MPI and Distributed DL

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CSCI-GA.3033-020 HPML

Performance Factors

Algorithms Performance

- Communication patterns
- Performance Modeling

Hyperparameters Performance

• Hyperparameters choice

Implementation Performance

• Implementation of the algorithms on top of a framework

Framework Performance

Python, PyTorch Distributed DL

Libraries Performance

• CUDA, cuDNN, cuBLAS, Communication Libraries (MPI, Gloo)

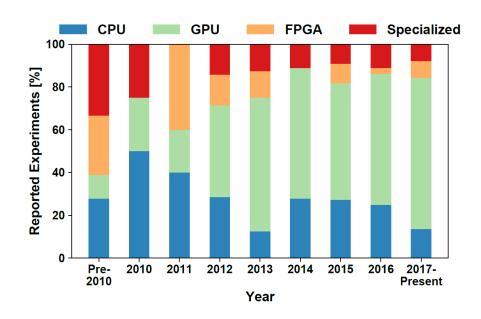
Hardware Performance

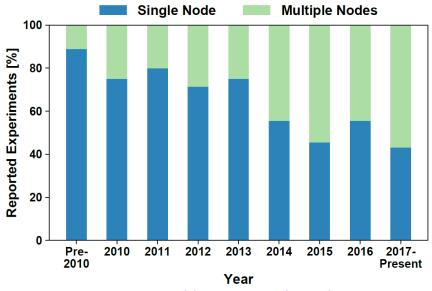
• CPU, DRAM, GPU, HBM, Tensor Units, Disk/Filesystem, Network

DL Hardware Trends

Trend: From Parallel to Distributed DL

- Deep Learning has always exploited parallel architectures
- During the years:
 - DL has been moving towards distributed architectures
 - GPUs have become the default compute architecture

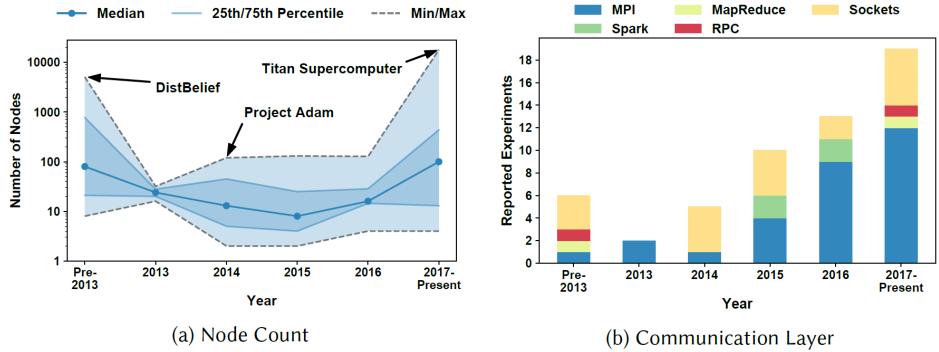




From:https://arxiv.org/abs/1802.09941

Trend: Growing scale for Distributed DL

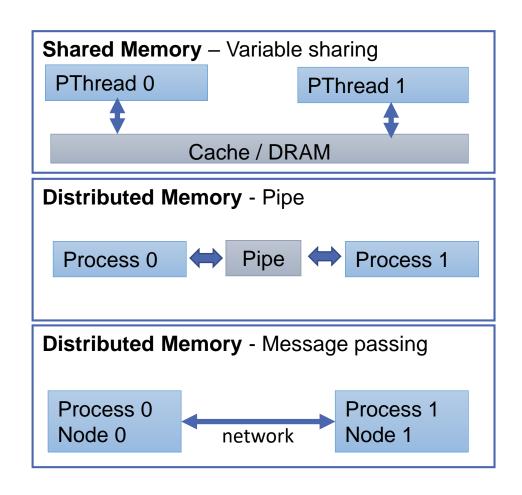
- GPUs are the main focus from 2013
- Node count has been growing since 2015
- MPI adoption becomes larger



Message Passing Interface

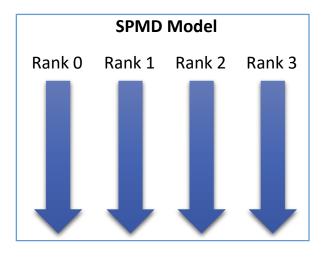
Distributed vs. Shared Memory Programming

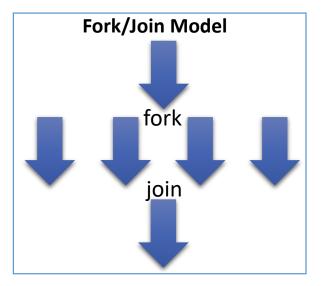
- Shared Memory:
 - Access the same virtual address space
 - Pass data by reference
 - Example:
 - Share a variable with pthreads
- Distributed Memory:
 - Separate Virtual Address Spaces
 - Cannot access shared data structures
 - Pass data by value (copy)
 - Examples:
 - Send an element through a process pipe
 - Send message across network



SPMD vs Fork/Join

- SPMD (Single Program Multiple Data): execution starts in parallel (different from fork-join style)
 - MPI implements SPMD
 - 1 program executed by multiple processes (MPI ranks)
 - Programmers need to think in parallel from the beginning of the execution
 - Static parallelism: number of processes does not change
- Fork/Join: execution starts serial new processes or threads are created at fork operation
 - pthread create()/fork() /OpenMP are examples of fork/join
 - Dynamic parallelism: number of processes can change at each fork





TCP vs MPI

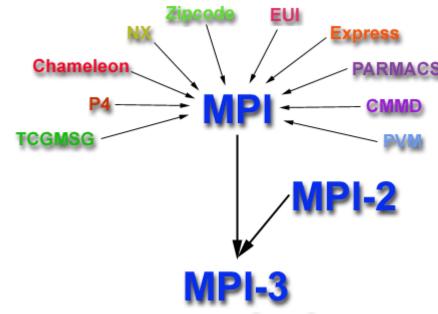
TCP stack	MPI stack
Connections based on IP addresses and ports	Based on rank number
Point-to-point communication	Point-to-point, collectives, one-sided
Stream-oriented	Message Oriented
Raw data (bytes/octets)	Typed messages
Network independent	Network independent
high latency	low latency

Message Passing Interface

What is MPI?

MPI is a **standard specification** of a message passing interface for large scale systems (Supercomputers)

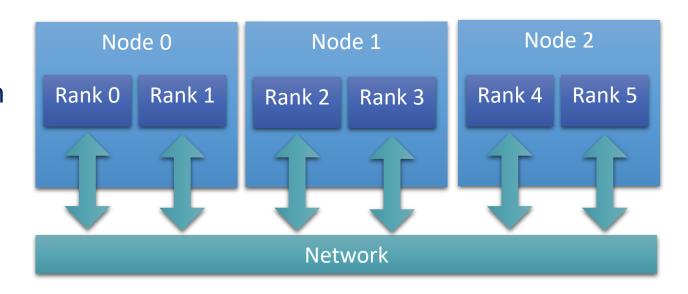
- Advantages
 - Standardization
 - Portability
 - Performance optimization
 - Functionality
- First version released: MPI-1.0 in 1994
- Today: MPI 3.1



From: https://computing.llnl.gov/tutorials/mpi/

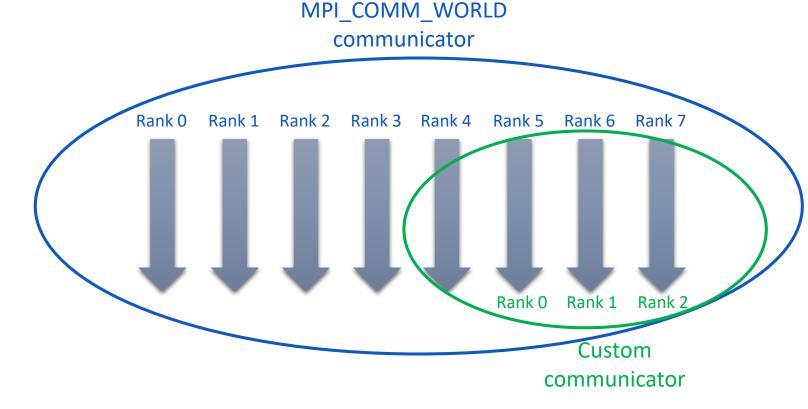
MPI – System components

- Node:
 - A single host on the network
- Rank:
 - A process executing the MPI program
- MPI is executed on multiple nodes (thousands easily)
- Each node can have many processes
 - Usually one per core



MPI Programmer View

- Nodes are transparent to programmer
- Only ranks matter
- Communicator:
 - A group of ranks that can communicate
- MPI_COMM_WORLD
 - Communicator that includes all the ranks



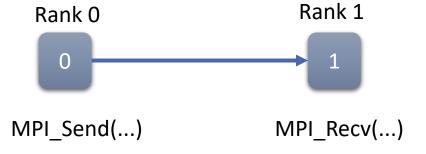
MPI Data Types

- MPI messages types and size is specified in advance
 - higher performance
 - less programming errors with types
- A message is always composed by one or more elements of MPI datatype size
- Definition of new types is possible
 - example: new data structures
- MPI_Byte and also dynamic sizing is also available for special cases

MPI datatype	C equivalent
MPI_SHORT	short int
MPI_INT	int
MPI_LONG	long int
MPI_LONG_LONG	long long int
MPI_UNSIGNED_CHAR	unsigned char
MPI_UNSIGNED_SHORT	unsigned short int
MPI_UNSIGNED	unsigned int
MPI_UNSIGNED_LONG	unsigned long int
MPI_UNSIGNED_LONG_LO	unsigned long long int
MPI_FLOAT	float
MPI_DOUBLE	double
MPI_LONG_DOUBLE	long double
MPI_BYTE	char

Point-to-Point

- MPI_Send() and MPI_Recv() can happen in any order: MPI runtime will take care to deliver the message
- Destination is only based on the rank and communicator (0 or 1)
- Message is typed, we are not sending just "bytes"
- Can multiple int (float, double) etc.



```
// Find out rank, size
int world rank;
MPI Comm rank(MPI COMM WORLD, &world rank);
int world size;
MPI_Comm_size(MPI_COMM_WORLD, &world_size);
int number;
if (world rank == 0) {
    number = -1;
    MPI Send(&number, 1, MPI_INT, 1, 0, MPI_COMM_WORLD);
} else if (world_rank == 1) {
    MPI_Recv(&number, 1, MPI_INT, 0, 0, MPI_COMM_WORLD,
             MPI STATUS IGNORE);
    printf("Process 1 received number %d from process 0\n",
           number);
```

int MPI_Send(const void *buf, int count, MPI_Datatype datatype, int dest, int tag, MPI_Comm comm)
int MPI_Recv(void *buf, int count, MPI_Datatype datatype, int source, int tag, MPI_Comm comm, MPI_Status * status)

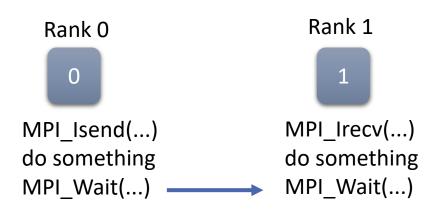
Point-to-Point – MPI_Send() Semantic

- When MPI_Send() returns:
 - We can reuse the communication buffers
 - It does not imply that the message arrived
 - It does not imply that the message left the local node
- How to know if a message actually arrived?
 - Need to send an MPI message back
 - Use one-sided MPI primitives to write directly to the receiver memory using RDMA (not part of the course)

```
// Find out rank, size
int world rank;
MPI Comm rank(MPI_COMM_WORLD, &world_rank);
int world size;
MPI Comm size(MPI_COMM_WORLD, &world_size);
int number;
if (world rank == 0) {
   number = -1;
   MPI Send(&number, 1, MPI INT, 1, 0, MPI COMM WORLD);
   number = 0 // reuse buffer
} else if (world rank == 1) {
   MPI_Recv(&number, 1, MPI_INT, 0, 0, MPI_COMM_WORLD,
             MPI STATUS IGNORE);
    printf("Process 1 received number %d from process 0\n",
           number);
   number = 0; // reuse buffer
```

Non Blocking Point-to-Point

- MPI_ISend() and MPI_IRecv() can happen in any order: MPI runtime will take care to deliver the message
- Isend and Irecv are non-blocking: process can continue execution and then wait later

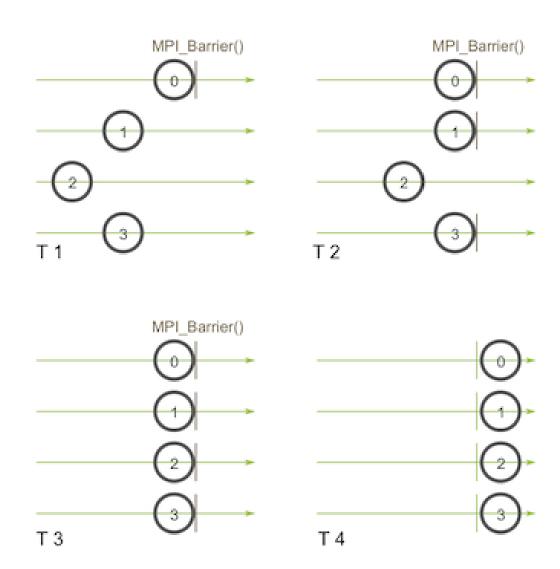


```
int myid, numprocs, left, right;
int buffer[10], buffer2[10];
MPI Request request, request2;
MPI Status status;
MPI Init(&argc,&argv);
MPI Comm size(MPI COMM WORLD, &numprocs);
MPI Comm rank(MPI COMM WORLD, &myid);
right = (myid + 1) % numprocs;
left = myid - 1;
if (left < 0)
     left = numprocs - 1;
MPI Irecv(buffer, 10, MPI INT, left, 123, MPI COMM WORLD, &request);
MPI Isend(buffer2, 10, MPI_INT, right, 123, MPI_COMM_WORLD, &request2);
MPI Wait(&request, &status);
MPI Wait(&request2, &status);
MPI Finalize();
```

Barriers and Synchronization

- MPI_Barrier() is used to synchronize ranks
- It is a fundamental primitive for parallel programming
- Barrier implementation and latency are key to many algorithms performance

MPI_Barrier(MPI_Comm communicator)



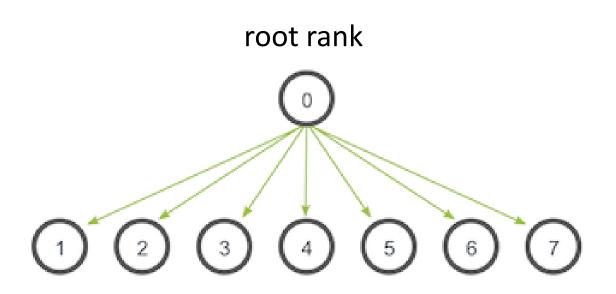
Collectives

- Collectives: communication patterns that involve data exchange across multiple ranks
- Type of collectives:
 - Reduce, AllReduce
 - Gather, AllGather
 - Scatter
 - AllToAll
 - Broadcast
- Collectives represent the biggest value of MPI implementations
- Some collectives can be hardware accelerated (ex barriers, or reduce)

Broadcast

- Root rank (can be any rank) sends the same single message to multiple receivers
- Message can contain multiple elements of type DataType

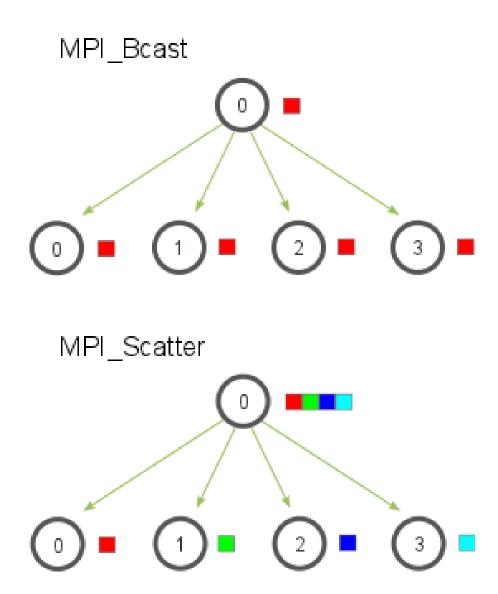
```
MPI_Bcast(
    void* data,
    int count,
    MPI_Datatype datatype,
    int root,
    MPI_Comm communicator)
```



Scatter

 Root rank sends the a different single message to each receiver

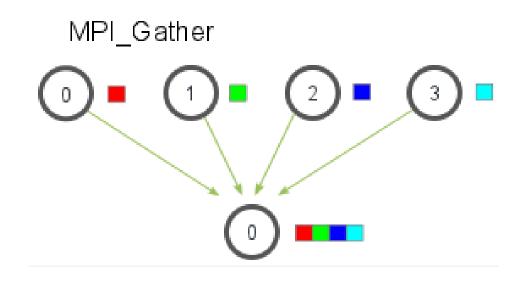
```
MPI_Scatter(
    void* send_data,
    int send_count,
    MPI_Datatype send_datatype,
    void* recv_data,
    int recv_count,
    MPI_Datatype recv_datatype,
    int root,
    MPI_Comm communicator)
```



Gather

 Root rank gather a different single message from each receiver

```
MPI_Gather(
    void* send_data,
    int send_count,
    MPI_Datatype send_datatype,
    void* recv_data,
    int recv_count,
    MPI_Datatype recv_datatype,
    int root,
    MPI_Comm communicator)
```



Average with Gather and Scatter

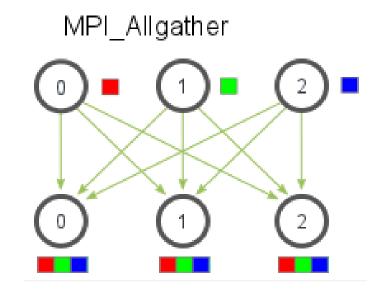
- Gather and Scatter example to compute the average of FLOAT numbers
- Ranks are in world_rank

```
if (world rank == 0) {
 rand nums = create rand nums(elements per proc * world size);
// Create a buffer that will hold a subset of the random numbers
float *sub rand nums = malloc(sizeof(float) * elements per proc);
// Scatter the random numbers to all processes
MPI Scatter(rand nums, elements per proc, MPI FLOAT, sub rand nums,
      elements per proc, MPI FLOAT, 0, MPI COMM WORLD);
// Compute the average of your subset
float sub avg = compute avg(sub rand nums, elements per proc);
// Gather all partial averages down to the root process
float *sub avgs = NULL;
if (world rank == 0) {
 sub avgs = malloc(sizeof(float) * world size);
MPI Gather(&sub avg, 1, MPI FLOAT, sub avgs, 1, MPI FLOAT, 0,
     MPI COMM WORLD);
// Compute the total average of all numbers.
if (world rank == 0) {
 float avg = compute avg(sub avgs, world size);
```

All Gather

- All Gather is composed of one gather for each rank
- Useful when all ranks need the result of the gather

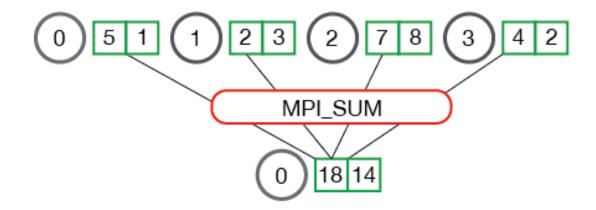
```
MPI_Allgather(
   void* send_data,
   int send_count,
   MPI_Datatype send_datatype,
   void* recv_data,
   int recv_count,
   MPI_Datatype recv_datatype,
   MPI_Comm communicator)
```



Reduce

- Reduces a set of numbers into a smaller set of numbers via a function
- In the picture MPI_SUM is used as reduce function
- Reduce can involve multiple elements per rank

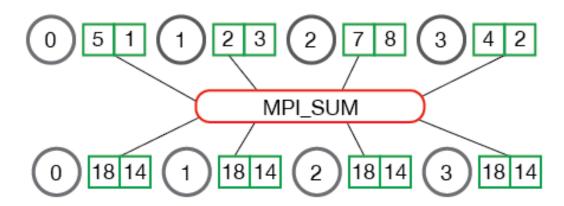
```
MPI_Reduce(
    void* send_data,
    void* recv_data,
    int count,
    MPI_Datatype datatype,
    MPI_Op op,
    int root,
    MPI_Comm communicator)
```



All Reduce

- Reduces a set of numbers into a smaller set of numbers via a function
- Each rank obtains the result
- In the picture MPI_SUM is used as reduce function
- All Reduce can involve multiple elements per rank

```
MPI_Allreduce(
    void* send_data,
    void* recv_data,
    int count,
    MPI_Datatype datatype,
    MPI_Op op,
    MPI_Comm communicator)
```



Reduce – Available Functions

- MPI_MAX Returns the maximum element
- MPI_MIN Returns the minimum element
- MPI_SUM Sums the elements
- MPI_PROD Multiplies all elements
- MPI_LAND Performs a logical and across the elements
- MPI_LOR Performs a logical or across the elements
- MPI_BAND Performs a bitwise and across the bits of the elements
- MPI_BOR Performs a bitwise or across the bits of the elements
- MPI_MAXLOC Returns the maximum value and the rank of the process that owns it
- MPI_MINLOC Returns the minimum value and the rank of the process that owns it

StdDev with All Reduce

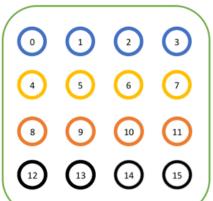
- Using all reduce to compute the standard deviation of a set of numbers
- Each rank obtains the result

```
rand nums = create rand nums(num elements per proc);
// Sum the numbers locally
float local sum = 0;
int i;
for (i = 0; i < num elements per proc; i++) {
  local sum += rand nums[i];
// Reduce all of the local sums into the global sum in order to
// calculate the mean
float global sum;
MPI Allreduce(&local_sum, &global_sum, 1, MPI_FLOAT, MPI_SUM,
              MPI COMM WORLD);
float mean = global sum / (num elements per proc * world size);
// Compute the local sum of the squared differences from the mean
float local sq diff = 0;
for (i = 0; i < num elements per proc; i++) {
  local sq diff += (rand nums[i] - mean) * (rand nums[i] - mean);
// Reduce the global sum of the squared differences to the root
// process and print off the answer
float global sq diff;
MPI_Reduce(&local_sq_diff, &global_sq_diff, 1, MPI_FLOAT, MPI_SUM, 0,
           MPI COMM WORLD);
// The standard deviation is the square root of the mean of the
// squared differences.
if (world rank == 0) {
  float stddev = sqrt(global_sq_diff /
                      (num elements per proc * world size));
  printf("Mean - %f, Standard deviation = %f\n", mean, stddev);
                                                                 27
```

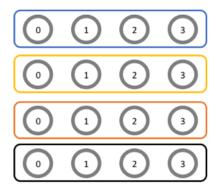
Multiple Communicators

- MPI_COMM_WORLD can be split in multiple communicators to allow communication in sub-groups of processes
- Rank numbers and communication are always associated with a communicator
- Example shows how to split communicators with MPI_Comm_Split()

MPI_COMM_WORLD communicator



Multiple communicators



```
// Get the rank and size in the original communicator
int world rank, world size;
MPI Comm rank(MPI COMM WORLD, &world rank);
MPI Comm size(MPI COMM WORLD, &world size);
int color = world rank / 4; // Determine color based on row
// Split the communicator based on the color and use the
// original rank for ordering
MPI Comm row comm;
MPI Comm split(MPI COMM WORLD, color, world rank,
&row comm);
int row rank, row size;
MPI Comm rank(row comm, &row rank);
MPI Comm size(row comm, &row size);
printf("WORLD RANK/SIZE: %d/%d \t ROW RANK/SIZE: %d/%d\n",
         world rank, world size, row rank, row size);
MPI Comm free(&row comm);
```

DL Performance Modeling

Performance Modeling for distributed systems

- Performance Modeling on current Large Scale Distributed Systems is extremely complex:
 - Network performance
 - Network Topologies
 - Network Traffic
 - Node performance
 - CPU, Multicores, Hardware Threading
 - GPU, Blocks, Shared memory
 - Memories:
 - Caches, DRAM, HBM

Performance Modeling with Cost Models

- Simplify reality with very strong assumption
- Make possible reasoning about algorithms and underlying systems
- Need to be validated with measurement and experimentation
- No substitute for actual implementation and real experiments

Work and Depth Cost Model

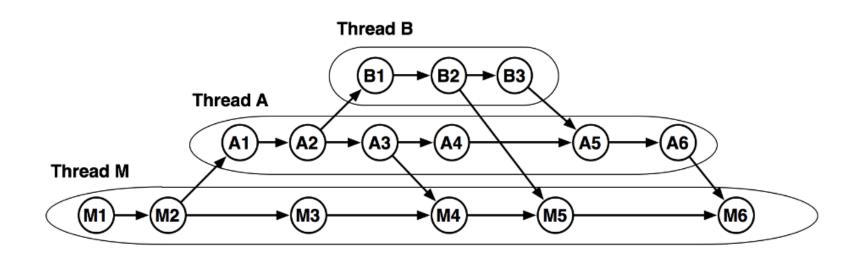
 Cost Model for Parallel Algorithms (ignores communication cost) executing on multiple processors

Assumptions:

- Communication time among processors ignored
- Memory accesses ignored
- Processors activity is clock-synchronized
- Computations steps are constant size

Work and Depth Cost Model

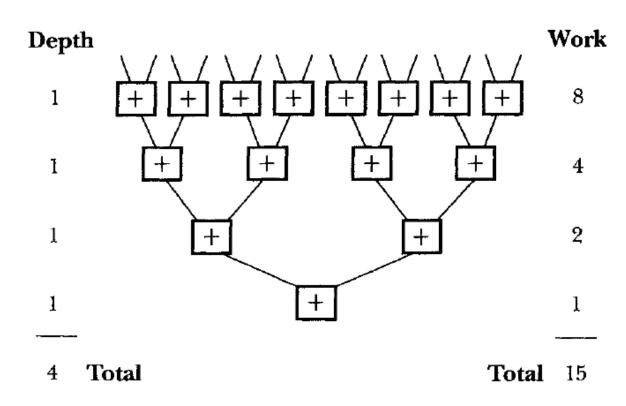
- The execution of a parallel algorithm can be represented by a directed acyclic graph - DAG
- Directed edges represent data dependencies
- Vertices represent a computation



from: http://www.cs.cmu.edu/afs/cs/academic/class/15210-f15/www/tapp.html# dag representation

Work and Depth Cost Model (1)

- Work w: the total number of operations executed by a computation
- Depth d (also called span): the longest chain of sequential dependencies
- Example:
 - Reduction with SUM function

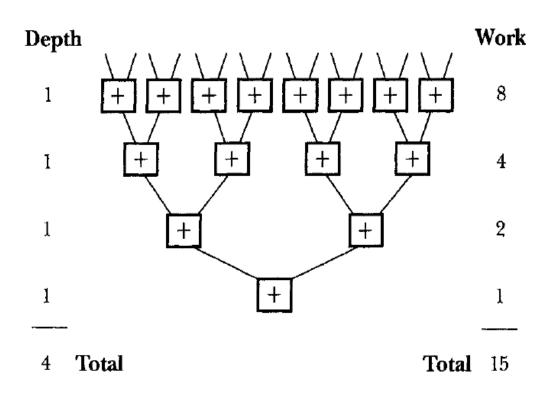


From:https://www.cs.cmu.edu/afs/cs/Web/People/blelloc h/papers/B85.pdf

Work and Depth Model (2)

- We assume 1 time unit per compute operation
- T₁: time units to compute work on a single processor
- T_{∞} : time units to **compute** work on a infinite number of processors
- Relationship to work and depth:

$$T_1 = W$$
 $T_{\infty} = D$

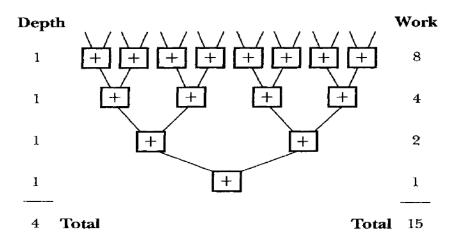


From:https://www.cs.cmu.edu/afs/cs/Web/People/blelloch/papers/B85.pdf

Work and Depth model bounds

- T_p : execution Time on p processes
 - Lower bound: max{W/p, D}
 - Upper bound: O(W/p + D)
 - where $\frac{W}{p} \ge 1$

$$\max\left\{\frac{W}{p},D\right\} \leq T_{p} \leq O\left(\frac{W}{p}+D\right)$$



From:https://www.cs.cmu.edu/afs/cs/Web/People/blelloch/papers/B85.pdf

Analysis of All-Reduce with Work and Depth (1)

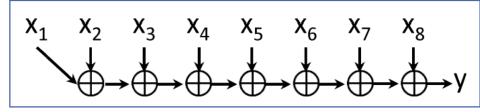
- All-Reduce with n operations using operator ⊕:
 - $Y = X_1 \oplus X_2 \oplus X_3 \oplus X_4 \oplus X_5 \oplus X_6 \oplus X_7 \oplus X_n$
- If \bigoplus is **non-associative** (ex. subtraction or division):
 - W = n 1 = 7
 - D = n 1 = 7
 - Average Parallelism: W/D = 1
 - T_p bounds:

$$\max\left\{\frac{W}{p}, D\right\} \le T_{p} \le O\left(\frac{W}{p} + D\right)$$

$$\max\left\{\frac{n-1}{p}, n-1\right\} \le T_{p} \le O\left(\frac{n-1}{p} + n - 1\right)$$

$$n-1 \le T_p \le O\left((n-1)\left(1-\frac{1}{p}\right)\right)$$

$$n-1 \le T_p \le O(n-1)$$



From:https://arxiv.org/abs/1802.09941

Analysis of All-Reduce with Work and Depth (3)

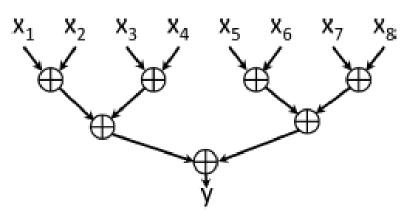
- All-Reduce with n operations using operator \oplus :
 - $Y = X_1 \oplus X_2 \oplus X_3 \oplus X_4 \oplus X_5 \oplus X_6 \oplus X_7 \oplus X_n$
- If \oplus is **associative** (ex. addition or multiplication):
 - W = n 1 = 7
 - $D = log_2(n) = 2.81$
 - Average Parallelism: W/D = 2.49
 - T_p bounds:

$$\max\left\{\frac{W}{p}, D\right\} \le T_p \le O\left(\frac{W}{p} + D\right)$$

$$\max\left\{\frac{n-1}{p}, log_2(n)\right\} \le T_p \le O\left(\frac{n-1}{p} + D\right)$$

$$log_2(n) \le T_p \le O\left(\frac{n-1}{p} + log_2(n)\right)$$
 assuming $p = n - 1$

$$\log_2(n) \le \boldsymbol{T_p} \le O(\log_2(n))$$



From:https://arxiv.org/abs/1802.09941

Alpha Beta Cost Model

 Network communication cost model based on latency and bandwidth only

Assumptions:

- Network costs are constant during the time
- Latency and Bandwidth are constant across different nodes/topologies
- No CPU costs involved in communication

Alpha Beta Cost Model

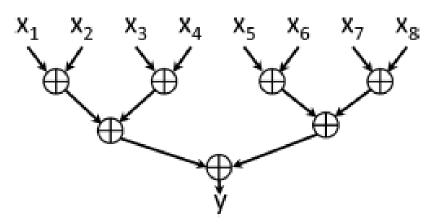
• Parameters:

- **P**: number of processors on the network (nodes)
- α : fixed communication latency (time to send zero-length msg)
- β : time to send one byte
- γ : size in bytes of message

- Time to transmit a message:
 - $T = \alpha + \beta \times \gamma$

Alpha Beta Cost Model

- Reduction analysis with Alpha-beta cost model:
 - E.g. all nodes on same switch
 - E.g. 1 Message with all elements in array (γ =N)
 - Phase (2->1, 4->3,...), phase (3->1, 7->5,...)...
 - Reduction-Time estimates:
 - $T_r \ge \alpha \log_2(P)$, latency time
 - $T_r \ge log_2(P) \gamma \beta$
 - Pipelining => more messages per node but communication overlap.



From: https://arxiv.org/abs/1802.09941

LogP Cost Model

- Cost model that includes Network Communication cost
- See: https://dl.acm.org/citation.cfm?doid=155332.155333
- Assumptions:
 - one processor per node (no intra-node communication)
 - message size is small
 - communication time (network time + cpu time) dominates execution
 - computation time usually assumed 1 cycle
 - memory access ignored

LogP Cost Model

- Parameters:
 - **P**: number of processors on the network (nodes)
 - L: communication latency to send one small message of one word over the network
 - o: cpu time spent to receive or send a message
 - g: minimum time gap between two network messages
 - 1/g = injection rate
 - word-size/g = bandwidth

LogP Cost Model (2)

- Example: Broadcast analysis with LogP model
- Optimal tree: unbalanced

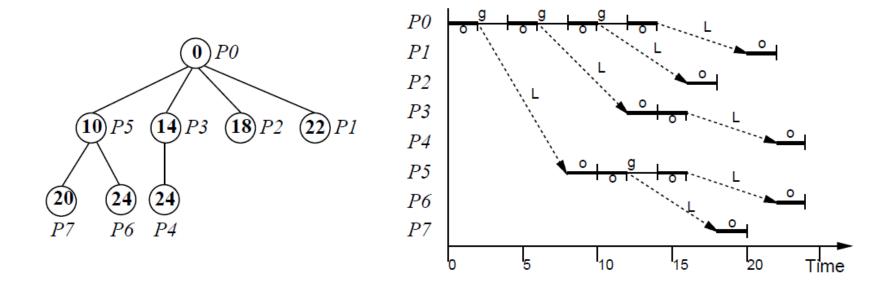


Figure 3: Optimal broadcast tree for P = 8, L = 6, g = 4, o = 2 (left) and the activity of each processor over time (right). The number shown for each node is the time at which it has received the datum and can begin sending it on. The last value is received at time 24.

From: https://dl.acm.org/citation.cfm?doid=155332.155333

DDL Performance Modeling

- DDL are composed of many parts
- For simplicity we can divide DDL performance modeling in
 - Layers Computation Modeling
 - Fully connected Layers (linear + activation)
 - Convolution Layers
 - Pooling
 - RNN
 - Communication Modeling
 - All-Reduce
 - Parameter server

Layer Computation Performance Modeling

- Layers Performance modeling is hard even with basic work models:
 - Work/Depth
- Example: cublasSgem performance for various sizes

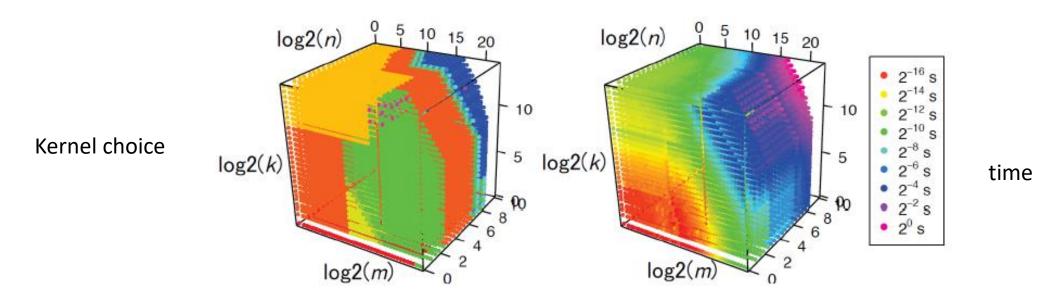
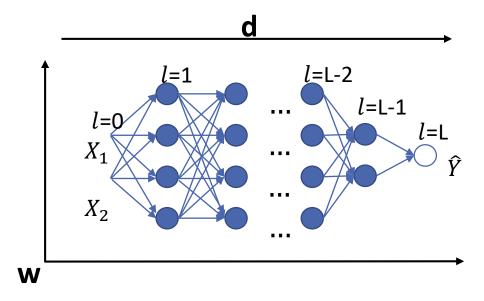


Fig. 17. Performance of cublasSgemm on an NVIDIA Tesla K80 for various matrix sizes (adapted from [Oyama et al. 2016])

From:https://arxiv.org/abs/1802.09941

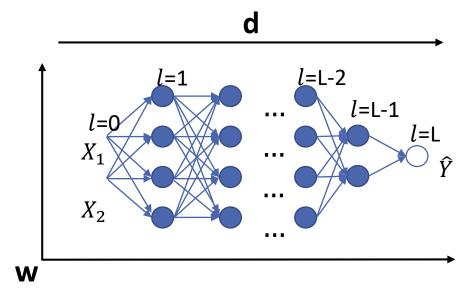
Layer Computation Performance Modeling

- Work and depth application to DL:
 - Work w is proportional to the size and depth of layers (tensors)
 - Proportional to samples/batch
 - Depth **d** is **proportional** to the depth of the network



Layer Computation Performance Modeling (d)

- Average parallelism: w/d
 - More features => higher w => higher average parallelism
 - More layers => higher w but also d => same average parallelism
 - More layers but same work => higher w but also d => less average parallelism
 - Large batchsize => expensive layers fully use GPU!



DL Parallelism Approaches

Model Parallelism

split model across multiple compute engines

Data Parallelism

split data across multiple compute engines

Pipelining

use layers as pipeline to keep all compute engines busy

Hybrid Parallelism

use multiple approaches together

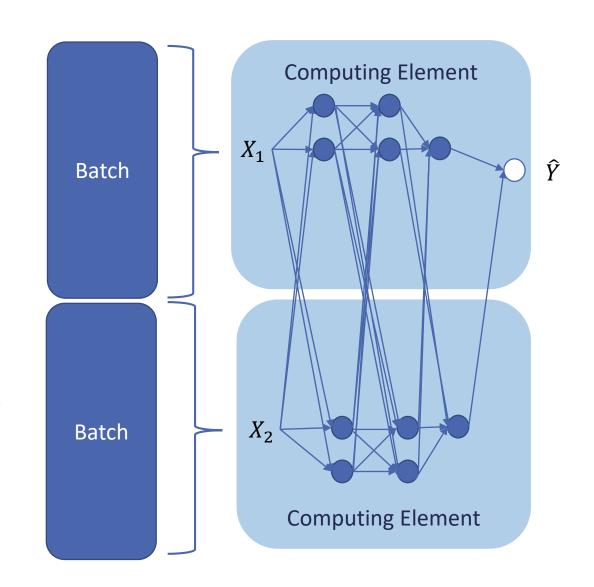
ML Model Parallelism

Model Parallelism:

- 1. Divide the model in parts
- Each computing element (CPU core or GPU thread) receives its part of the model
- 3. Send same batch to the computing elements
- 4. Model merges at the end

Characteristics:

- Latency of communication between the computing elements (fine-gran communication) degrades performance
- Harder to obtain performance if computing elements are far apart
- Used among GPU threads or CPU cores/threads

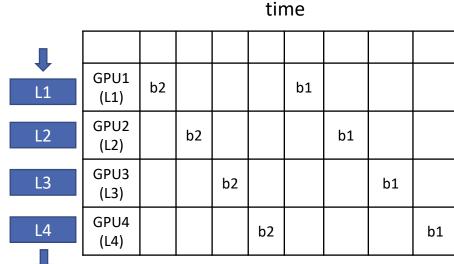


DL Pipelining

- Pipelining approach:
 - Split layers among compute engines
 - Each minibatch *b* (or sample s) goes from one compute engine to the next one: no need to wait for next one to exit the pipeline
- Is a form of **Model Parallelism**
- Pipelining performance

Ideal pipelining speedup:
$$S = \frac{time \ without \ pipeline}{number \ of \ pipeline \ stages}$$

- Speedup is higher for deeper networks 🤝
- Ideal pipelining never reached because of "bubbles" that cause idle CPUs
- SGD pipeline bubble:
 - Before weights update, all batches need to have completed forward (otherwise accept **staleness**)



Non-pipelined execution

time

GPU1 b8 b7 b6 b4 b3 b2 b5 b1 L1 (L1) GPU₂ L2 b8 b5 b2 b7 b6 b4 b3 (L2) GPU3 L3 b6 b8 b5 b3 b7 b4 (L3) GPU4 L4 b8 b7 b6 b5 b4 (L4)

Pipelined execution

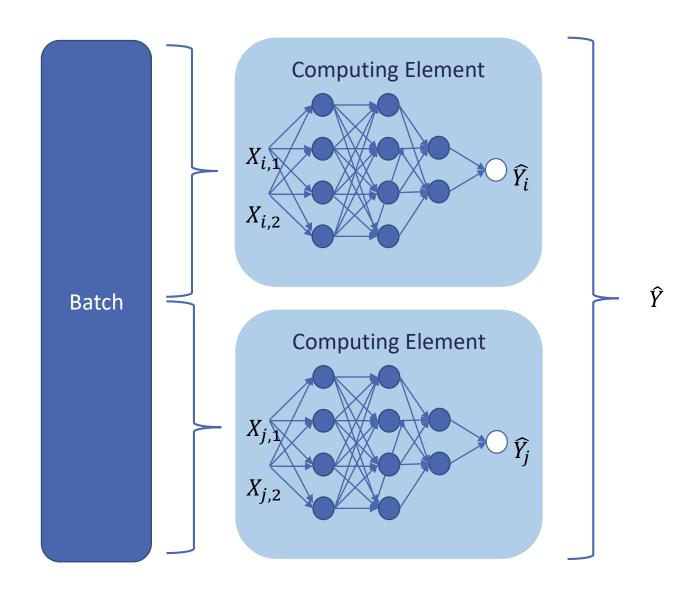
ML Data Parallelism

Data Parallelism:

- 1. replicate model on each computing element (CPU core, GPU thread, or Cluster node)
- 2. Each computing element gets a portion of the batch
- 3. Each computing element trains/infers in parallel on the model
- 4. Gather the results at the end.

Characteristics:

- Used among GPUs devices or among cluster nodes
- PyTorch: DataParallel already implemented
- Can be also implemented using different batches instead of parts of one batch (typically among nodes in a cluster)



Lesson Key Points

- DL Hardware Trends
 - GPU and Communication trends
- MPI
 - Interface
 - Communication primitives
 - API Semantic
- Performance Models
 - Work Depth model
 - Alpha Beta model
 - LogP model