Practical Parallel Computing (実践的並列コンピューティング)

Part3: MPI (3)
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"mm" sample: Matrix Multiply (Revisited, related to [M2])

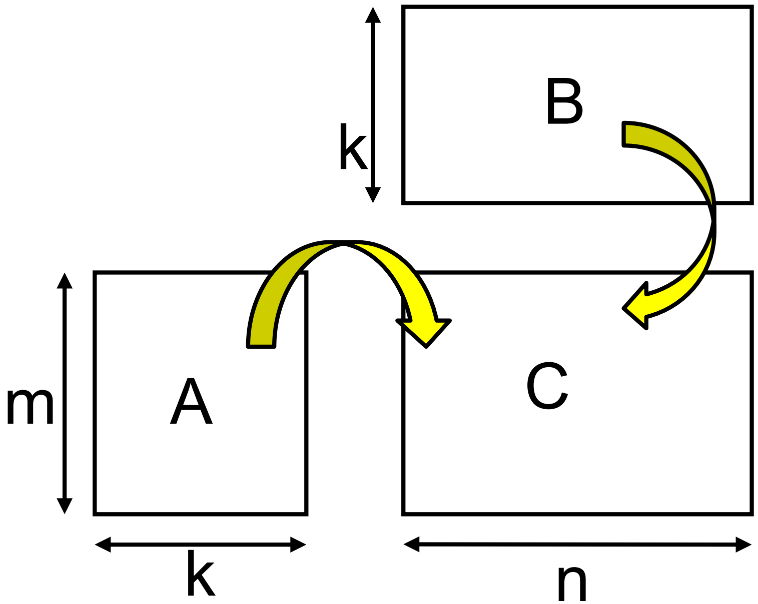
MPI version available at /gs/hs1/tga-ppcomp/20/mm-mpi/

A: a $(m \times k)$ matrix, B: a $(k \times n)$ matrix

C: a $(m \times n)$ matrix

$C \leftarrow A \times B$

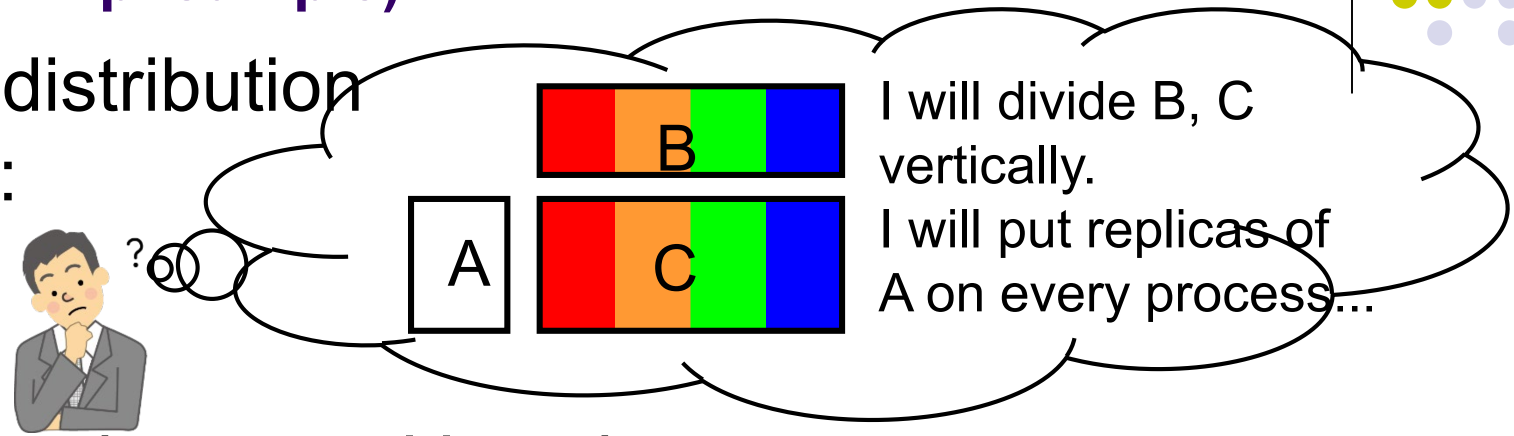
- Algorithm with a triple for loop
- Supports variable matrix size.
  - Each matrix is expressed as a 1D array by *column-major* format



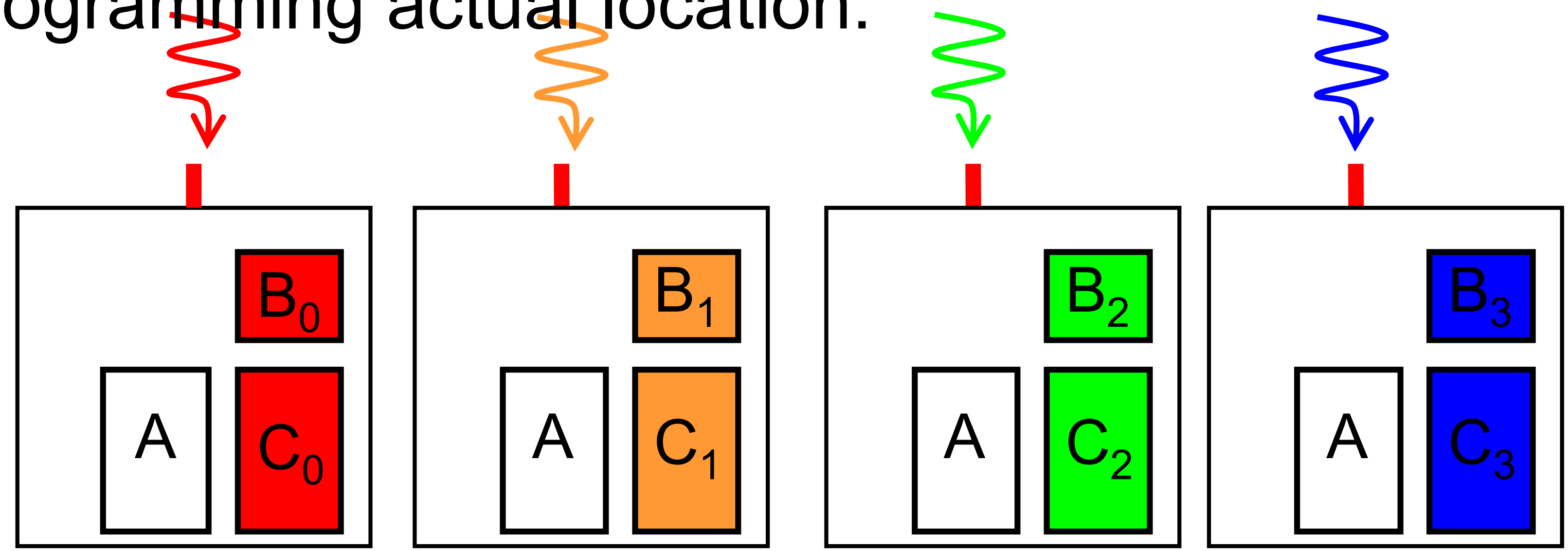
Execution: mpiexec -n [#proc] ./mm [m] [n] [k]

Programming Data Distribution
(for mm-mpi sample)

Design distribution method:



Programming actual location:



This is not a unique solution. How about other solutions?

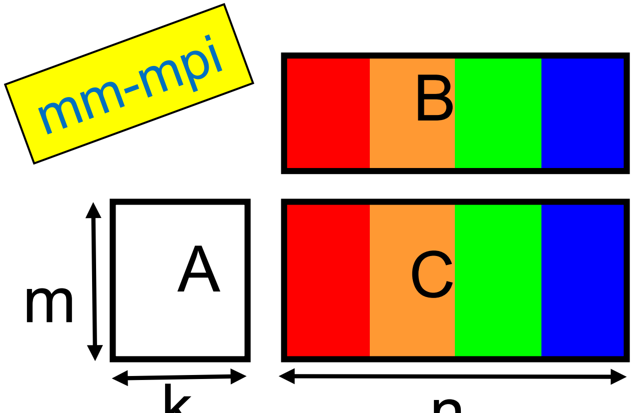
Discussion on Considering Data Distribution

- Choice of data distribution have impact on
  - Communication cost
  - Memory consumption cost
    - In mm-mpi, every process has a coppy of matrix A → memory consumption is large
  - (Sometimes, computation cost)

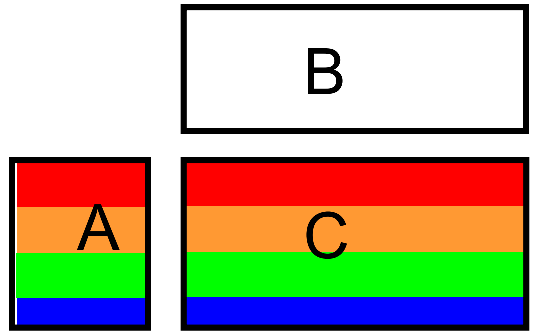
- Smaller cost is better

Other Data Distribution Methods?

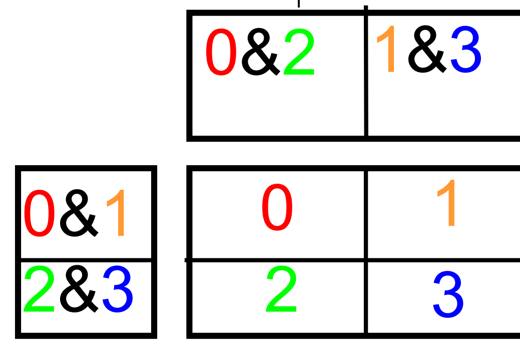
- $C_{i,j}$ requires <u>*i*-th row of A</u> and <u>*j*-th column of B</u>



C is divided in col-wise
⇒ Similarly B
A is replicated



C is divided in row-wise
⇒ Similarly A
B is replicated



C is divided in 2D
⇒ A:row-wise + replica
B:col-wise + replica

Total Comm.	0	0	0
Totel Mem.	O(mkp+nk+mn)	O(mk+nkp+mn)	$O(mkp^{1/2}+nkp^{1/2}+mn)$

p: the number of processes
Note: If initial matrix is owned by one process, we need communication before computation

Among them, the third version has lowest memory consumption

Reducing Memory Consumption Further

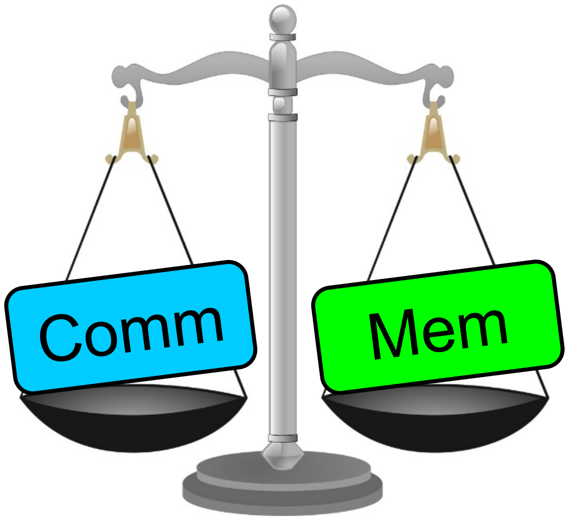
- Even in the third version, memory consumption is $O(mkp^{1/2}+nkp^{1/2}+mn)$ > $O(mk+nk+mn)$ (theoretical minimum)
- If p=10000, we consume 100x larger memory ☹

→ we cannot solve larger problems on supercomputers

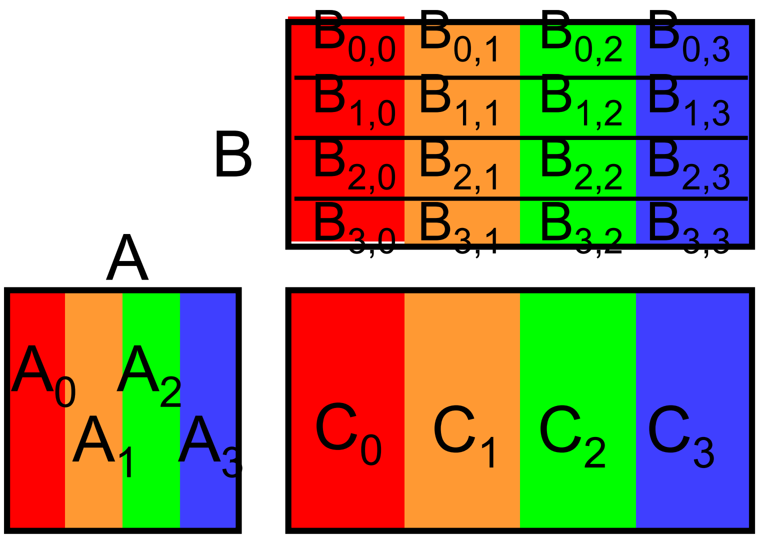
- To reduce memory consumption, we want to eliminate replica!

→ But this increases communication costs

Trade-off: a balance achieved between two desirable but incompatible features



Data Distribution with Less Memory Consumption



Not only B/C, but A is divided among all processes

(In this example, column-wise)

⇒ We need communication!

Algorithm

__Step 0 :__

P_0 sends A_0 to all other processes

Every process P_r computes

C_r += $A_0 \times B_{0,r}$

__Step 1 :__

P_1 sends A_1 to all other processes

Every process P_r computes

C_r += $A_1 \times B_{1,r}$

:

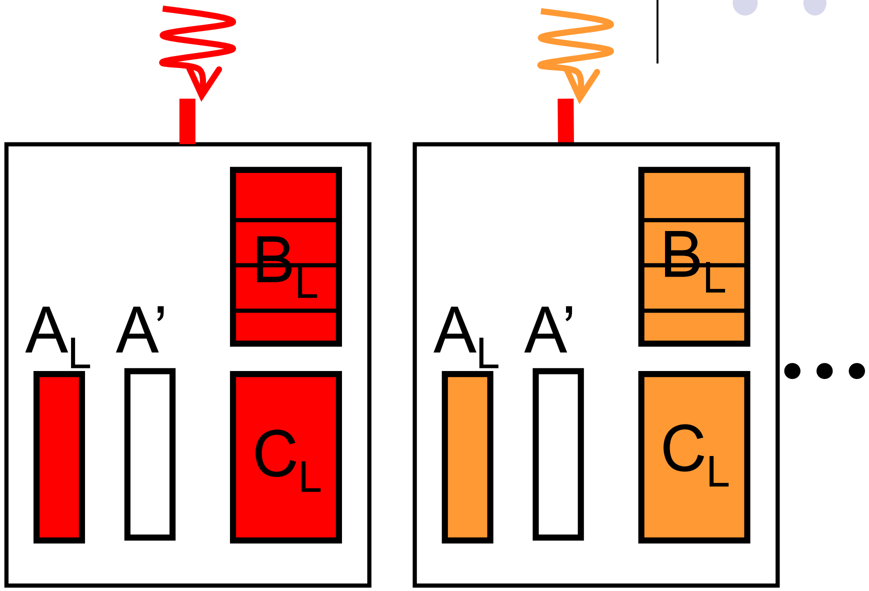
Repeat until *__Step (p-1)__*

Total Comm: O(mkp) Total Mem: O(mk+nk+mn)

Actual Data Distribution of Memory Reduced Version

Every process has partial A, B, C

- A_L on process r ⇔ A_r
- B_L on process r ⇔ B_r
- C_L on process r ⇔ C_r



- Additionally, every process should prepare a receive buffer ➔ A' in the figure
  - A' (instead of A) is used for arguments of MPI_Recv()
  - On receivers, A' is used for computation

[Q] What if a process uses A_L for MPI_Recv() ?

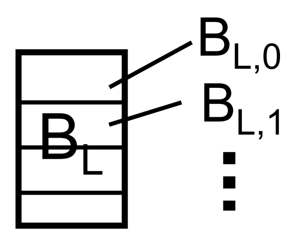
Programming Memory Reduced Matrix Multiplication

On every process r:

```
for (i = 0; i < size; i++) {   // size: number of processes
    if (r == i) {
        for (dest = 0; dest < size; dest++)
            if (dest != r) MPI_Send(A_L, …, dest, …);
    } else
        MPI_Recv(A’, …, i, …);

    if (r == i)
        Compute C_L += A_L × B_L,i
    else
        Compute C_L += A’ × B_L,i
}
```

P_i sends its A_L to all other processes



Improvements of Memory Reduced Version

Followings are options (NOT mandatory) in assignments [M2]

1. To use collective communications (explained hereafter)

2. To use SUMMA: scalable universal matrix multiplication algorithm
   - See http://www.netlib.org/lapack/lawnspdf/lawn96.pdf
   - Replica is eliminated, and matrices are divided in 2D

Peer-to-peer Communications vs Collective Communications

- Communications we have learned are called peer-to-peer communications
- A process sends a message. A process receives it

※ MPI_Irecv, MPI_Isend are also peer-to-peer communications

	Blocking	Non-Blocking
Peer-to-Peer	MPI_Send, MPI_Recv…	MPI_Isend, MPI_Irecv…
Collective	MPI_Bcast, MPI_Reduce…	(MPI_Ibcast, MPI_Ireduce…)

Collective Communications (Group Communications)

- Collective communications involves many processes
  - MPI provides several collective communication patterns
    - Bcast, Reduce, Gather, Scatter, Barrier・・・
  - All processes must call the same communication function

→ Something happens for all of them

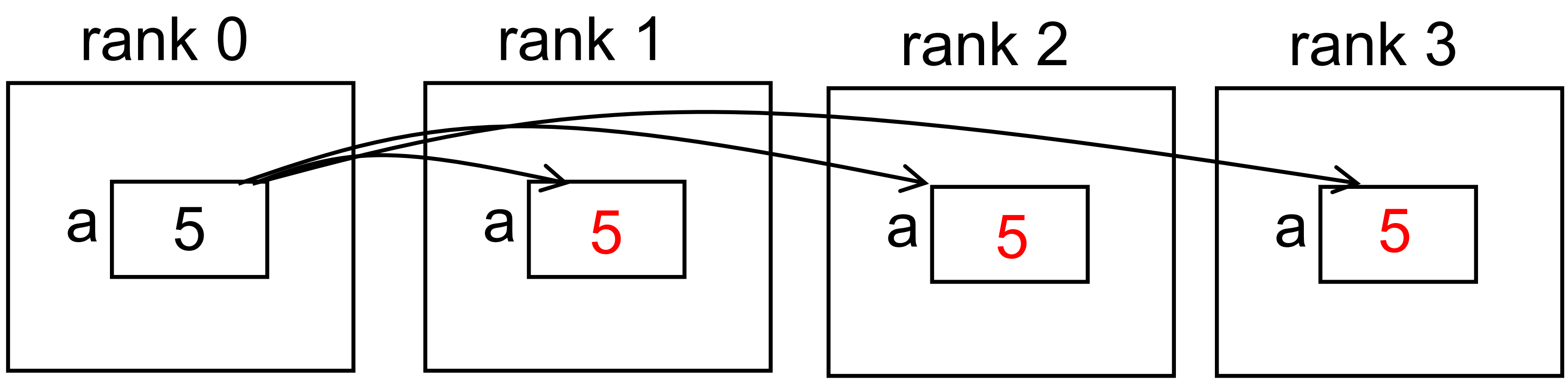
One of Collective Communications: Broadcast by MPI_Bcast

cf) rank 0 has "int a" (called root process). We want to send it to all other processes

```
MPI_Bcast(&a, 1, MPI_INT, 0, MPI_COMM_WORLD);
```

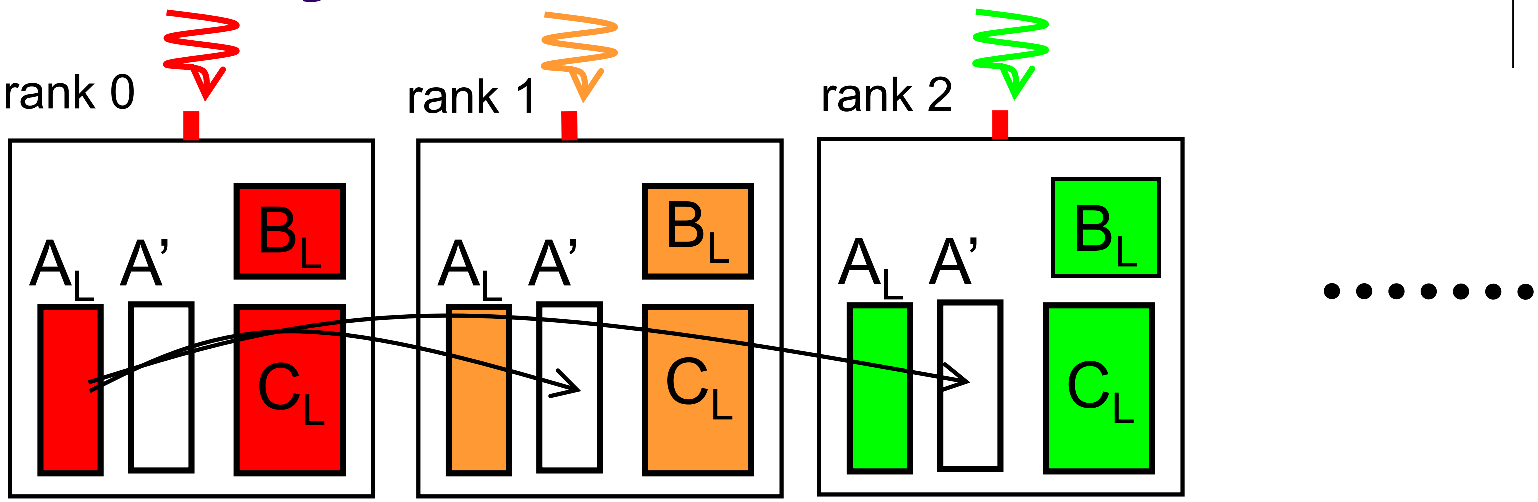
- All processes (in the communicator) must call MPI_Bcast(), including rank 0

→ All other process will receive the value on memory region a



※ What is the role of 1st argument?
it is "input" on the root process, and "output" on other processes

MPI_Bcast Can Be Used in Memory Reduced MM



- In Step i, rank i becomes the root
- It sends A_L to all other processes

→ This is “broadcast” pattern. We can use MPI_Bcast!

Note: Root wants to send A_L. Others want to receive data into A’
→ Different pointers

Solution 1:
if (I am rank i) copies A_L to A’
MPI_Bcast(A’, …);

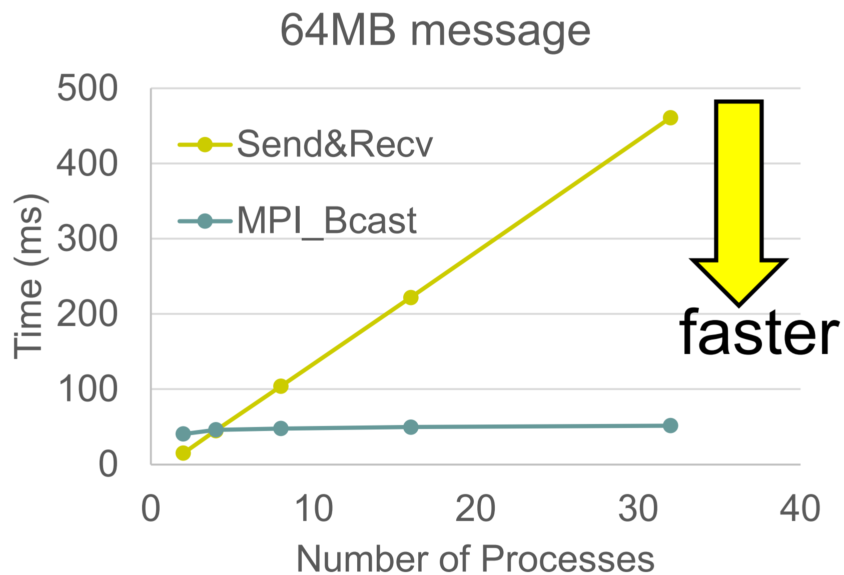
Solution 2:
if (I am rank i) {MPI_Bcast(A_L, …); }
else {MPI_Bcast(A’, …); }

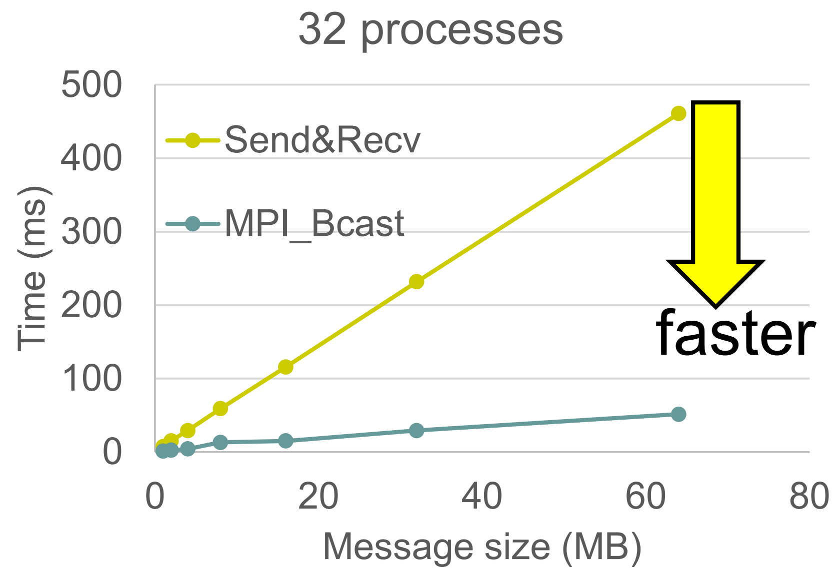
“Do I Really Need to Learn New Functions?”

- You can still use MPI_Send/MPI_Recv multiple times, but collective functions are often faster

In the graph, rank 0 called MPI_Send for p-1 times to other processes

measured on TSUBAME2





- MPI_Bcast are faster, especially when p is larger !
- The reason is MPI uses “scalable” communication algorithms

  cf) http://www.mcs.anl.gov/~thakur/papers/mpi-coll.pdf

Reduction by MPI_Reduce

cf) Every process has “int a”. We want the sum of them

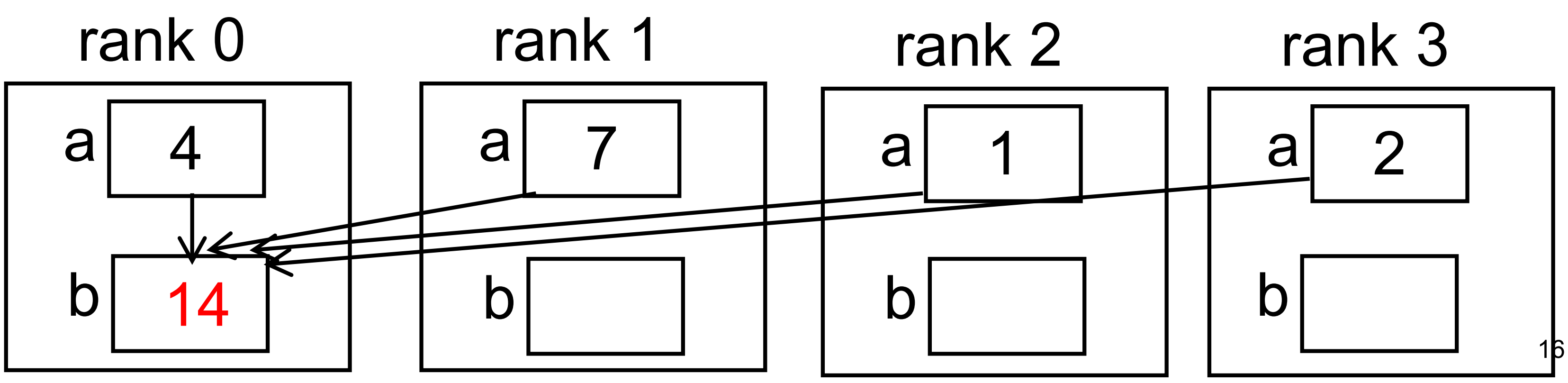
```
MPI_Reduce(&a, &b, 1, MPI_INT, MPI_SUM, 0,
           MPI_COMM_WORLD);
```

operation *root process*

- Every process must call MPI_Reduce()

→ The sum is put on b on root process (rank 0 now)

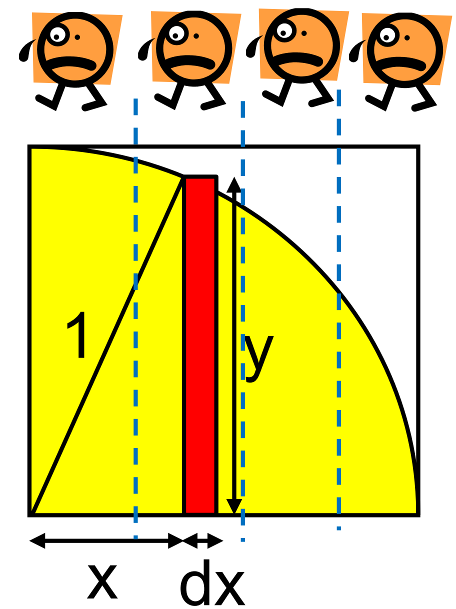
- Operation is one of MPI_SUM, MPI_PROD(product), MPI_MAX, MPI_MIN, MPI_LAND (logical and), etc.



MPI Version of "pi" Sample

/gs/hs1/tga-ppcomp/20/pi-mpi/

- Execution : mpiexec -n [#procs] ./pi [n]
  - n: Number of division
  - Cf) ./pi 100000000



- We divide *n* tasks among processes and calculate total yellow area

dx = 1/n
y = sqrt(1-x*x)

1. Each process calculates local sum
2. Rank 0 obtains the final sum by MPI_Reduce

Note: Differences with “omp for reduction” in OpenMP

- Syntaxes are completely different
- Computations are also different
  - #pragma omp for reduction(…) in OpenMP
    - Do “sum += a[i]” in parallel for loop with reduction(+:s)

4	7	2	3	0	1	5	6	5

⇒ sum=33

  - MPI_Reduce(…) in MPI
    - If each input is an array, output is also an array
    - Operations are done for each index

4	7	2

3	0	1

5	6	5

⇒

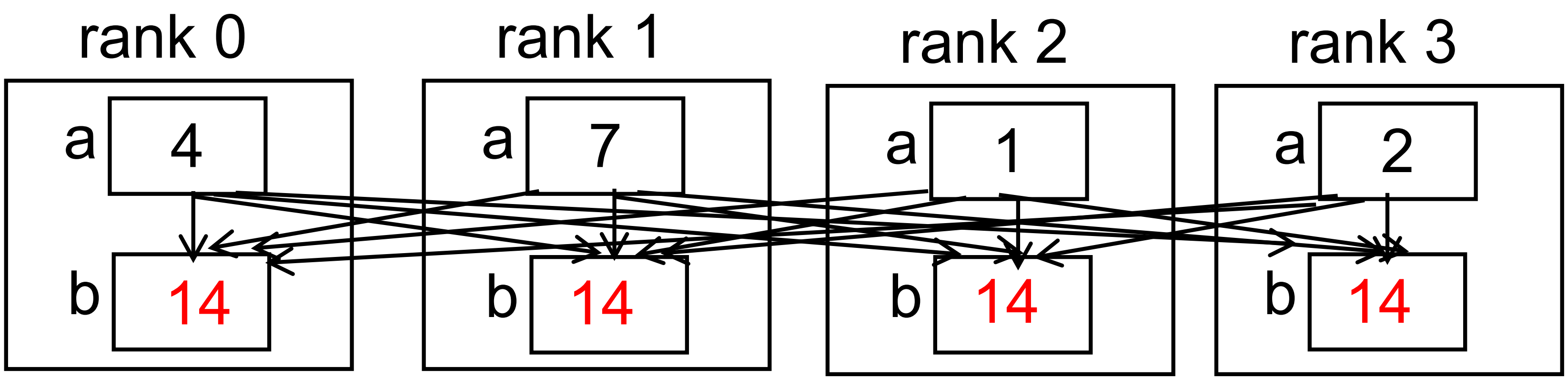
12	13	8

MPI_Allreduce

- Allreduce = Reduction + Bcast

```
MPI_Allreduce(&a, &b, 1, MPI_INT, MPI_SUM,
              MPI_COMM_WORLD);
```

  - The sum is put on b on all processes



Important communication pattern for distributed deep learning → Google “allreduce deep learning”

MPI_Barrier

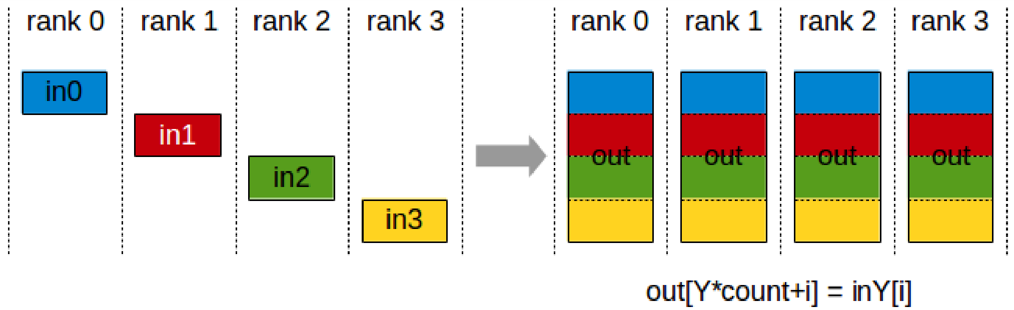
- Barrier synchronization: processes are stopped until all processes reach the point

```
MPI_Barrier(MPI_COMM_WORLD);
```

  - Used in sample programs, to measure execution time more precisely

Other Collective Communications

- MPI_Scatter
  - An array on a process is “scattered” to all processes
  - cf) Process 0 has an array of length 10,000. There are 10 processes. The array is divided to parts of length 1,000 and scattered
- MPI_Gather
  - Data on all processes are “gathered” to the root process.
  - Contrary to MPI_Scatter
- MPI_Allgather
  - Similar to MPI_Gather. Gathered data are put on all processes

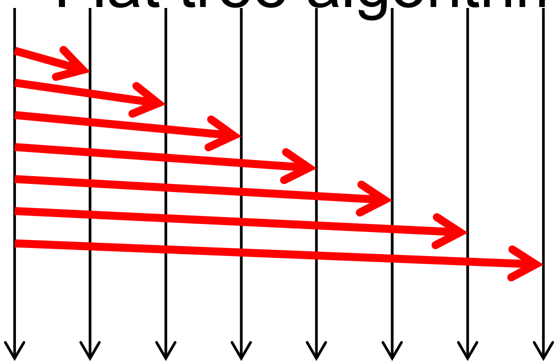


NCCL manual at docs.nvidia.com

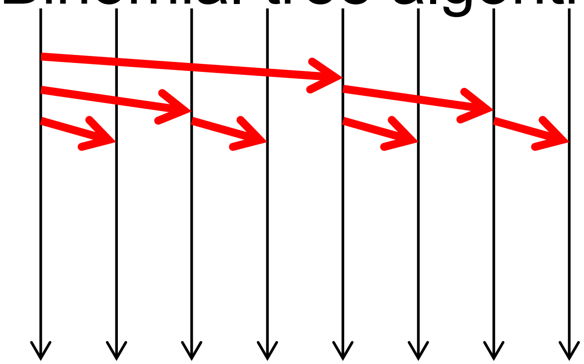
Why are Collective Communications Fast?

- Since MPI library uses scalable communication algorithms
  - Case of broadcast:

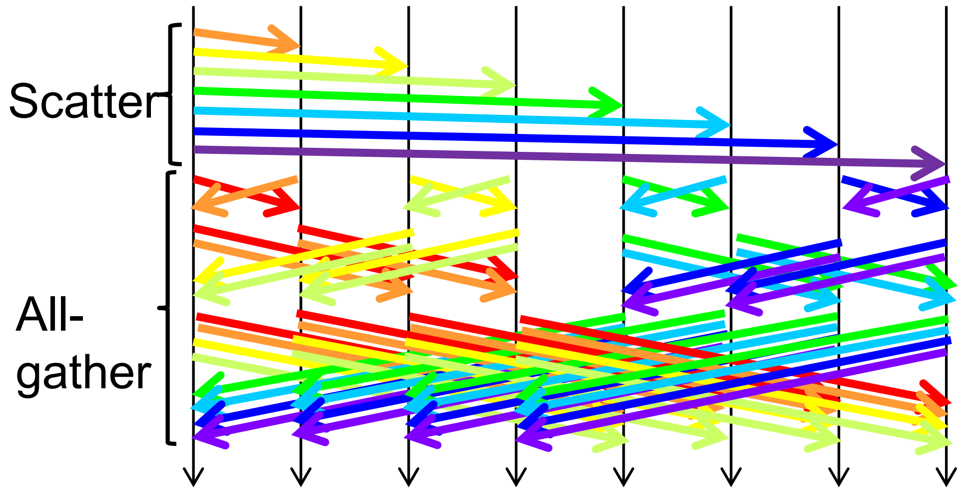
Flat tree algorithm



Binomial tree algorithm

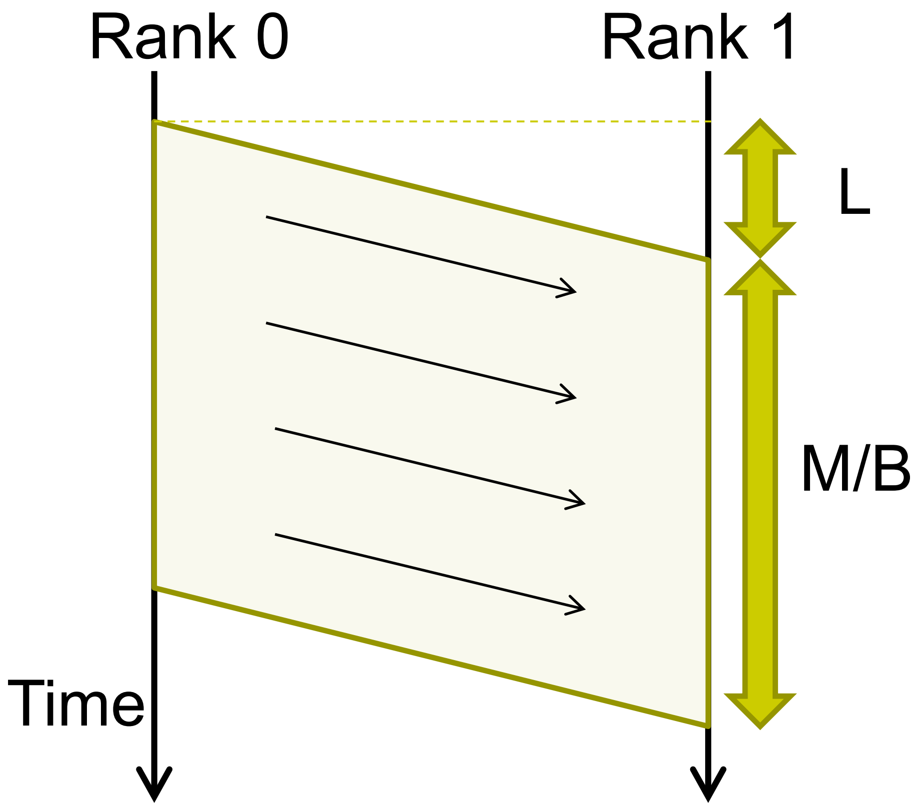


Scatter&Allgather algorithm



Model of Communication Time

Illustration of peer-to-peer communication of data size M



$$T = M / B + L$$

T: Communication time

M: Data size

B: Bandwidth

L: Network latency

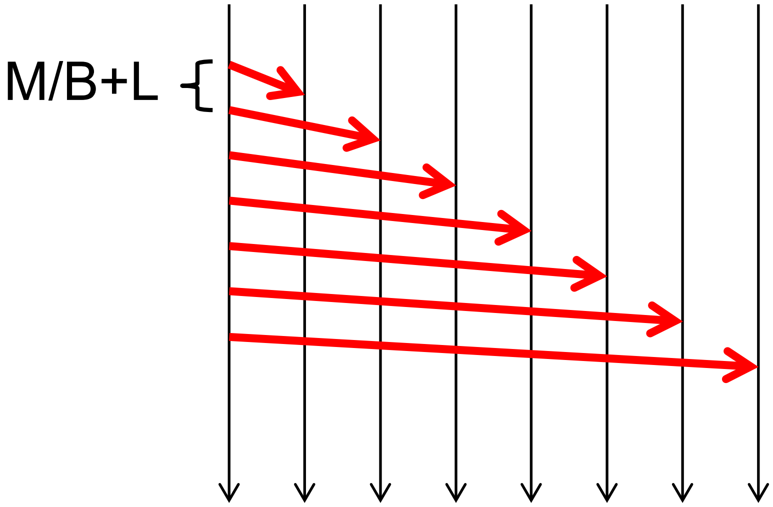
※ Be aware of difference between "Byte" and "bit": 1Byte=8bit

※ Actually it is more complex for effects of network topology, congestion, packet size, error correction…

Cost Model of Broadcast Algorithms

- Case of “broadcast” of size M data
  - p: number of processes, B: network bandwidth, L: network latency

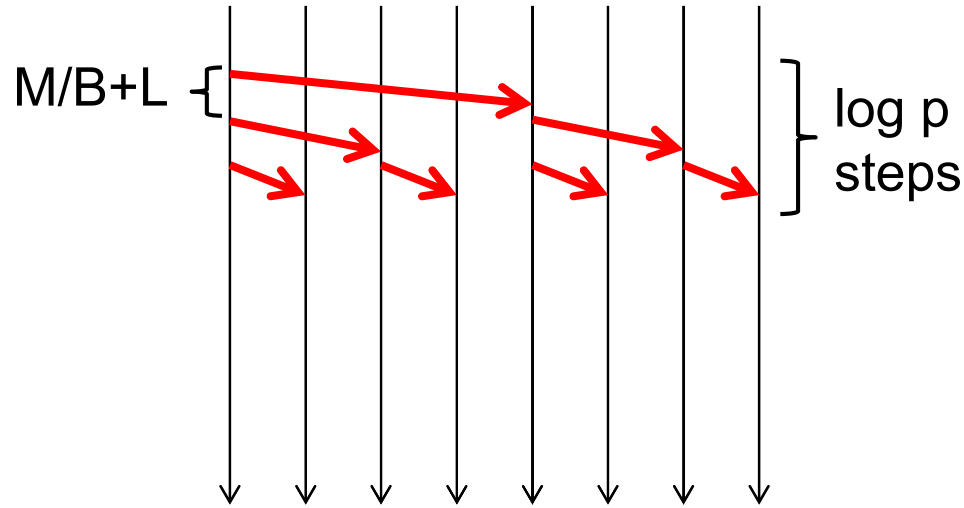
Flat tree algorithm



$p(M/B+L)$

→ *Slow*

Binomial tree algorithm

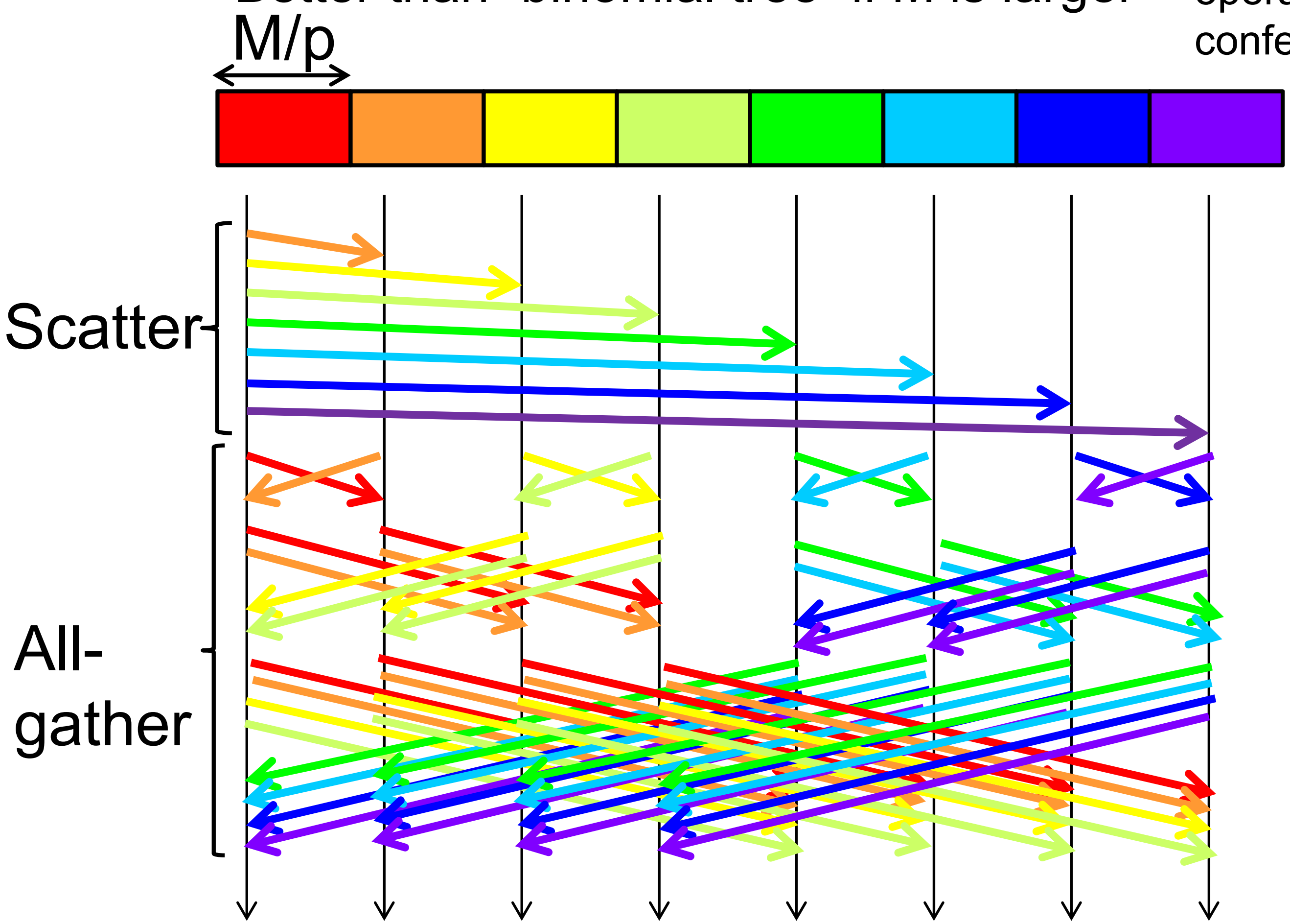


$(\log p)(M/B+L)$

One of Scalable Broadcast Algorithms

- Scatter&Allgather algorithm
  - Message is divided into p parts
  - Better than "binomial tree" if M is larger

R. Thakur and W. Gropp. Improving the performance of collective operations in mpich. EuroPVM/MPI conference, 2003.



$$\overbrace{M/B + pL}^{\text{Scatter}} + \underbrace{M/B + (\log p)L}_{\text{All-gather}}$$

Comparison of Broadcast Algorithms

- Consider two extreme cases
  - If M is sufficiently large: *M/B+L → M/B*
  - If M is close to zero: *M/B+L → L*

	Flat Tree	Binomial Tree	Scatter& All-gather
Cost (General)	p(M/B+L)	(log p) (M/B+L)	2M/B + (p + log p)L
Cost with very large M	p M/B	(log p) M/B	2 M/B → Fastest
Cost with very small M	p L	(log p) L → Fastest	(p + log p) L

Many MPI libraries implement multiple algorithms
They switch them automatically according to message size M ☺

We Have Learned

- Part 1: Shared memory parallel programming with OpenMP
- Part 2: GPU programming with OpenACC and CUDA
- Part 3: Distributed memory parallel programming with MPI

Many common strategies towards faster software:

- To understand source of bottleneck
- Reducing computation and communication
- Overlapping computation and communication
- To understand property of architecture

Let’s enjoy high performance computing!

Assignments in MPI Part (Abstract)

Choose *one of* [M1]—[M3], and submit a report

Due date: 11AM, June 29 (Monday)

[M1] Parallelize “diffusion” sample program by MPI.

[M2] Improve mm-mpi sample in order to reduce memory consumption.

[M3] (Freestyle) Parallelize *any* program by MPI.

For more detail, please see June 11 slides