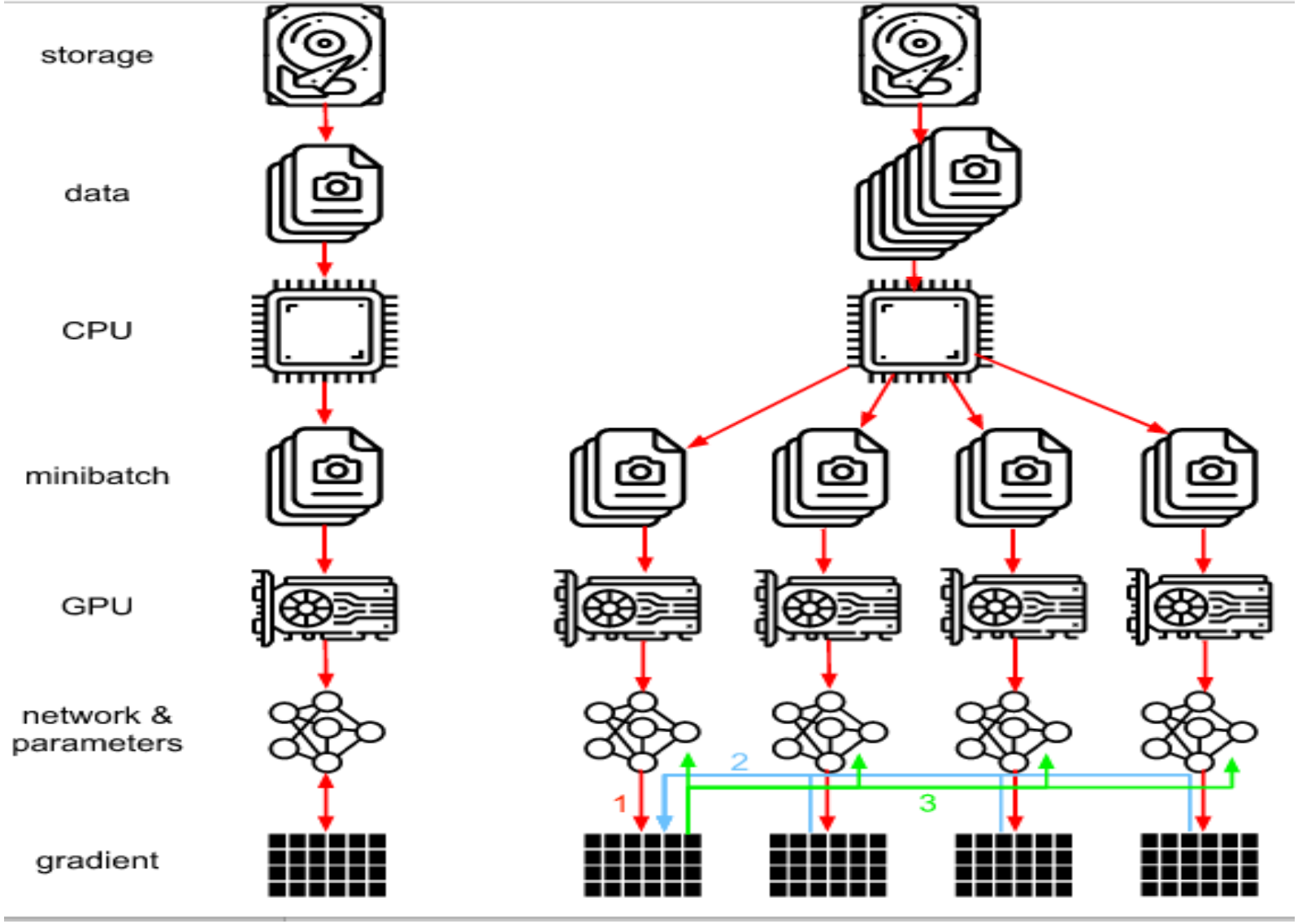


- **How to divide/distribute batches to workers**
- **When to synchronize workers**
- **How to maintain consistency in states**

Data Parallel



Data Parallel

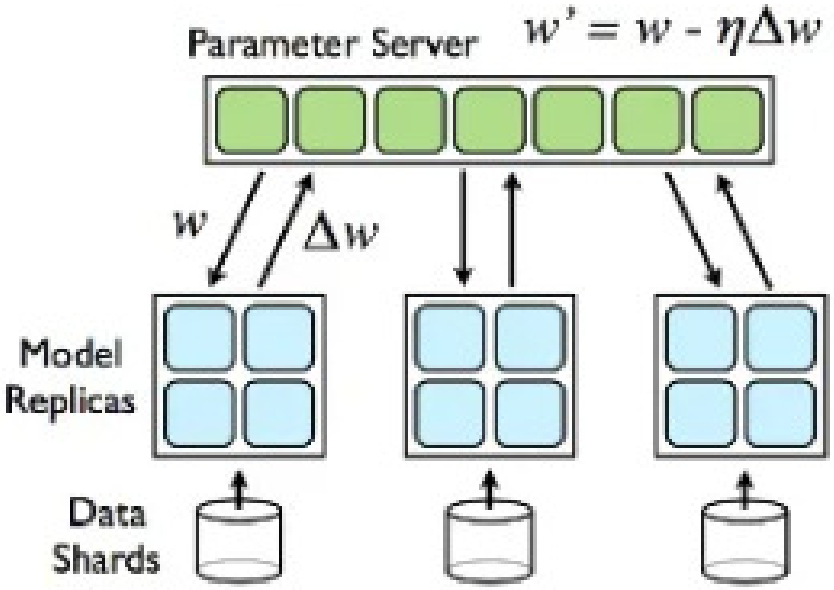


How to synchronize model parameters

- **Parameter Server (centralized)**
  - Synchronous
  - Asynchronous
- **Ring AllReduce (decentralized)**

Parameter Server (PS)

1. **Split the training data into shards** and assign a model replica to each data shard
2. For each model replica, fetch the parameters from the centralized **sharded parameter server**
3. Gradients are computed per model and pushed back to the parameter server



Each data shard stores a subset of the complete training data

Synchronous vs. Asynchronous PS

Downpour SGD:
Online Asynchronous Stochastic Gradient Descent

Sandblaset L- BFGS:
Batch Distributed Parameter Storage and Manupulation

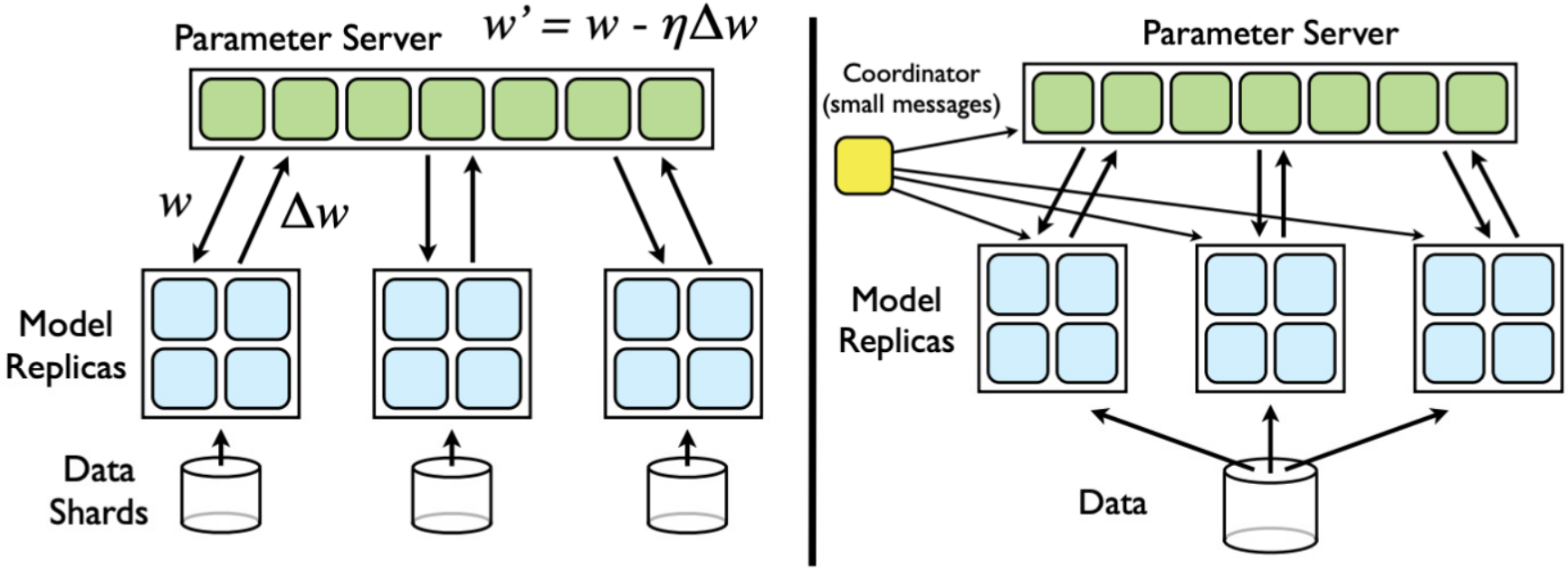
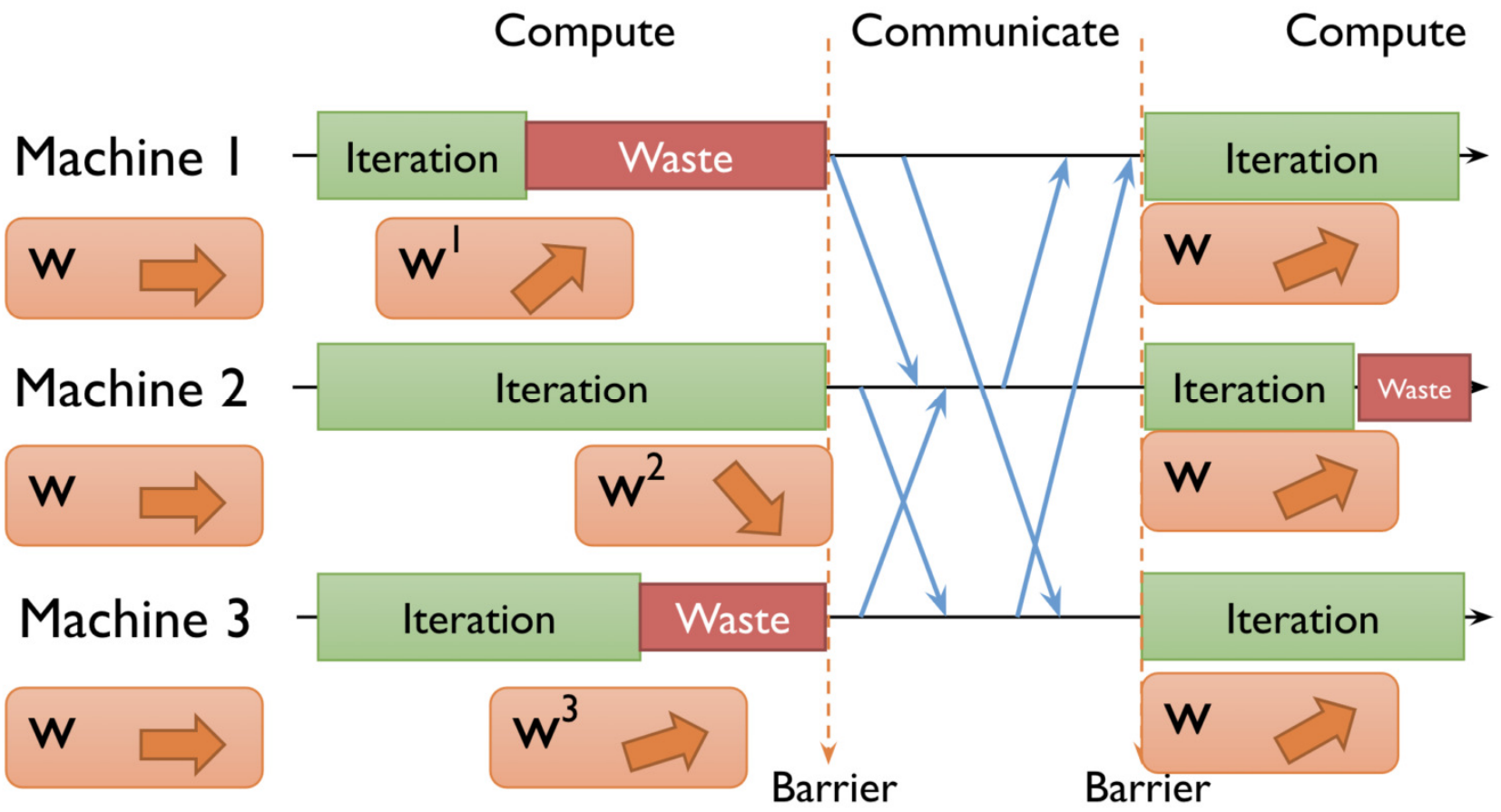


Figure 2: Left: Downpour SGD. Model replicas asynchronously fetch parameters w and push gradients Δw to the parameter server. Right: Sandblaster L-BFGS. A single 'coordinator' sends small messages to replicas and the parameter server to orchestrate batch optimization.

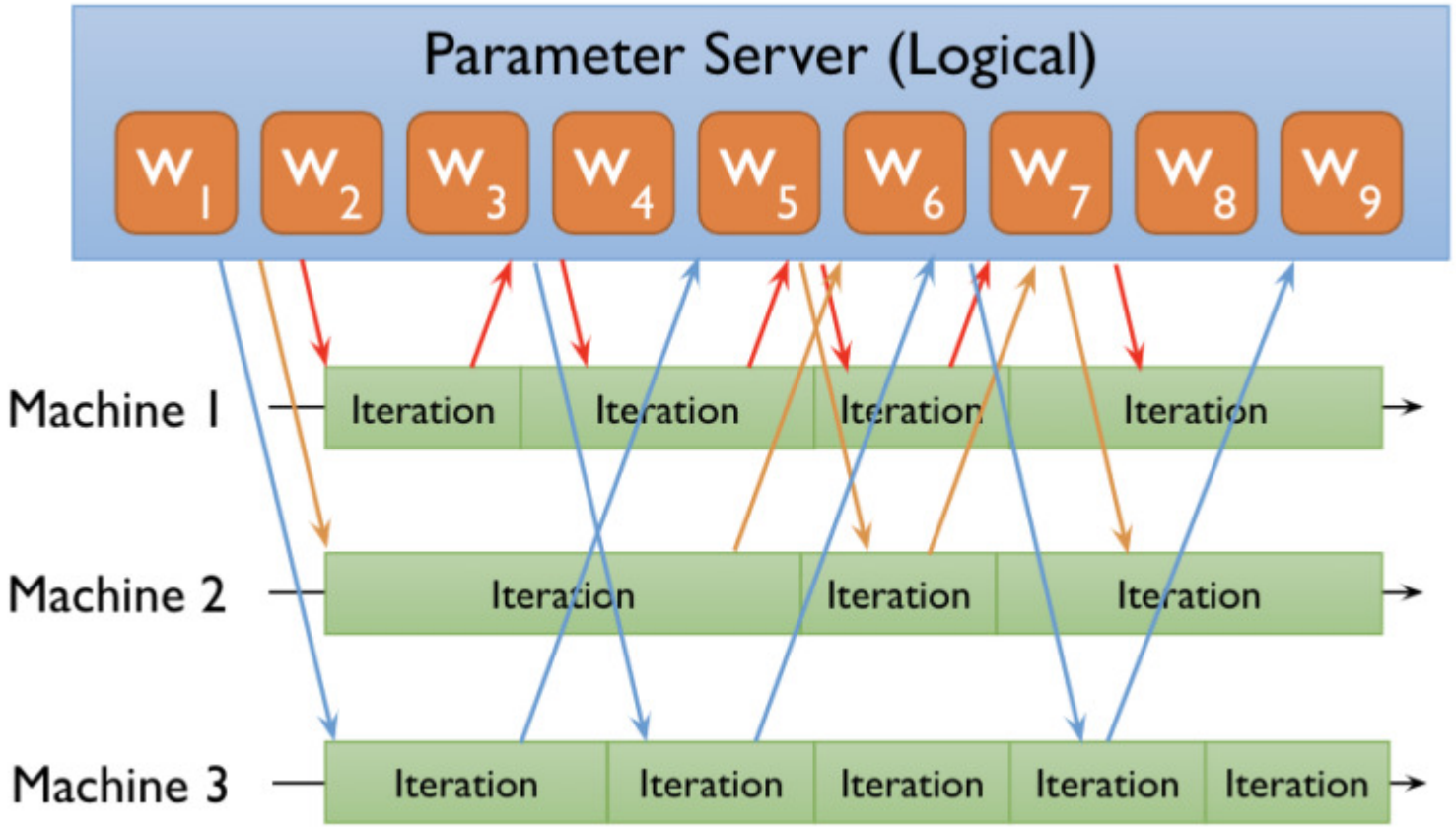
Figure from Large Scale Distributed Deep Networks

https://static.googleusercontent.com/media/research.google.com/ko//archive/large_deep_networks_nips2012.pdf

Synchronous PS



Asynchronous PS



Ring AllReduce

- **Synchronized w/o parameter server(s)**

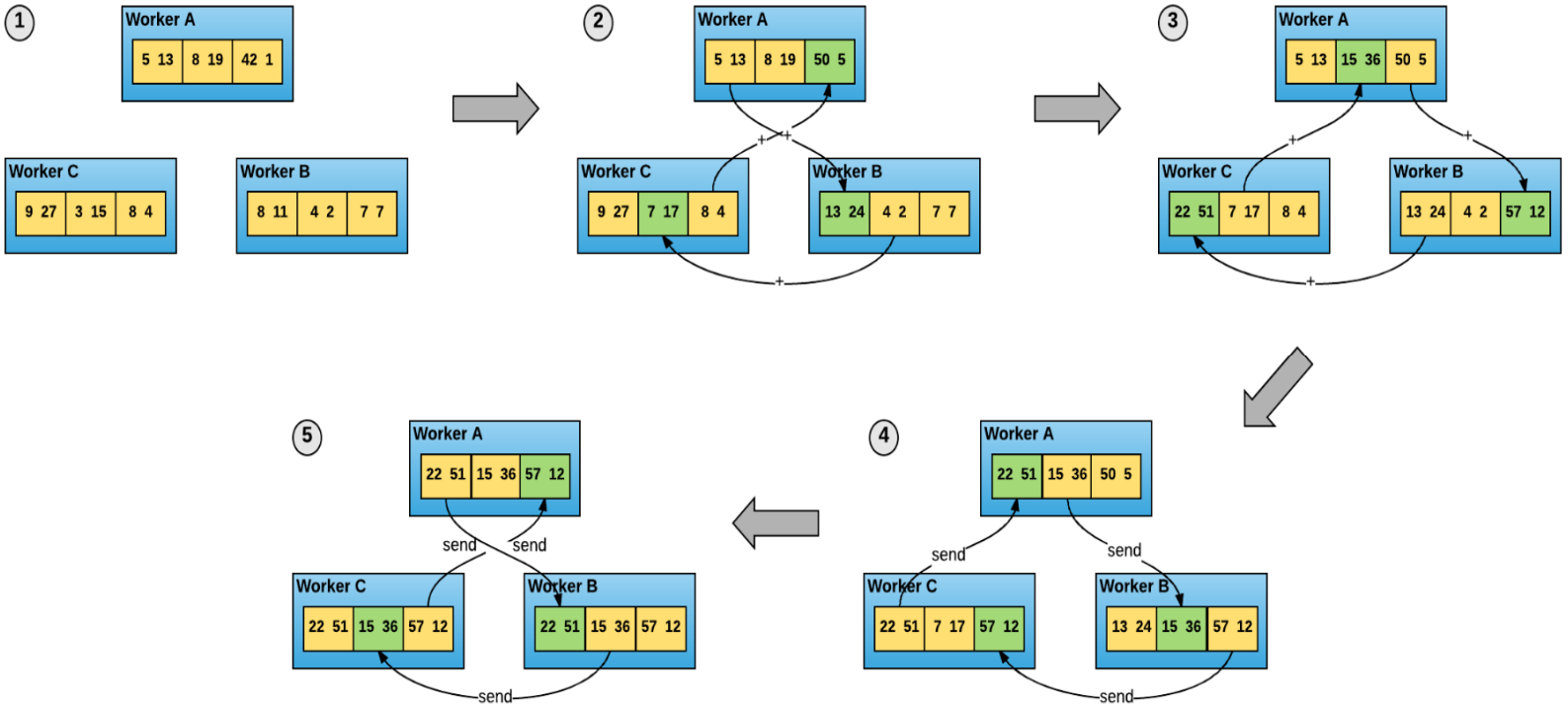
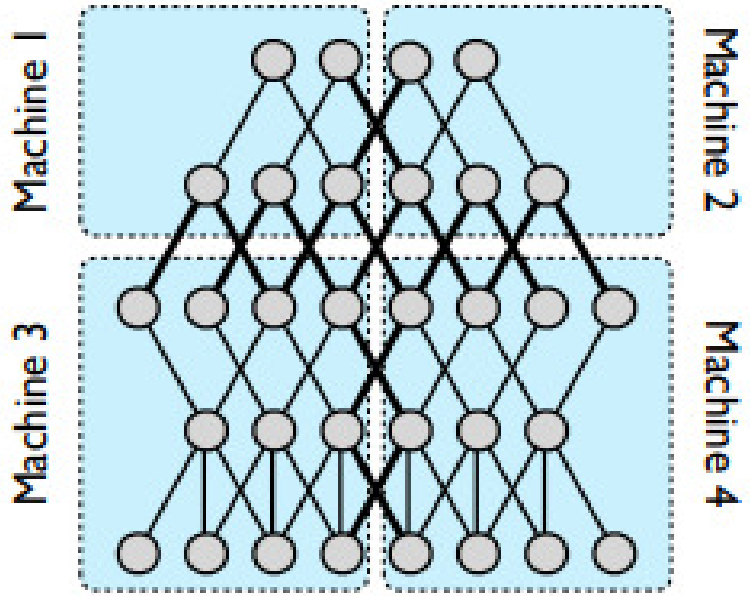


Figure 4: The ring-allreduce algorithm allows worker nodes to average gradients and disperse them to all nodes without the need for a parameter server.

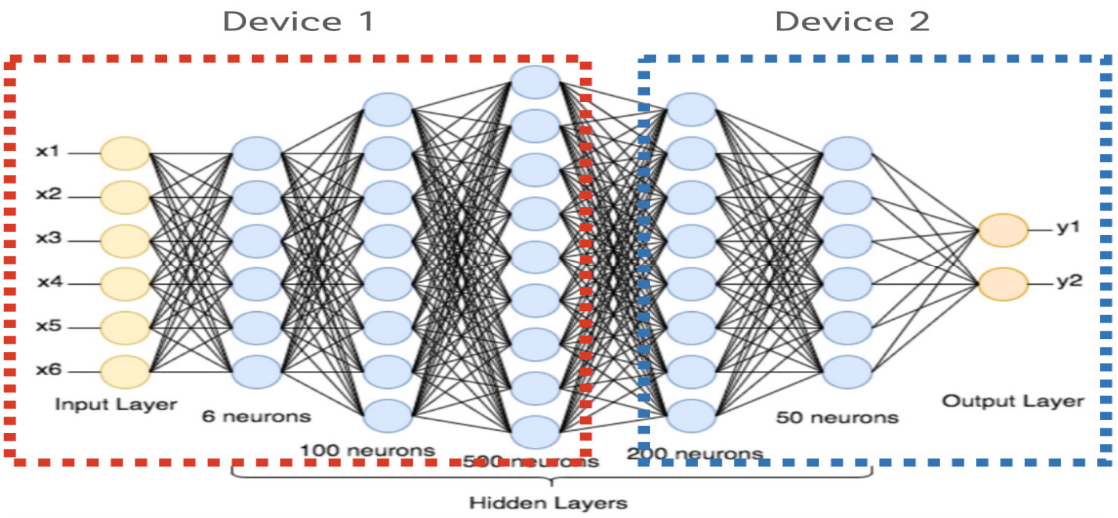
Horovod: fast and easy distributed deep learning in Tensorflow
https://arxiv.org/pdf/1802.05799.pdf

Model Parallel

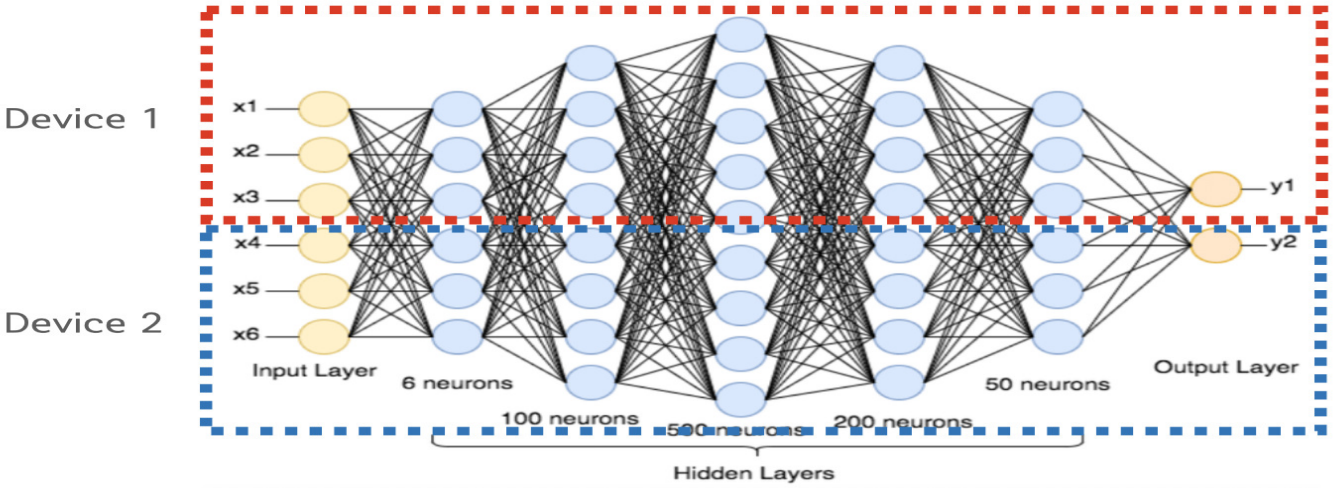
- **Inter-layer Model Parallel**
  - pipeline parallel
- **Intra-layer Model Parallel**
  - Tensor parallel
- **Multi-dimensional Parallel**
  - 3D parallel



Inter/Intra-layer Model Parallel

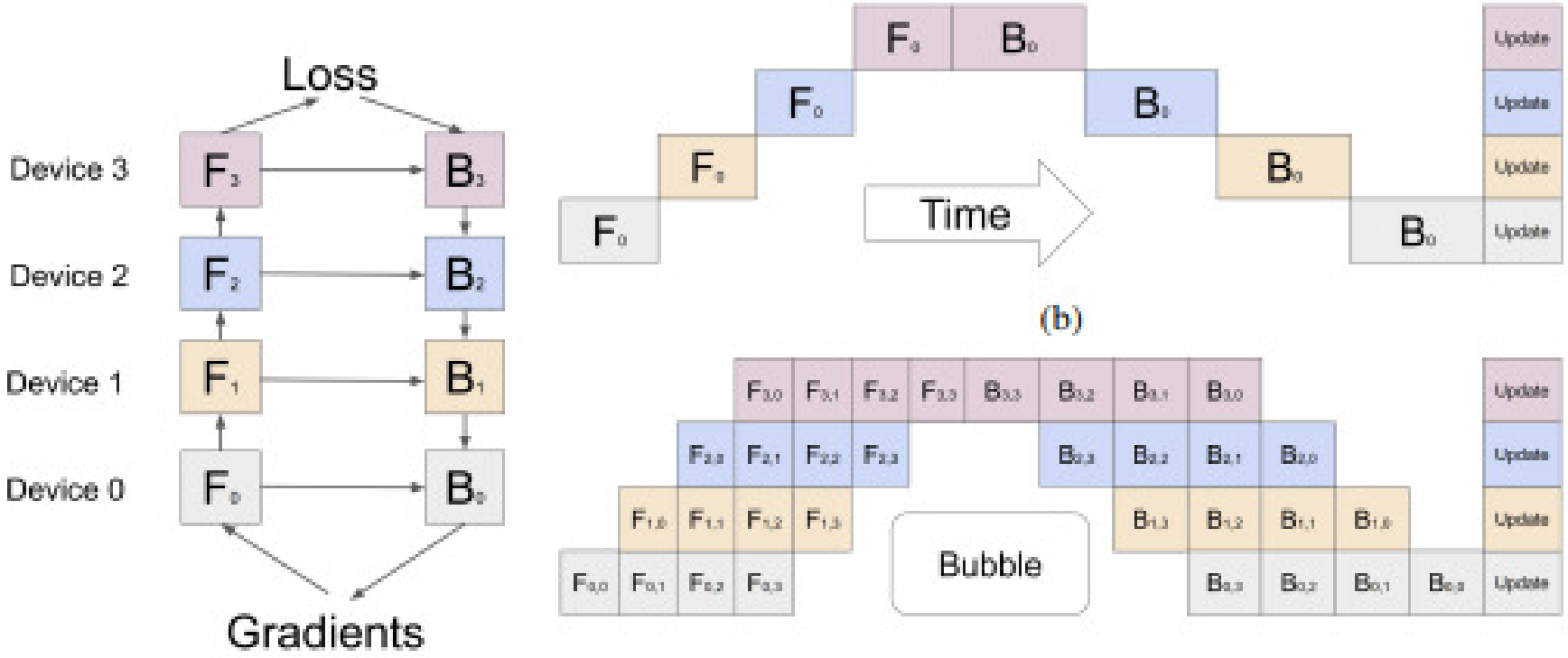


Inter- layer model parallel



Intra- layer model paralle

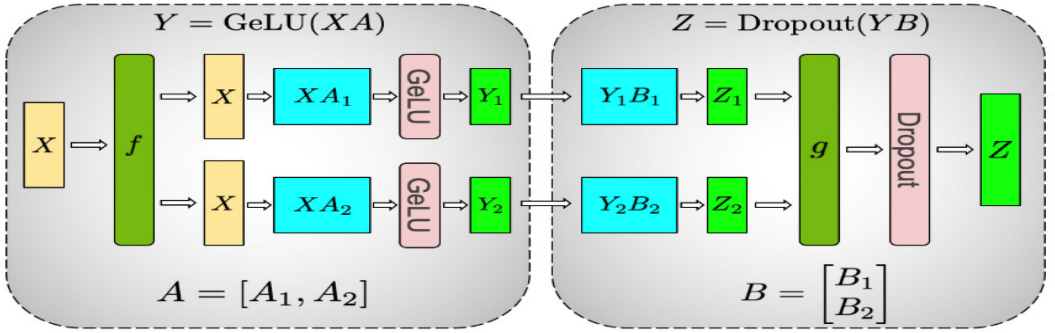
Pipeline Model Parallel



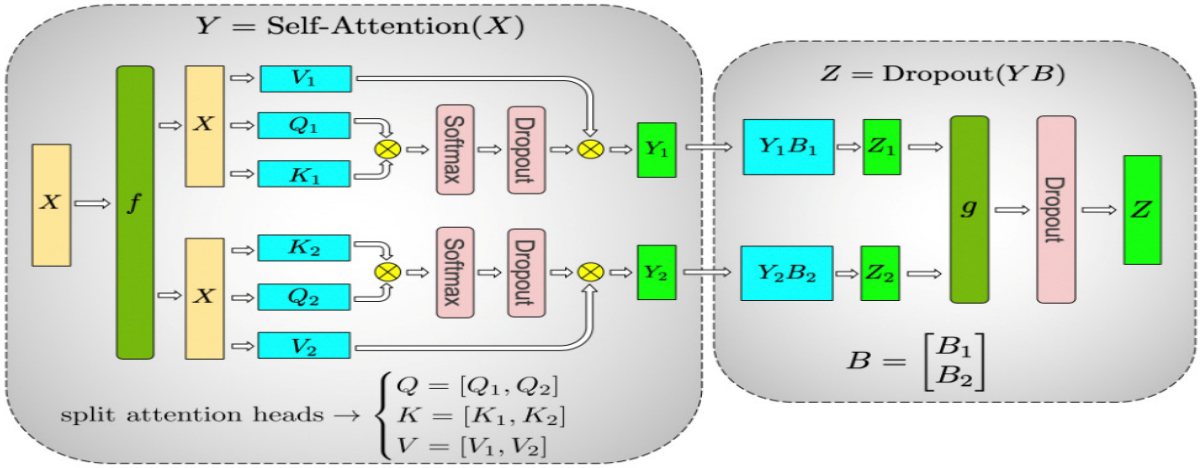
GPipe: Easy Scaling with Micro- Batch Pipeline Parallelism
https://arxiv.org/pdf/1811.06965.pdf

PipeDream: Fast and Efficient Pipeline Parallel DNN Training
https://arxiv.org/pdf/1806.03377.pdf

Tensor Parallel



(a) MLP

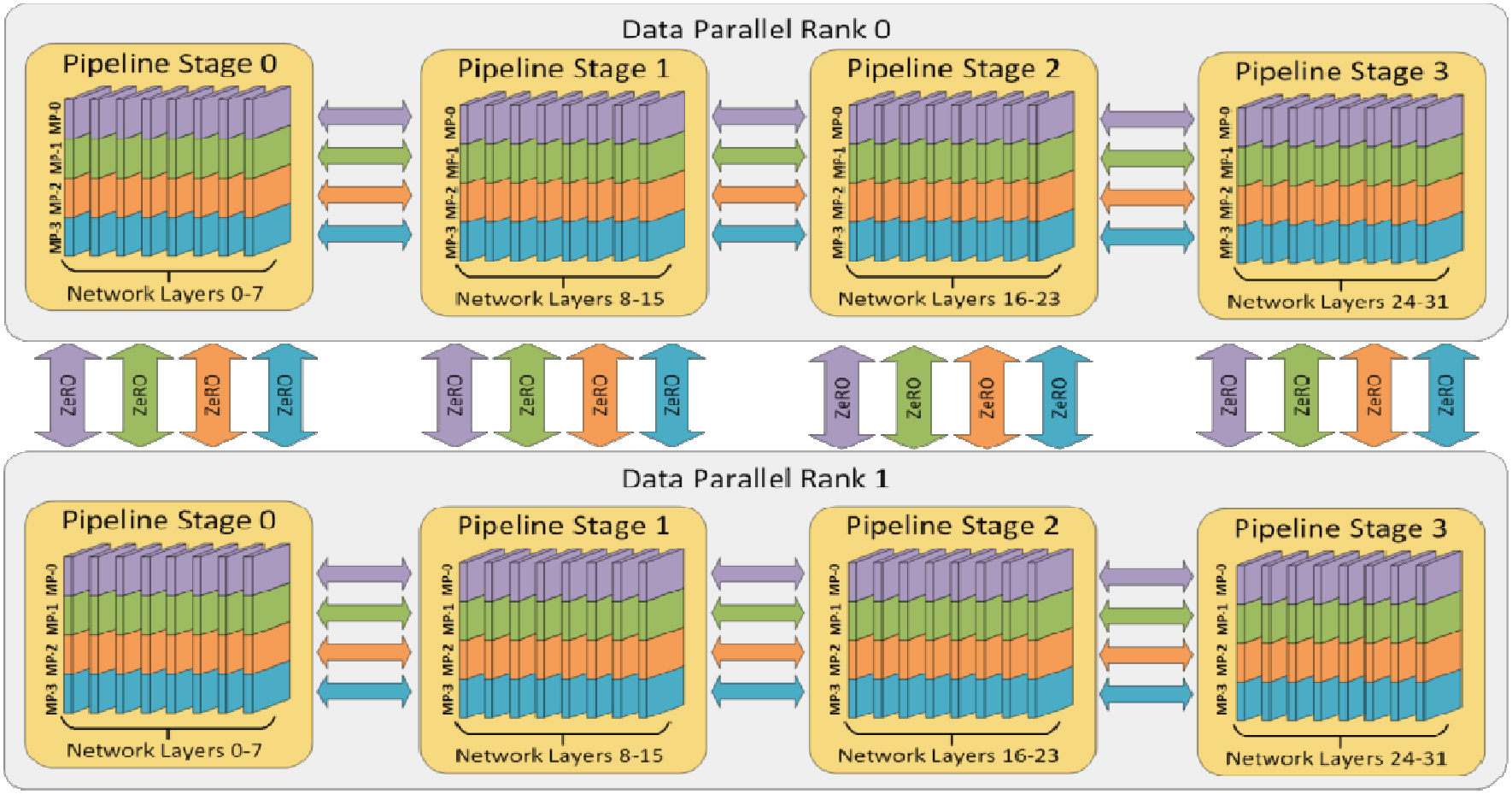


(b) Self attention

Megatron- LM: Training Multi- Billion Parameter Language Models Using Model Parallelism
https://arxiv.org/pdf/1909.08053.pdf

3D Parallel

- **Data Parallel + Pipeline Parallel + Tensor Parallel**

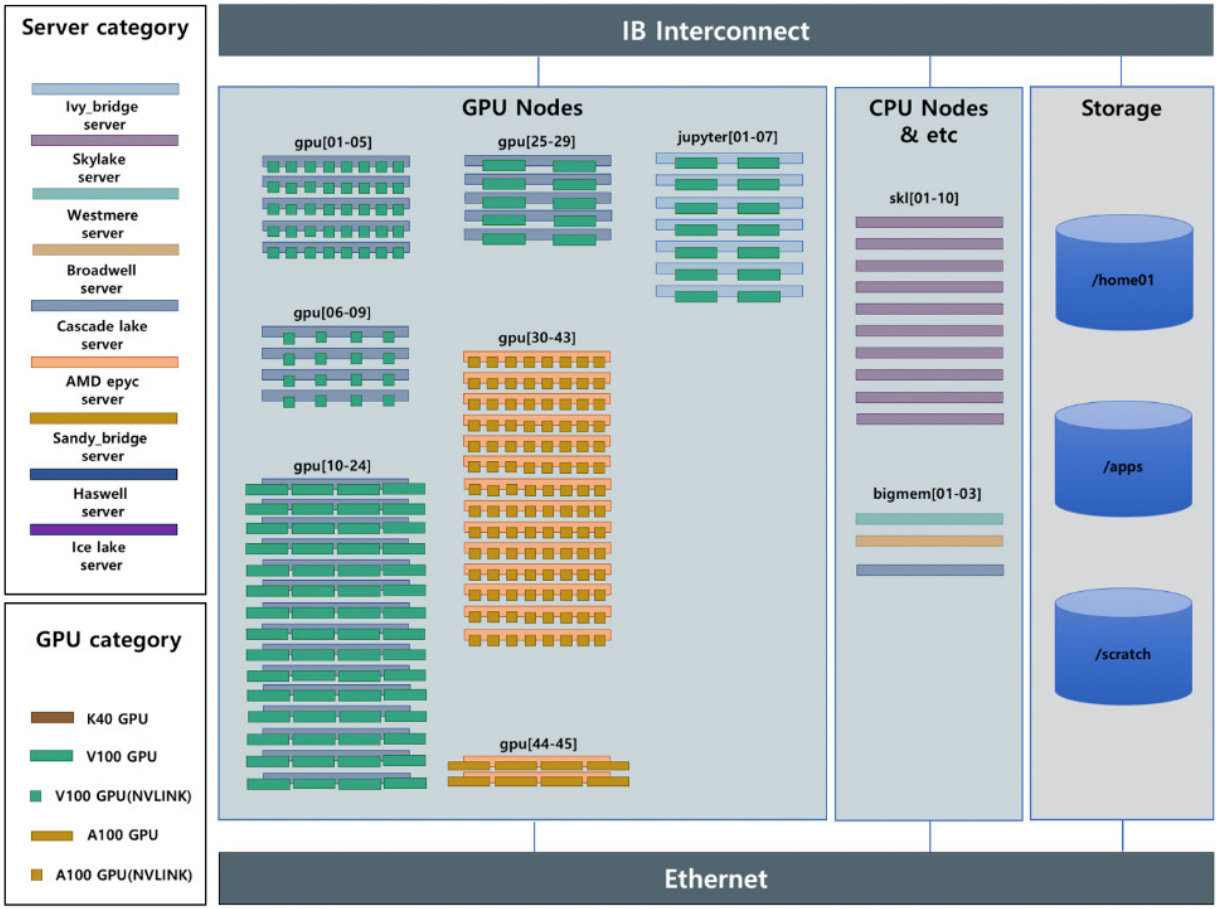


DeepSpeed: Extreme- scale model training for everyone

https://www.microsoft.com/en- us/research/blog/deepspeed- extreme- scale- model- training- for- everyone

KISTI GPU Cluster: Neuron

KISTI GPU Cluster: Neuron



year	#node	#GPU	#Flops
2018	44	53	312.8TF
2019	63	99	698.8TF
2020	78	163	1.24PF
2021	59	200	2.34PF
2022	65	260	3.53PF

Slurm Queues on Neuron

Queue Name (CPU_GPU_GPU#)	#Node	#Total CPU Core	#Job Submission Limit per User	#GPU allocation Limit per User	
cas_v100nv_8	5	160	2	40	V100 (NVlink) 8ea
cas_v100nv_4	4	160	2	16	V100 (NVlink) 4ea
cas_v100_4	15	600	4	40	V100 4ea
cas_v100_2	5	160	2	10	V100 2ea
amd_a100nv_8	14	868	4	64	A100 (Nvlink) 8ea
amd_a100_4	2	128	1	8	A100 4ea
amd_a100_2	2	128	1	4	A100 2ea
skl	10	360	2	-	
bigmem	3	120	1	-	

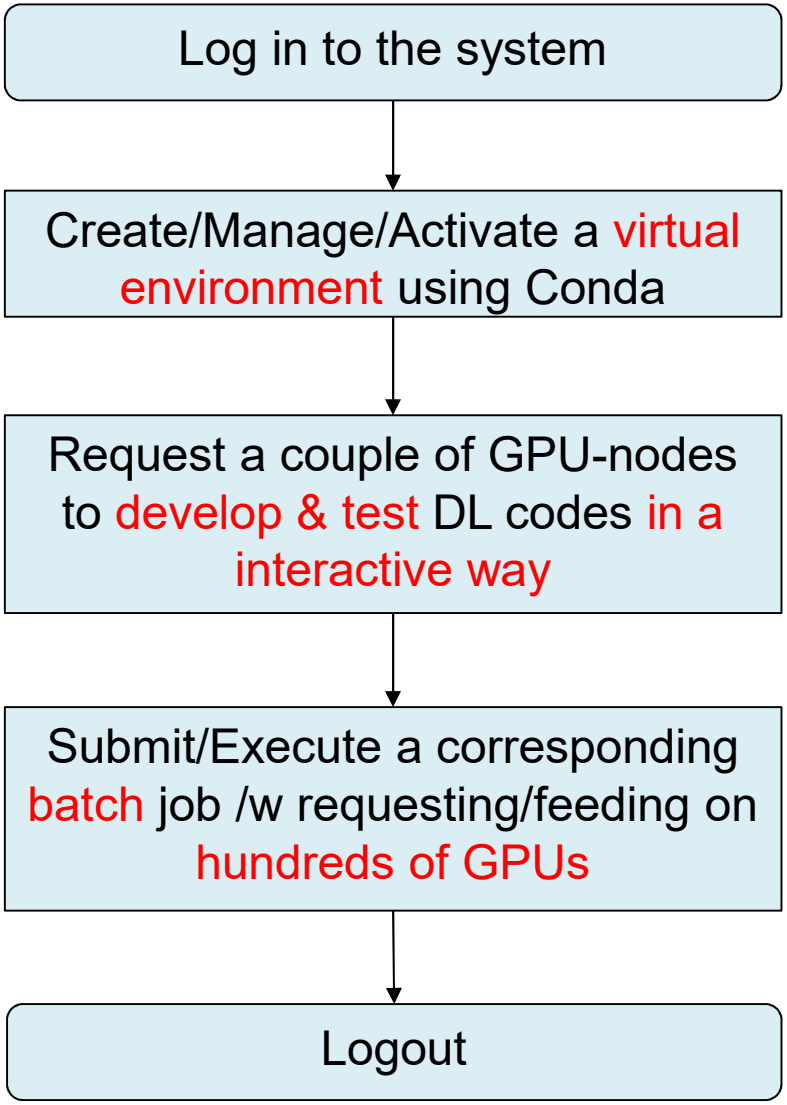
Slurm Queues & available GPUs on Neuron

```
$ sinfo
PARTITION    AVAIL  TIMELIMIT  NODES  STATE NODELIST
jupyter        up 2-00:00:00      3    mix jupyter[02-04]
jupyter        up 2-00:00:00      1   idle jupyter01
cas_v100nv_8    up 2-00:00:00      1    mix gpu01
cas_v100nv_8    up 2-00:00:00      4  alloc gpu[02-05]
cas_v100nv_4    up 2-00:00:00      1    mix gpu09
cas_v100nv_4    up 2-00:00:00      2  alloc gpu[07-08]
cas_v100_4      up 2-00:00:00      2    mix gpu[13,17]
cas_v100_4      up 2-00:00:00     10  alloc gpu[10-12,18-24]
cas_v100_4      up 2-00:00:00      2   idle gpu[14-15]
cas_v100_2      up 2-00:00:00      1    mix gpu25
cas_v100_2      up 2-00:00:00      1  alloc gpu26
amd_a100nv_8    up 2-00:00:00      2    mix gpu[36-37]
amd_a100nv_8    up 2-00:00:00      6  alloc gpu[30,32-33,39-41]
amd_a100nv_8    up 2-00:00:00      1   idle gpu42
amd_a100_4      up 2-00:00:00      1    mix gpu44
amd_a100_4      up 2-00:00:00      1  alloc gpu45
skl           up 2-00:00:00      8   idle skl[01-06,08-09]
bigmem         up 2-00:00:00      2   idle bigmem[01-02]
exclusive       up   infinite      1    mix gpu06
scidebert       up   infinite      1    mix gpu35
scidebert       up   infinite      1  alloc gpu34
new_service     up   infinite      4  down* bigmem03,jupyter[05-06],skl07
maintenance     up   infinite      6   idle gpu[16,29,31,38,43],jupyter07
```

- **Slurm Quick Start User Guide**
  - https://slurm.schedmd.com/quickstart.html
- **KISTI User Guide**
  - https://www.ksc.re.kr/gsjw/jcs/hd

Distributed Training Workflow on Supercomputer

Distributed Training Workflow on Neuron




```
## create/activate a virtual environment
$ conda create -n pt_env python=3.7
$ conda activate pt_env
$ (pt_env) conda install pytorch
$ (pt_env) python train.py
```

```
## request 2 nodes for interactive job
$ salloc --nodes=2 --time=8:00:00 --
gres=gpu:4 # available GPU-nodes allocated

## run& test ML/DL codes interactively
$ (pt_env) srun -n 8 python train_ddp.py
```

```
## submit a batch job script requesting 20
nodes with 8 GPUs each node
$ (pt_env) sbatch train_ddp_script.sh

## monitor/check the job status
$ (pt_env) squeue
```

Conda Virtual Environment

Conda Virtual Environment

- **Download & Install Conda on /scratch/userID directory**

```
## Miniconda
$ wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh
$ chmod 755 Miniconda3-latest-Linux-x86_64.sh
$ ./Miniconda3-latest-Linux-x86_64.sh
```

- ✓ Type your Conda installation directory to "/scratch/userID/miniconda3"
  - ✓ Conda default installation directory: $HOME/miniconda3
- ✓ Type Conda init: "yes", which will add conda init scripts to ~/.bashrc

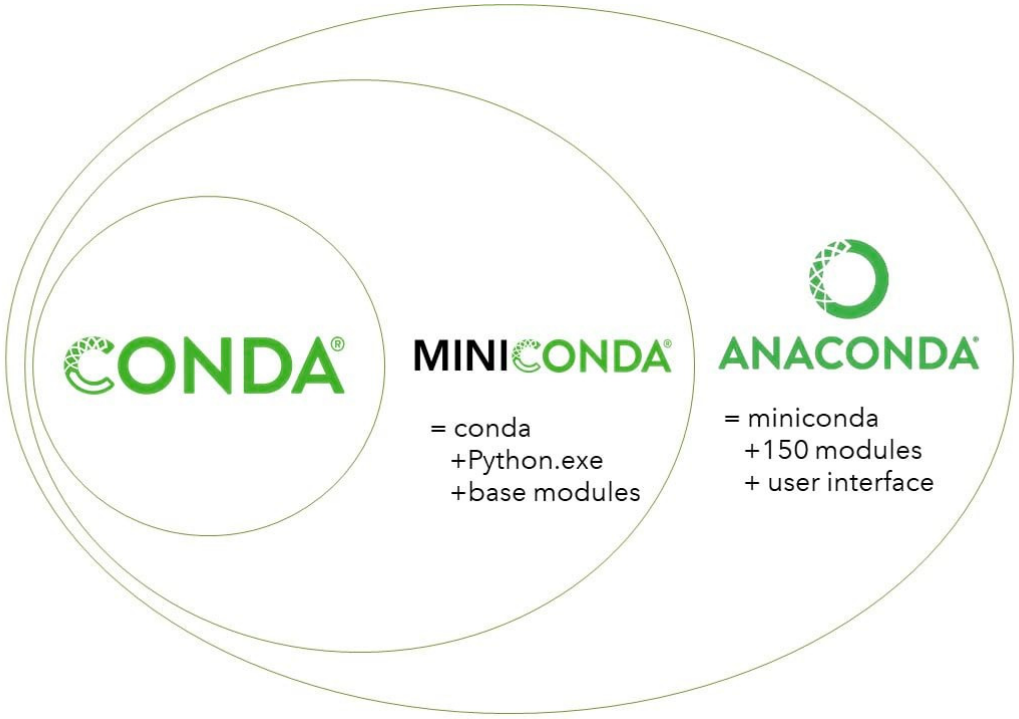
```
$ source ~/.bashrc    # set conda path
$ conda config --set auto_activate_base false
$ which conda
/scratch/$USER/miniconda3/condabin/conda
$ conda --version
conda 4.12.0
$ ls /scratch/$USER/miniconda3
./              conda-meta/  lib/        mkspecs/     qml/        ssl/
../             doc/         libexec/    phrasebooks/ resources/  translations/
bin/            envs/        LICENSE.txt pkgs/        sbin/       var/
....
```

Anaconda

- **Anaconda**
  - distribution of the Python and R programming languages for scientific computing
    - data science, machine learning applications, large-scale data processing, predictive analytics, etc
  - aims to simplify package management and deployment
- **Conda**
  - open source package management system and environment management system
  - runs on Windows, macOS, Linux and z/OS
  - quickly installs, runs and updates packages and their dependencies.
- **PIP**
  - package installer for Python
  - use pip to install packages from the Python Package Index and other indexes.

Miniconda

- **a small, bootstrap version of Anaconda**
  - includes only conda, Python, the packages they depend on
- **a free minimal installer for conda**



Anaconda vs Miniconda

- **Number of packages**
  - Anaconda comes with over 150 data science packages, whereas miniconda comes with only a handful
- **Interface**
  - Anaconda has a graphical user interface (GUI) called the Navigator, while miniconda has a command-line interface

```
### Anaconda Download
$ wget https://repo.anaconda.com/archive/Anaconda3-2022.10-Linux-x86_64.sh

### Miniconda Download
$ wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh
```

Conda command

clean	Remove unused packages and caches.
config	Modify configuration values in .condarc. This is modeled after the git config Writes to the user .condarc file (/home01/userID/.condarc) by default.
create	Create a new conda environment from a list of specified packages.
help	Displays a list of available conda commands and their help strings.
info	Display information about current conda install.
init	Initialize conda for shell interaction. [Experimental]
install	Installs a list of packages into a specified conda environment.
list	List linked packages in a conda environment.
package	Low-level conda package utility. (EXPERIMENTAL)
remove	Remove a list of packages from a specified conda environment.
uninstall	Alias for conda remove.
run	Run an executable in a conda environment. [Experimental]
search	Search for packages and display associated information. The input is a MatchSpec, a query language for conda packages. See examples below.
update	Updates conda packages to the latest compatible version.
upgrade	Alias for conda update

Horovod

Horovod

- **distributed deep learning training framework for TensorFlow, Keras, PyTorch, and Apache MXNet**
  - developed by Uber
- **aims to make distributed deep learning fast and easy to use**

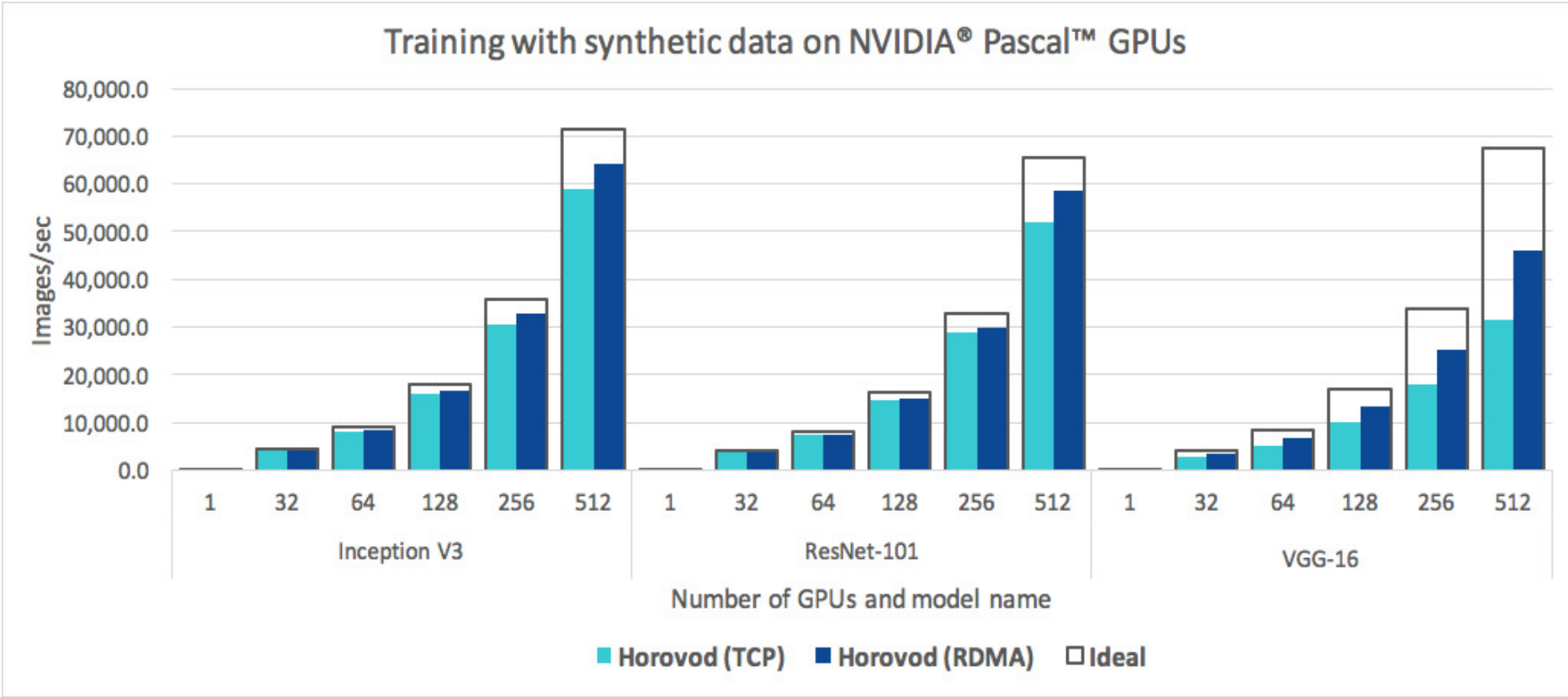
Why Horovod?

- **The primary motivation for this project is to make it easy to take a single-GPU training script and successfully scale it to train across many GPUs in parallel**
  - ✓ How much modification does one have to make to a program to make it distributed, and how easy is it to run it?
  - ✓ How much faster would it run in distributed mode?

- **Internally at Uber we found the MPI model to be much more straightforward and require far less code changes than previous solutions such as Distributed TensorFlow with parameter servers.**

Why Horovod?

- easy to use and fast
- scalling with Horovod



Horovod Usage

- **5 steps/lines to be added in your code**
  - Initialize Horovod
  - Pin GPU to each worker
  - Wrap the optimizer
  - Synchroize state across workers
  - Checkpoint on the first worker

Initialize Horovod

- **Tensorflow**
  - import horovod.tensorflow as hvd
  - hvd.init()
- **Kera**
  - import horovod.keras as hvd
  - hvd.init()
- **Pytorch**
  - import horovod.torch as hvd
  - hvd.init()

Pin a GPU for each worker

- **Tensorflow**
  - tf.config.experimental.set_visible_devices(gpus[hvd.local_rank()], 'GPU')
- **Keras**
  - tf.config.experimental.set_visible_devices(gpus[hvd.local_rank()], 'GPU')
- **Pytorch**
  - torch.cuda.set_device(hvd.local_rank())

Adjust learning rate and wrap the optimizer

- **Tensorflow**
  - opt = tf.optimizers.Adam(0.01 * hvd.size())
  - opt = hvd.DistributedOptimizer(opt,…)
- **Keras**
  - opt = keras.optimizers.Adadelta(0.01 * hvd.size())
  - opt = hvd.DistributedOptimizer(opt,…)
- **Pytorch**
  - opt = optim.SGD(model.parameters(), 0.01 * hvd.size())
  - opt= hvd.DistributedOptimizer(opt, …)

Synchronize state across workers

- **Tensorflow/Kera**
  - callbacks = [hvd.callbacks.BroadcastGlobalVariablesCallback(0)]
- **Pytorch**
  - hvd.broadcast_parameters(model.state_dict(), root_rank=0)
  - hvd.broadcast_optimizer_state(optimizer, root_rank=0)

- **Ensure all workers start with the same weights**

Checkpoint on the first worker (rank 0)

- **Tensorflow/Keras**
  - if hvd.rank() == 0:
    callbacks.append(keras.callbacks.ModelCheckpoint(args.checkpoint_format))
- **Pytorch**
  - if hvd.rank() == 0:

```
state = {'model': model.state_dict(),
         'optimizer': optimizer.state_dict(), }
torch.save(state, filepath)
```

Pytorch Example

```
import torch
import horovod.torch as hvd

# Initialize Horovod
hvd.init()

# Horovod: pin GPU to local rank.
torch.cuda.set_device(hvd.local_rank())

# Build model.
model = Net()
model.cuda()
optimizer = optim.SGD(model.parameters())

# Horovod: wrap optimizer with DistributedOptimizer.
optimizer = hvd.DistributedOptimizer(
    optimizer,
    named_parameters=model.named_parameters())
```

```
# Horovod: broadcast parameters.
hvd.broadcast_parameters(
    model.state_dict(),
    root_rank=0)

for epoch in range(100):
  for batch_idx, (data, target) in enumerate(...):
      optimizer.zero_grad()
      output = model(data)
      loss = F.nll_loss(output, target)
      loss.backward()
      optimizer.step()
```

Horovod execution command

- **MPI takes care of launching processes on all nodes**
- **Run on a 4-GPU machine**
  - $ salloc …
  - $ mpirun -np 4 -H localhost:4 python train_hvd.py
  - $ horovodrun -np 4 -H localhost:4 python train_hvd.py
  - $ srun -n python train_hvd.py
- **Run on 4 machines with 4-GPUs each**
  - $ salloc …
  - $ mpirun/horovodrun -np 4 -H node1:4,node2:4,node3:4,node4:4 python train_hvd.py
  - $ srun -n 16 python train_hvd.py

Horovod Installation on Neuron

```
$ module load gcc/10.2.0 cuda/11.4 cudampi/openmpi-4.1.1 cmake/3.16.9
$ conda create -n horovod
$ conda activate horovod
$ conda install pytorch==1.12.0 torchvision==0.13.0 torchaudio==0.12.0 cudatoolkit=11.3 -c pytorch
$ pip install tensorflow-gpu==2.10.0
$ HOROVOD_GPU_OPERATIONS=NCCL HOROVOD_WITH_TENSORFLOW=1
HOROVOD_WITH_PYTORCH=1 \
HOROVOD_WITH_MPI=1 HOROVOD_WITH_GLOO=1 pip install --no-cache-dir horovod
$ horovodrun -cb
Horovod v0.26.1:

Available Frameworks:
    [X] TensorFlow
    [X] PyTorch
    [ ] MXNet

Available Controllers:
    [X] MPI
    [X] Gloo

Available Tensor Operations:
    [X] NCCL
    [ ] DDL
    [ ] CCL
    [X] MPI
    [X] Gloo
```

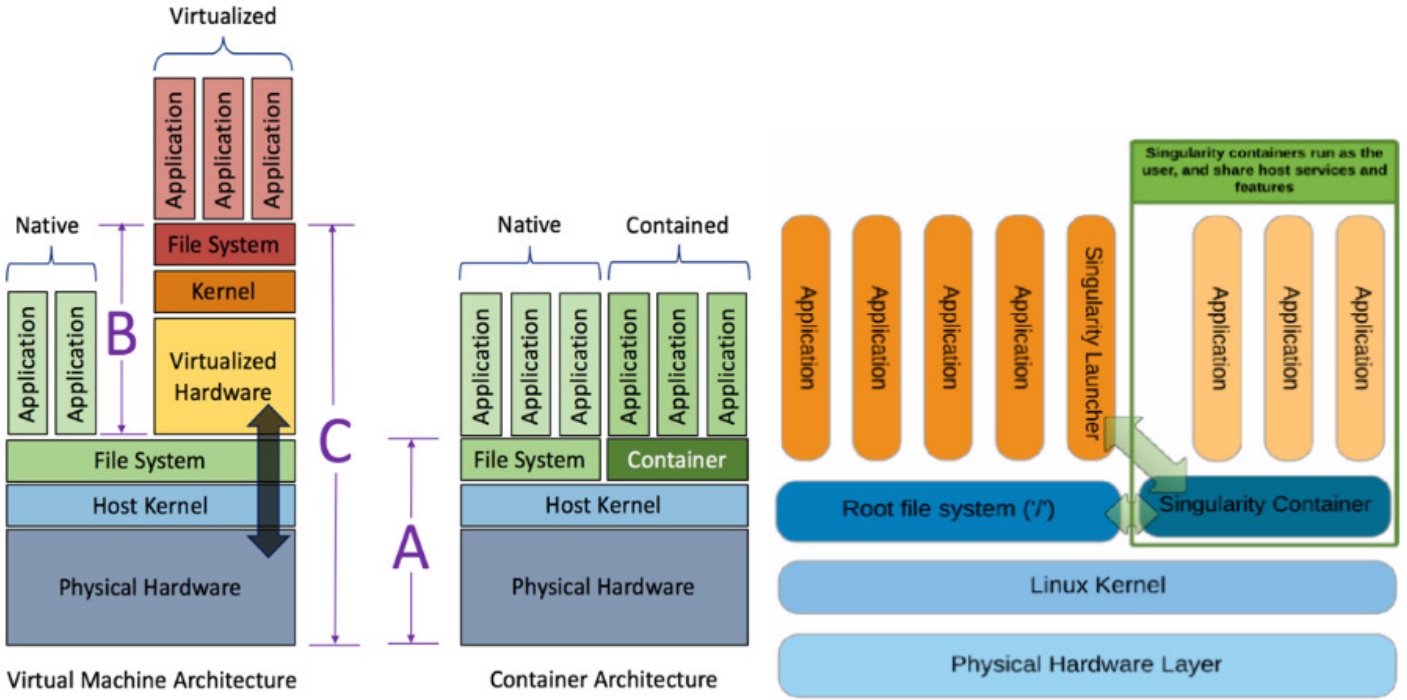
Horovod execution on Neuron

```
1) request an allocation of available on neuron
$ salloc --partition=amd_a100nv_8 -J debug --nodes=2 --time=2:00:00 --
gres=gpu:4 --comment=horovod

2) load modules
$ module load gcc/10.2.0 cuda/11.4 cudampi/openmpi-4.1.1 cmake/3.16.9

3) activate the horovod virtual environment
$ conda activate horovod

4) run horovod applications
(horovod) $ mpirun/horovod -np 8 -H gpu#:4,gpu#:4 python train_hvd.py
(horovod) $ srun -n python train_hvd.py
```

Singularity Container

Singularity

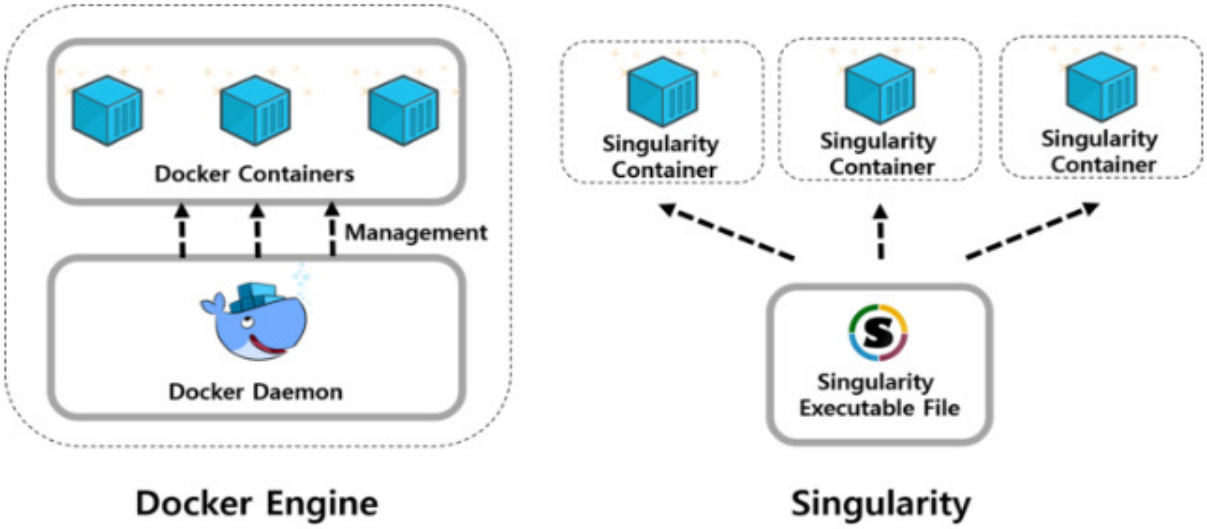
- **a container platform for HPC**



Container-based applications have *direct access* to the host kernel and hardware and, thus, are able to achieve similar performance to native applications. In contrast, VM-based applications only have *indirect access* via the guest OS and hypervisor, which creates a significant performance overhead.

Why Singularity?

- **A container platform for HPC**
  - Each container is a single image file
  - No root owned daemon processes
  - Support shared/multi-tenant resource environment
  - Support HPC hardware
    - Infiniband, GPUs
  - Support HPC applications
    - MPI



Running Horovod using Singularity on Neuron

- **No bother to deal with conda & horovod**
- **Just allocate nodes using salloc and run singularity container. That's it!!!**

```
$ salloc --partition=amd_a100nv_8 -J debug --nodes=2 --time=2:00:00 --
gres=gpu:4 --comment=horovod

$ srun -n 8 singularity run --nv
/apps/applications/singularity_images/ngc/pytorch_22.03-hd-py3.sif python
pytorch_imagenet_resnet50.py
/usr/bin/rm: cannot remove '/usr/local/cuda/compat/lib': Read-only file system
/usr/bin/rm: cannot remove '/usr/local/cuda/compat/lib': Read-only file system
…….
Train Epoch     #10:   0%|          | 1/5005 [00:13<19:03:52, 13.72s/it, loss=2.29, accurTrain Epoch
#10:   0%|          | 1/5005 [00:13<19:03:52, 13.72s/it, loss=2.22, accurTrain Epoch     #10:   0%|          |
2/5005 [00:13<19:03:38, 13.72s/it, loss=2.16, accurTrain Epoch     #10:   0%|          | 3/5005
[00:13<5:00:52,  3.61s/it, loss=2.16, accuraTrain Epoch     #10:   0%|          | 3/5005 [00:13<5:00:52,
3.61s/it, loss=2.17, accuraTrain Epoch     #10:   0%|          | 4/5005 [00:13<5:00:48,  3.61s/it, loss=2.23,
accura
……..
```

Singularity Usage on Neuron

- **Web site: https://www.ksc.re.kr/gsjw/jcs/hd**

- **DDL training job scripts directory**
  - /apps/applications/singularity_images/examples
- **Singularity Container Images directory**
  - /apps/applications/singularity_images/ngc
- **Pytorch examples directory**
  - Single node
    - /apps/applications/singularity_images/examples/pytorch/resnet50v1.5
  - Multiple nodes
    - /apps/applications/singularity_images/examples/horovod/examples/pytorch
- **Imagenet datasets directory**
  - Training data
    - /apps/applications/singularity_images/imagenet/train
  - Validation data
    - /apps/applications/singularity_images/imagenet/val

Thank you

Contact: Soonwook Hwang <hwang@kisti.re.kr>

github.com/hwang2006/KISTI-DL-tutorial-using-horovod