MPI

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1. MPI Overview

1.1 What is MPI (Message Passing Interface)?

- A standard API for message passing between distributed memories in parallel computing.
- MPI assumes a distributed-memory computing system
- MPI can run on shared-memory computing system
- MPI programming model (basically) uses **SPMD**(Single Program, Multiple Data).

1.2 Parallel Programming Classification

- Multi-Process: MPI(Message Passing Interface), HPF(High Performance Fortran)
- Multi-Thread: OpenMP, Pthread(POSIX Thread)

| Aspect | MPI | HPF |
|---------------------|--------------------------------|----------------------------|
| Type | Parallel communication library | Fortran language extension |
| Language | C / C++ / Fortran | Fortran only |
| Parallelism Control | Fully manual by programmer | Mostly compiler-driven |
| Flexibility | Very high | Limited |
| Maintainability | Hard but highly tunable | Simpler but harder to tune |
| Learning Curve | High | Low to medium |
| Current Usage | Mainstream in HPC | Obsolete / deprecated |

1.3 MPI Features

- Communication Model:
 - Uses message passing for communication between processes.
- Distributed Memory Support:
 - Each process has its own memory space, no shared memory.
- Multi-node Capacity:
 - Can run across multiple nodes; abstracts network communication.
- Standardized API:
 - Standardized interface in C, C++, and Fortran; highly portable.
- Multiple Implementation:
 - Available implementations include OpenMPI, MPICH, and Intel MPI, etc.
- Difficult to Debug:
 - Debugging is challenging due to concurrency and communication complexity.

1.4 Typical example of Usage

- Simulation on a supercomputer
 - ▶ Physics, Meteorology, Chemistry, etc.
- Data processing in large-scale data analysis
 - e.g., genomics, astronomy
- Machine learning training on large datasets
 - e.g., distributed deep learning

1.5 Comparison between implementations

| | OpenMPI | MPICH | Intel MPI | |
|----------------------------|-----------------------------------|----------------------------------|-----------------------------------|--|
| Developer | Universities, Companies | Argonne National Laboratory | Intel Corporation | |
| Distribution | Open source | Open source | Closed source | |
| Optimization Target | General purpose | Lightweight, stable | Optimized for Intel architecture | |
| Performance | Medium to high | Lightweight, stable, scalable | Best performance on Intel CPUs | |
| Main Use | Academic clusters, general HPC | Research, education | Commercial HPC, Intel clusters | |

- <u>Miyabi uses OpenMPI</u> as the default MPI implementation.(Miyabiis the supercomputer system of the University of Tokyo)
- To be more specific, mpicc on Miyabi is bound to nvc compiler (NVIDIA HPC SDK C compiler), which means NVIDIA HPC SDK + MPI environment is used.

1.6 Key Communication Primitives

- System function:
 - ► MPI_Init, MPI_Finalize, MPI_Comm_size, MPI_Comm_rank
- Point-to-point communication:
 - ► MPI_Send, MPI_Recv
- Collective communication:
 - ▶ MPI Bcast, MPI Reduce, MPI Alltoall
- Synchronization:
 - ► MPI_Barrier, MPI_Wait, MPI_Test
- Derived data types:
 - ► MPI_Type_create_struct, MPI_Type_vector
- Non-blocking communication:
 - ► MPI_Isend, MPI_Irecv
- Remote memory access:
 - ► MPI Put, MPI Get
- Process management:
 - ► MPI_Comm_spawn, MPI_Comm_free

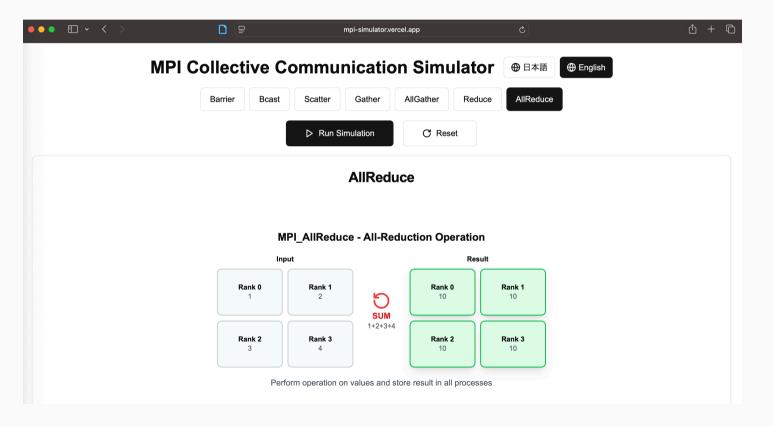
1.7 Internal Mechanisms of MPI Communication

- MPI implementations (e.g., MPICH, OpenMPI) rely on various OS system calls and low-level libraries for communication.
- Intra-node Communication (within the same node):
 - Shared memory: mmap, shm_open, memfd_create, System V shm
 - Event waiting: futex, poll, epoll, select
 - ▶ Pipes & sockets: write, read
 - UNIX domain sockets: sendmsg, recvmsg
 - Synchronization: sem_open, pthread_mutex, spinlock
- Inter-node Communication (across nodes):
 - ► TCP/IP sockets: socket, bind, listen, accept, connect, send, recv, sendto, recvfrom
 - ▶ RDMA & verbs API (e.g., InfiniBand) for zero-copy communication
- High-Performance Cluster Communication:
 - ► Libraries: libibverbs, UCX, OFI (Libfabric), XPMEM, NVLink
 - Kernel bypass with DMA (Direct Memory Access) for low-latency, high-throughput transfers

2. Basic Learning of MPI

2.1 MPI Simulation Website

- I developed a simple MPI simulation website for learning MPI.
- Please Click on: Izawa MPI Simulation Website



2.2 Tutorial Programs

• The following programs are available below.

MPI Tutorial GitHub Repository

2.3.1 MPI Language Differences

| | С | C++ | Fortran |
|----------------------|-------------------------------------|-------------------------------------|---------------------------|
| MPI Header | <pre>#include <mpi.h></mpi.h></pre> | <pre>#include <mpi.h></mpi.h></pre> | use mpiorinclude 'mpif.h' |
| Official MPI support | 0 | A | 0 |
| Syntax intuitiveness | Explicit C syntax | Almost same as C | call and subroutine based |
| Compiler | mpicc | mpicxx or mpic++ | mpif90 or mpifort |
| Scientific computing | 0 | A | |

- C++
 - ► MPI-3.0 abolished C++ only bindings.
 - Currently, C++ also uses C interface.
- Fortran
 - Considering readability, type safety, and portability, use mpi is recommended.

2.3.2 Hello World (C)

```
#include <mpi.h>
#include <stdio.h>
#include <stdlib.h>
int main(int argc, char *argv[])
    MPI Init(&argc, &argv);
    int num procs;
    int my rank;
    MPI Comm size(MPI COMM WORLD, &num procs);
    MPI Comm rank(MPI COMM WORLD, &my rank);
    printf("Num of Proc : %d\n", num procs);
    printf("My Rank : %d\n", my rank);
   MPI Finalize();
    return EXIT_SUCCESS;
```

```
mpicc mpi_hello.c -o mpi_hello
mpirun -np 4 ./mpi_hello
Num of Proc : 4
My Rank : 3
Num of Proc : 4
My Rank : 2
Num of Proc : 4
My Rank : 0
Num of Proc : 4
My Rank : 1
```

2.3.3 Hello World (C++)

```
#include <mpi.h>
#include <iostream>
#include <cstdlib>
int main(int argc, char *argv[])
{
    MPI Init(&argc, &argv);
    int num procs;
    int my rank;
    MPI Comm size(MPI COMM WORLD, &num procs);
    MPI Comm rank(MPI COMM WORLD, &my rank);
    std::cout << "Num of Proc : " << num procs <<</pre>
std::endl:
    std::cout << "My Rank : " << my rank << std::endl;</pre>
    MPI Finalize();
    return EXIT_SUCCESS;
```

```
mpic++ mpi_hello.cpp -o mpi_hello
mpirun -np 4 ./mpi_hello
Num of Proc : 4
My Rank : 3
Num of Proc : 4
My Rank : 1
Num of Proc : 4
My Rank : 0
Num of Proc : 4
My Rank : 0
Num of Proc : 4
My Rank : 2
```

2.3.4 Hello World (Fortran)

```
program hello mpi
 use mpi
 implicit none
 integer :: ierr, rank, size
 call MPI Init(ierr)
 call MPI Comm rank(MPI COMM WORLD, rank, ierr)
 call MPI Comm size(MPI COMM WORLD, size, ierr)
 print *, "Num of Proc:", size
 print *, "My Rank: ", rank
 call MPI Finalize(ierr)
end program hello mpi
```

```
mpif90 mpi_hello.f90 -o mpi_hello
mpirun -np 4 ./mpi_hello
Num of Proc: 4
My Rank: 2
Num of Proc: 4
My Rank: 0
Num of Proc: 4
My Rank: 3
Num of Proc: 4
My Rank: 1
```

2.4.1 Overview

- Process:
 - computing unit in parallel computing in MPI.
 - process num is determined by mpirun -np
- Group:
 - a set of processes that can communicate with each other.
- Communicator:
 - a group of processes that can communicate with each other.
- Rank:
 - unique identifier for each process in MPI.
 - ► Ranks are assigned from 0 to num_procs 1.

2.4.2 Communicator Image

- Each process belongs to some **group**.
- A group is associated with a **communicator**.
- Each process in a communicator has a unique rank.

```
- Example:
- Process 0, 1, 2, 3 belong to a group.
- Communicator: MPI_COMM_WORLD
- Group: [P0, P1, P2, P3]
- Rank: 0, 1, 2, 3

MPI_COMM_WORLD (communicator)

├ Group: { P0, P1, P2, P3 }

│ ├ P0 (rank 0)

│ ├ P1 (rank 1)

│ ├ P2 (rank 2)

│ └ P3 (rank 3)
```

2.4.3 Communicator and Group

- **Group** is a set(list) of processes. It is just a list, it does not have any communication capability.
- Communicator containes a group and communication capability. It is a unit of communication.
- A group can create multiple communicators.
- A communicator cannnot communicate with other communicators.

Q&A

- Q: Q: Can processes be added to an existing group?
- A: No. You cannot add processes to an existing group.

Attention

- A single process can belong to multiple groups and communications.
- In such cases, the process has a unique rank within each communicator.

```
MPI COMM WORLD
    |- Group A: {0, 1, 2, 3, 4}
↓ Communicator B (created from Group A)
    |- Group B {0, 1, 2, 3}
↓ Communicator C (created from Group A)
    |- Group C {0, 1, 2, 4}
- \circ 0, 1, 2 \leftrightarrow 3 (via Communicator B)
- ○ 0, 1, 2 ↔ 4 (via Communicator C)
- ○ 3 ↔ 4 (via Communicator A)
- x 3 ↔ 4 (via Communicator B and C)
```

- In the above example, process 0 belongs to three communicators:
 - ► MPI_COMM_WORLD (Group A), Communicator B (Group B), Communicator C (Group C)

2.4.4 MPI Functions for Communicator

- MPI_COMM_WORLD:
 - the default communicator that includes all processes.
 - all processes first belong to this communicator.
 - becomes the default communicator for most MPI functions.
- MPI_Comm_rank():
 - retrieves the rank of the calling process in specified communicator.
 - ▶ usually use MPI_COMM_WORLD as the communicator.
- MPI_Comm_size():
 - retrieves the number of processes in the specified communicator.
 - ▶ usually use MPI_COMM_WORLD as the communicator.
- MPI_Comm_split():
 - creates a new communicator by splitting the existing one based on a color and key.
 - in other words, create a new communicator with the same color processes.

MPI_Comm_rank and MPI_Comm_size

```
int rank;
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
printf("I am process %d\n", rank);
```

MPI_Comm_size

```
int size;
MPI_Comm_size(MPI_COMM_WORLD, &size);
printf("There are %d processes\n", size);
```

MPI_Comm_split

```
// ランクの3の剰余を基に color=0, 1, 2 に分ける
int color = rank % 3;
MPI Comm new comm;
MPI Comm split(MPI COMM WORLD, color, rank, &new comm);
int new rank, new size;
MPI Comm rank(new comm, &new rank);
MPI Comm size(new comm, &new size);
printf("World Rank %d => Group %d, New Rank %d of %d\n",
       rank, color, new rank, new size);
MPI_Comm_free(&new_comm); // 新しいコミュニケータの解放
```

```
$ mpicc comm_split.c -o comm_split
$ mpirun -np 8 ./comm_split

World Rank 5 => Group 2, New Rank 1 of 2
World Rank 2 => Group 2, New Rank 0 of 2
World Rank 1 => Group 1, New Rank 0 of 3
World Rank 4 => Group 1, New Rank 1 of 3
World Rank 7 => Group 1, New Rank 2 of 3
World Rank 3 => Group 0, New Rank 1 of 3
World Rank 6 => Group 0, New Rank 2 of 3
World Rank 6 => Group 0, New Rank 2 of 3
World Rank 0 => Group 0, New Rank 0 of 3
```

| World Rank | color(= rank % 3) | new group | new rank | new_size |
|------------|-------------------|-----------|----------|----------|
| 0 | 0 | {0, 3, 6} | 0 | 3 |
| 1 | 1 | {1, 4, 7} | 0 | 3 |
| 2 | 2 | {2, 5} | 0 | 2 |
| 3 | 0 | {0, 3, 6} | 1 | 3 |
| 4 | 1 | {1, 4, 7} | 1 | 3 |
| 5 | 2 | {2, 5} | 1 | 2 |
| 6 | 0 | {0, 3, 6} | 2 | 3 |
| 7 | 1 | {1, 4, 7} | 2 | 3 |

- Many MPI functions have the following signature
- MPI_Send sends data to a specific process.
- MPI_Recv receives data from a specific process.

```
MPI_Recv(
    void* data,
    int count,
    MPI_Datatype datatype,
    int source,
    int tag,
    MPI_Comm communicator,
    MPI_Status* status);
```

| MPI Data Type | C Type |
|------------------------|------------------------|
| 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_LONG | unsigned long long int |
| MPI_FLOAT | float |
| MPI_DOUBLE | double |
| MPI_LONG_DOUBLE | long double |
| MPI_BYTE | char |

```
send_data()
```

```
int send_data[10];
for (int i = 0; i < 10; i++)
    send_data[i] = i + 1;
int data_count = 10;

printf("Rank 0: Sending data.\n");
printf("send_data: [");
for (int i = 0; i < 10; i++)
    printf(" %d", send_data[i]);
printf(" ]\n");

MPI_Send((void*)send_data, data_count, MPI_INT,
1, 0, MPI_COMM_WORLD);</pre>
```

```
recv_data()

int data[10];
int data_count = 10;
MPI_Status st;

printf("Rank 1: Receiving data.\n");
MPI_Recv((void*)data, data_count, MPI_INT, 0, 0,
MPI_COMM_WORLD, &st);
printf("recv_data: [");
for (int i = 0; i < 10; i++)
    printf(" %d", data[i]);
printf(" ]\n");</pre>
```

```
$ mpicc send_recv.c -o mpi_send_recv
$ mpirun -np 2 ./mpi_send_recv
Rank 0: Sending data.
send_data: [ 1 2 3 4 5 6 7 8 9 10 ]
Rank 1: Receiving data.
recv_data: [ 1 2 3 4 5 6 7 8 9 10 ]
```

- We can combine send_data() and recv_data() into a single program.
- The program can be run with mpirun -np 2 ./mpi_send_recv2

```
int data count = 10;
int numbers[data count];
if (world rank == 0) {
    for (int i = 0; i < 10; i++) numbers[i] = i + 1;
    printf("Send Data:");
    for (int i = 0; i < 10; i++)
        printf(" %d", numbers[i]);
    printf("\n");
    MPI Send((void *)&numbers, data count, MPI INT, 1, 0, MPI COMM WORLD);
} else if (world rank == 1) {
    MPI Recv(&numbers, data count, MPI INT, 0, 0, MPI COMM WORLD, MPI STATUS IGNORE);
    printf("Received Data:");
    for (int i = 0; i < 10; i++)
        printf(" %d", numbers[i]);
    printf("\n");
}
```

```
$ mpicc send_recv2.c -o mpi_send_recv2
$ mpirun -np 2 ./mpi_send_recv2

Send Data: 1 2 3 4 5 6 7 8 9 10
Received Data: 1 2 3 4 5 6 7 8 9 10
```

3. Collective Communication

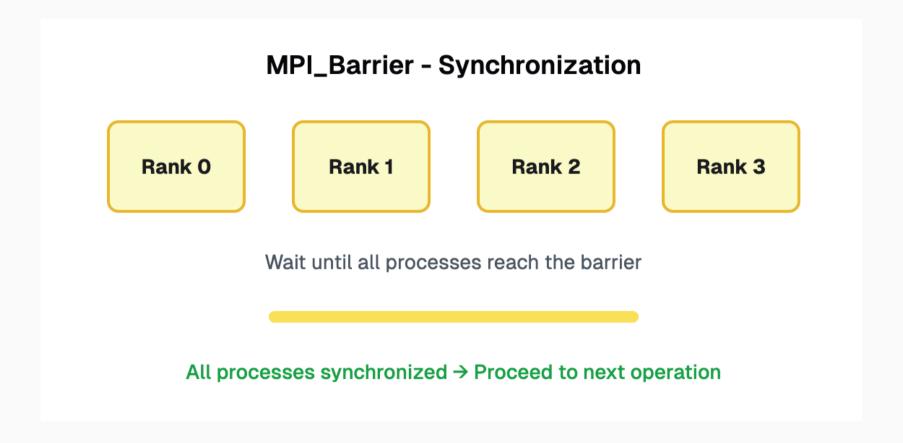
3.1 synchronization

- Collective communication is a communication method that <u>involves all processes in a communicator</u>.
- In collective communication, synchronization among all process is required.
- · All process cannot proceed until all processes reach the same point.
- To achieve this, MPI provides several collective communication functions.

3.2 MPI_Barrier

- MPI_Barrier is a collective communication function that synchronizes all processes in a communicator.
- All processes must call MPI_Barrier to ensure that all processes reach the same point before proceeding.
- It is often used to ensure that all processes have completed their previous tasks before moving on to the next step.
- The most basic usage of MPI_Barrier is for precise time measurement.
- If you do not call MPI_Barrier in all processes, the program will block and cannot proceed.
- MPI_Barrier(MPI_Comm communicator);

3.2 MPI_Barrier



3.2 MPI_Barrier

```
int rank, size;
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_size(MPI_COMM_WORLD, &size);

printf("Rank %d: before barrier\n", rank);

sleep(rank);

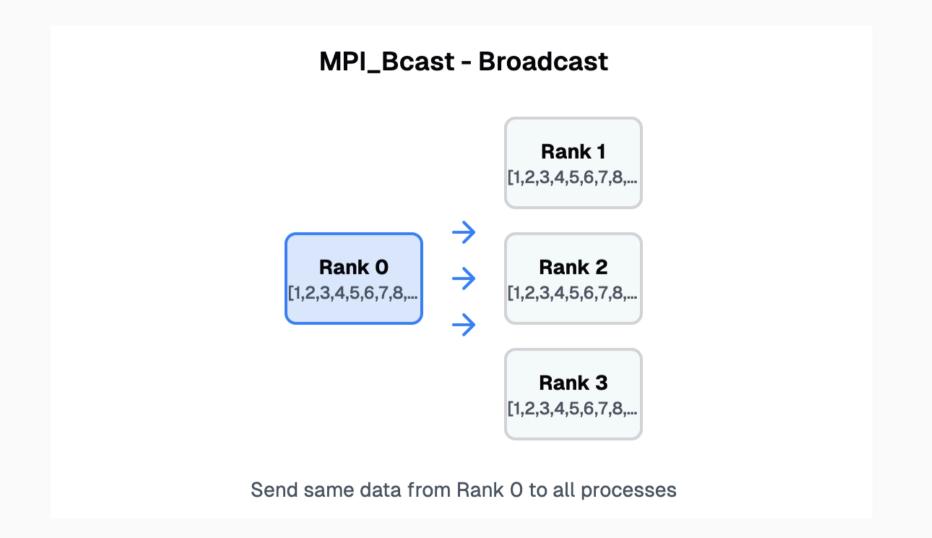
MPI_Barrier(MPI_COMM_WORLD);
printf("Rank %d: after barrier\n", rank);
```

```
$ mpicc barrier.c -o barrier
$ mpirun -np 4 ./barrier

Rank 2: before barrier
Rank 3: before barrier
Rank 0: before barrier
Rank 1: before barrier
Rank 3: after barrier
Rank 1: after barrier
Rank 0: after barrier
Rank 0: after barrier
```

- MPI_Bcast is a collective communication function that broadcasts data from one process to all other processes in a communicator.
- It is used to distribute data from a root process to all other processes.
- All processes in the communicator must call MPI_Bcast with the same parameters.

- Root Process: Sends the data to all other processes.
- Other Processes: Receive the data from the root process.



```
int rank, size;
MPI Comm rank(MPI COMM WORLD, &rank);
MPI Comm size(MPI COMM WORLD, &size);
int data[10]:
if (rank == 0) {
    for (int i = 0; i < 10; i++) {
        data[i] = i + 1;
    printf("Rank 0: broadcasting data = [");
    for (int i = 0; i < 10; i++)
        printf(" %d", data[i]);
    printf(" ]\n");
}
MPI Bcast(data, 10, MPI INT, 0, MPI COMM WORLD);
printf("Rank %d: received data = [", rank);
for (int i = 0; i < 10; i++)
    printf(" %d", data[i]);
printf(" ]\n");
```

```
$ mpicc bcast.c -o bcast
$ mpirun -np 4 ./bcast

Rank 0: broadcasting data = [ 1 2 3 4 5 6 7 8 9 10 ]
Rank 0: received data = [ 1 2 3 4 5 6 7 8 9 10 ]
Rank 2: received data = [ 1 2 3 4 5 6 7 8 9 10 ]
Rank 3: received data = [ 1 2 3 4 5 6 7 8 9 10 ]
Rank 1: received data = [ 1 2 3 4 5 6 7 8 9 10 ]
```

We can implement MPI_Bcast wrapper using MPI_Send and MPI_Recv.

```
void my bcast(void* data, int count, MPI Datatype datatype, int root, MPI Comm communicator) {
  int world rank;
 MPI Comm rank(communicator, &world rank);
 int world size;
 MPI Comm size(communicator, &world_size);
  if (world rank == root) {
   for (int i = 0; i < world_size; i++) {</pre>
     if (i != world rank) {
       MPI Send(data, count, datatype, i, 0, communicator);
 } else {
    MPI Recv(data, count, datatype, root, 0, communicator, MPI STATUS IGNORE);
```

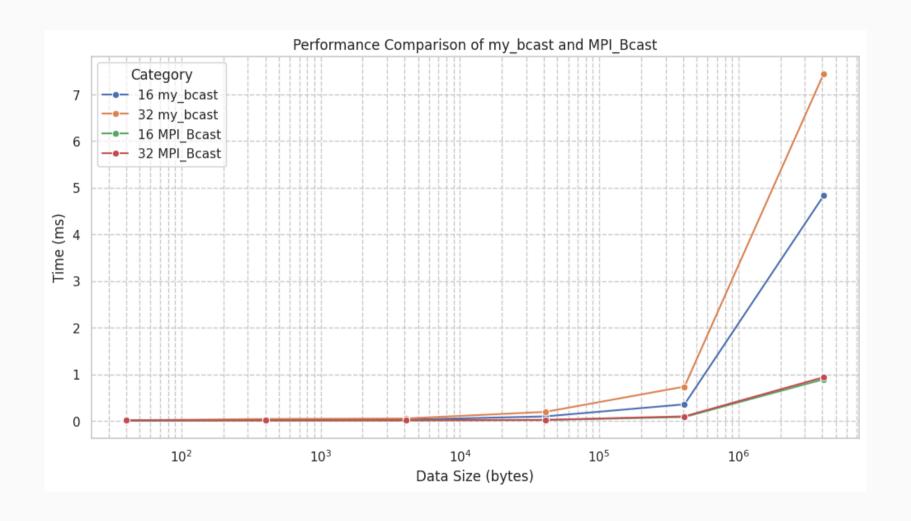
• Q: Is this equivalent to MPI_Bcast?

- A: No, it is less efficient than MPI_Bcast.
- This implementation has only one network communication link. The process with root rank sends data to all other processes one by one.
- MPI_Bcast uses Tree-based broadcast algorithm.
- 1. The root process sends data to process 1.
- 2. The root process sends data to process 2, process 1 sends data to process 3.
- 3. The root process sends data to process 4, process 1 sends data to process 5, process 2 sends data to process 6, process 3 sends data to process 7.

. . .

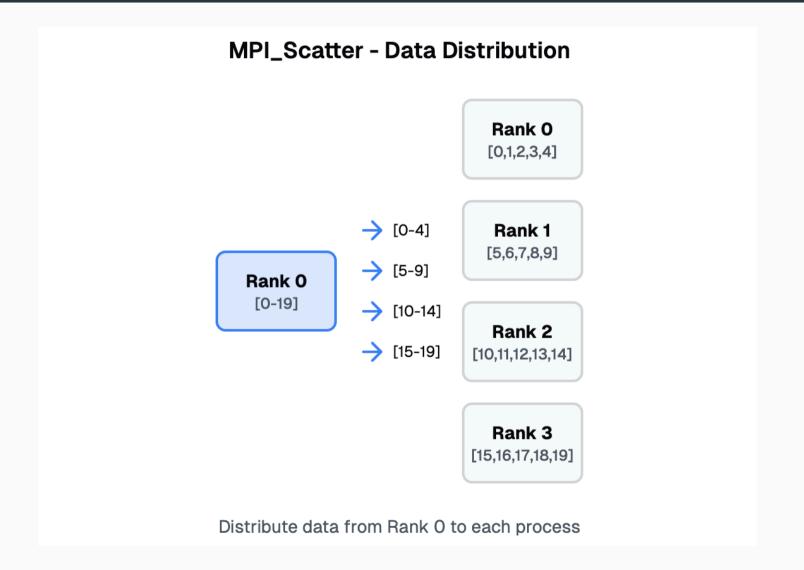
- Comparison of MPI_Bcast and my_bcast
- Average time of 10 trials

| Procs | Data Size | my_bcast (ms) | MPI_Bcast (ms) |
|-------|-----------|---------------|----------------|
| 16 | 40 | 0.008 | 0.009 |
| 16 | 400 | 0.022 | 0.009 |
| 16 | 4k | 0.026 | 0.010 |
| 16 | 40k | 0.096 | 0.018 |
| 16 | 400k | 0.355 | 0.084 |
| 16 | 4000k | 4.832 | 0.893 |
| 32 | 40 | 0.012 | 0.012 |
| 32 | 400 | 0.041 | 0.011 |
| 32 | 4k | 0.052 | 0.013 |
| 32 | 40k | 0.193 | 0.022 |
| 32 | 400k | 0.735 | 0.097 |
| 32 | 4000k | 7.447 | 0.937 |



- MPI_Scatter is a collective communication function that distributes data from a root process to all other processes in a communicator.
- MPI_Bcast sends the same data to all processes, while MPI_Scatter sends different chunks of data to each process.

- send_count: the number of elements to send to each process.
- recv_count: the number of elements to receive from each process.



```
#define TOTAL DATA 20
MPI Comm rank(MPI COMM WORLD, &rank);
MPI Comm size(MPI COMM WORLD, &size);
int send data[TOTAL DATA];
int recv count = TOTAL DATA / size;
int recv data[recv count];
if (rank == 0) {
    for (int i = 0; i < TOTAL DATA; i++)
        send data[i] = i;
    printf("Rank 0: Scattering data...\n");
}
MPI Scatter(send data, recv count, MPI INT,
            recv data, recv count, MPI INT,
            0, MPI COMM WORLD);
printf("Rank %d received:", rank);
for (int i = 0; i < recv count; i++)
    printf(" %d", recv data[i]);
printf("\n");
```

```
// send_data == 5

$ mpicc scatter.c -o scatter
$ mpirun -np 4 ./scatter

Rank 0: Scattering data...
Rank 0 received: 0 1 2 3 4
Rank 1 received: 5 6 7 8 9
Rank 2 received: 10 11 12 13 14
Rank 3 received: 14 15 16 17 18
```

if send_data cannot divide by size, the last process will receive the remaining data.

```
// send_data == recv_data == 6

Rank 0 received: 0 1 2 3 4 5
Rank 1 received: 6 7 8 9 10 11
Rank 2 received: 12 13 14 15 16 17
Rank 3 received: 18 19 20 -875497504 65535 20
```

What happens if send_count is not the same as recv_count?

```
int send_data[TOTAL_DATA];
int send count = TOTAL DATA / size;
int recv count = TOTAL DATA / size;
int recv data[recv count];
if (rank == 0) {
    for (int i = 0; i < TOTAL DATA; i++) {
        send data[i] = i;
    printf("Rank 0: Scattering data...\n");
}
if (rank == 3) {
    recv count = 4;
MPI Scatter(send data, send count, MPI INT,
            recv data, recv count, MPI INT,
            0, MPI COMM WORLD);
```

• A: It will cause an error.

```
$ mpicc scatter2.c -o scatter2
$ mpirun -np 4 ./scatter2

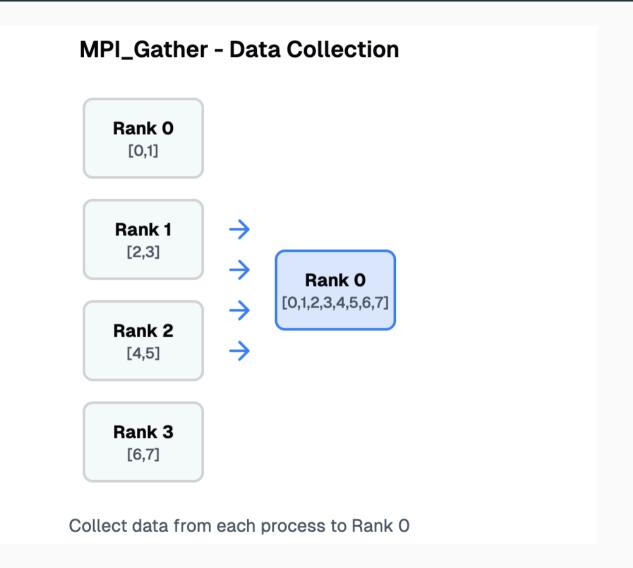
Rank 0: Scattering data...
Rank 0 received: 0 1 2 3 4
Rank 1 received: 5 6 7 8 9
Rank 2 received: 10 11 12 13 14
[miyabi-g3:1978858] *** An error occurred in MPI_Scatter
[miyabi-g3:1978858] *** reported by process [1190789121,3]
[miyabi-g3:1978858] *** on communicator MPI_COMM_WORLD
[miyabi-g3:1978858] *** MPI_ERR_TRUNCATE: message truncated
[miyabi-g3:1978858] *** MPI_ERR_TRUNCATE: message truncated
[miyabi-g3:1978858] *** mPI_ERRORS_ARE_FATAL (processes in this communicator will now abort,
[miyabi-g3:1978858] *** and potentially your MPI job)
```

3.5 MPI_Gather

- MPI_Gather is a collective communication function that collects data from all processes in a communicator and sends it to a root process.
- It is the reverse operation of MPI_Scatter.
- This is used in parallel sorting, parallel searching, and other parallel algorithms.

- Except for the root process, pass NULL for recv_data is allowed.
- recv_count is the number of elements to receive from each process, not the total number of elements.

3.5 MPI_Gather



3.5 MPI_Gather

```
#define ITEMS PER PROC 2
. . .
int send data[ITEMS PER PROC];
send data[0] = rank * 2;
send data[1] = rank * 2 + 1;
int recv data[ITEMS PER PROC * size];
MPI Gather(send data, ITEMS PER PROC, MPI INT,
            recv data, ITEMS PER PROC, MPI INT,
            0, MPI COMM WORLD);
if (rank == 0) {
    printf("Rank 0 gathered data: ");
    for (int i = 0; i < ITEMS PER PROC * size;</pre>
i++)
        printf("%d ", recv data[i]);
    printf("\n");
} else {
    printf("Rank %d sent data: %d %d\n", rank,
send data[0], send data[1]);
```

```
$ mpicc gather.c -o gather
$ mpirun -np 4 ./gather

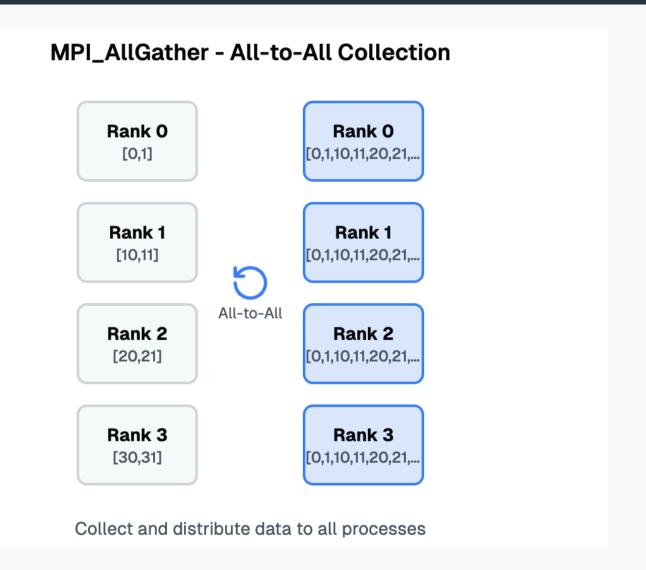
Rank 1 sent data: 2 3
Rank 3 sent data: 6 7
Rank 2 sent data: 4 5
Rank 0 gathered data: 0 1 2 3 4 5 6 7
```

3.6 MPI_Allgather

- MPI_Scatter and MPI_Gather conduct many-to-one or one-to-many communication.
- It is useful if you send data from multiple processes to multiple processes.
- MPI_Allgather is a collective communication function that collects data from all processes in a communicator and sends it to all other processes.
- It is like first MPI_Gather and then MPI_Bcast. Collect data by process rank order.

MPI_Allgather does not have a root process parameter.

3.6 MPI_Allgather



3.6 MPI_Allgather

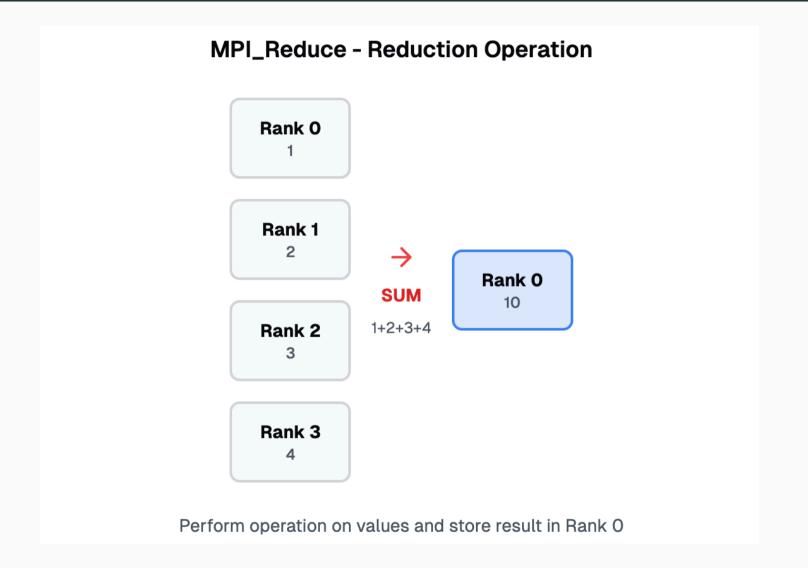
```
#define ITEMS PER PROC 2
. . .
int rank, size;
MPI Comm rank(MPI_COMM_WORLD, &rank);
MPI Comm size(MPI COMM WORLD, &size);
int send data[ITEMS PER PROC];
send data[0] = rank * 10;
send data[1] = rank * 10 + 1;
int recv data[ITEMS PER PROC * size];
MPI_Allgather(send data, ITEMS PER PROC,
MPI INT,
              recv data, ITEMS PER PROC,
MPI INT,
              MPI COMM WORLD);
printf("Rank %d received:", rank);
for (int i = 0; i < ITEMS PER PROC * size; i++)</pre>
    printf(" %d", recv data[i]);
printf("\n");
```

```
$ mpicc allgather.c -o allgather
$ mpirun -np 4 ./allgather

Rank 2 received: 0 1 10 11 20 21 30 31
Rank 3 received: 0 1 10 11 20 21 30 31
Rank 0 received: 0 1 10 11 20 21 30 31
Rank 1 received: 0 1 10 11 20 21 30 31
```

- reduce is a basic concept in functional programming. It transforms a set of numbers into a smaller set of numbers.
 - \rightarrow reduce([1, 2, 3, 4, 5], sum) = 15
 - ▶ reduce([1, 2, 3, 4, 5], multiply) = 120
- Collect dictributed data and apply a reduction operation is a tough task. However, MPI provides a simple interface to do this.
- MPI_Reduce is a collective communication function that collects data from all processes in a communicator to the root process, and applies a reduction operation to the data.

- MPI Reduction Operations:
 - ► MPI_MAX maximum value
 - ► MPI_MIN minimum value
 - ► MPI_SUM sum of values
 - MPI_PROD product of values
 - MPI_LAND logical AND of values
 - ► MPI_LOR logical OR of values
 - ► MPI_BAND bitwise AND of values
 - MPI_BOR bitwise OR of values
 - ► MPI_MAXLOC maximum value and its rank



```
int rank, size;
MPI Comm rank(MPI COMM WORLD, &rank);
MPI Comm size(MPI COMM WORLD, &size);
int value = rank + 1;
int sum;
MPI Reduce(&value, &sum, 1, MPI INT, MPI SUM, 0,
MPI COMM WORLD);
double average = (double)sum / size;
if (rank == 0) {
    printf("Rank %d: sum = %d, avg = %.2f\n",
rank, sum, average);
} else {
    printf("Rank %d: sum = %d, avg = %.2f\n",
rank, sum, average);
```

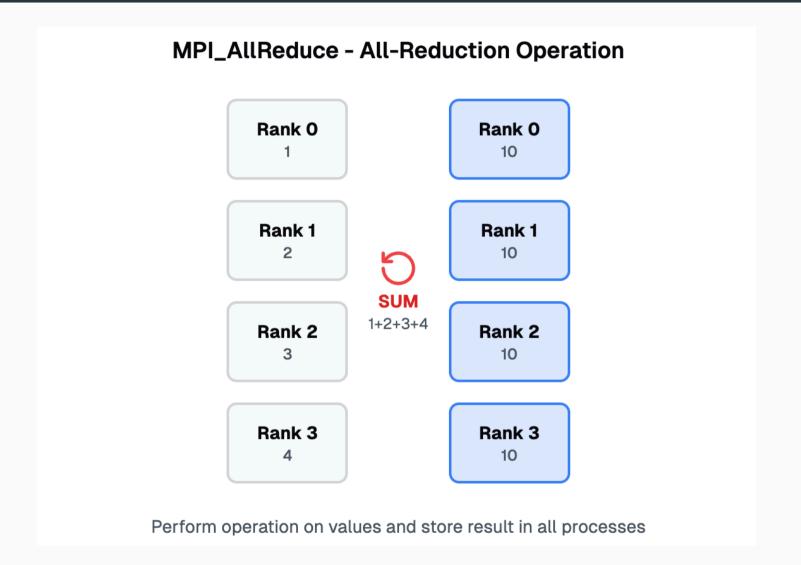
```
$ mpicc reduce.c -o reduce
$ mpirun -np 4 ./reduce

Rank 1: sum = 4197236, avg = 1049309.00
Rank 0: sum = 10, avg = 2.50
Rank 2: sum = 4197236, avg = 1049309.00
Rank 3: sum = 4197236, avg = 1049309.00
```

3.8 MPI_Allreduce

- MPI_Allreduce is a collective communication function that collects data from all processes in a communicator, applies a reduction operation to the data, and distributes the result to all processes.
- It is similar to MPI_Reduce, but the result is available to all processes, not just the root process.
- This is useful when all processes need to know the result of the reduction operation.

3.8 MPI_Allreduce



3.8 MPI_Allreduce

```
int rank, size;
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_size(MPI_COMM_WORLD, &size);

int value = rank + 1;
int total_sum = 0;

MPI_Allreduce(&value, &total_sum, 1, MPI_INT,
MPI_SUM, MPI_COMM_WORLD);

double average = (double)total_sum / size;
printf("Rank %d: total sum = %d, average =
%.2f\n", rank, total_sum, average);
```

```
$ mpicc allreduce.c -o allreduce
$ mpirun -np 4 ./allreduce

Rank 2: total sum = 10, average = 2.50
Rank 1: total sum = 10, average = 2.50
Rank 0: total sum = 10, average = 2.50
Rank 3: total sum = 10, average = 2.50
```

4. Application Example

4.1 How to Run Multi-node program on Miyabi

- The following is an example of how to run the Page Rank calculation on a multi-node cluster.
- When you submit a job to Miyabi-G cluster, you can specify the number of node and the number of process per node using -l select={num_nodes}:mpiprocs={num_procs_per_node} option.
- When you run a MPI program on a multi-node cluster, you need to specify the number of processes using mpirun -np {num_procs} option.

Example run.sh script:

```
#!/bin/bash
#PBS -q debug-g
#PBS -l select=16:mpiprocs=4
#PBS -W group_list=gc64
#PBS -o latest_result.txt
#PBS -j oe
...
mpirun -np 64 ./naive/pagerank_naive
```

4.1 How to Run Multi-node program on Miyabi

- If you want to run a MPI program on another process-per-node than mpiprocs, you can use --host option or --hostfile option.
- --host option allows you to specify the hostnames and the number of processes per host.
- --hostfile option allows you to specify a file that contains the hostnames and the number of processes per host.

Example -- host option:

```
$ mpirun -np 4 --host node1:2,node2:2 ./your_mpi_program
→node1 and node2 each run 2 processes.
```

Example -- hostfile option: hostfile.txt:

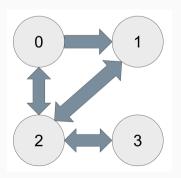
```
node1 slots=2
node2 slots=2/

$ mpirun -np 4 --hostfile hostfile.txt ./your_mpi_program
```

- For a simple application example of MPI, I will introduce the Page Rank calculation.
- Page Rank is an algorithm <u>used by Google to rank web pages</u> in search results.
- The concept of Page Rank is that "The page is important if it is linked from many other important pages."

$$x^{\{(k+1)\}} = dMx^{\{(k)\}} + (1-d)v$$

- M is the link matrix, each element represents the link between pages,
- x is the Page Rank vector, each element represents the Page Rank of a page,
- d is the damping factor, usually set to 0.85,
- v is the uniform distribution vector (initial vector).



$$d = 0.85, M = \begin{pmatrix} 0 & 0 & \frac{1}{3} & 0 \\ \frac{1}{2} & 0 & \frac{1}{3} & 0 \\ \frac{1}{2} & 1 & \frac{1}{3} & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}, v = \begin{pmatrix} \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \end{pmatrix}$$

$$M = \begin{pmatrix} 0 & 0 & \frac{1}{3} & 0 \\ \frac{1}{2} & 0 & \frac{1}{3} & 0 \\ \frac{1}{2} & 1 & \frac{1}{3} & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

- The sum of each column in matrix M is 1 because M represents a transition probability matrix, where each column corresponds to a node and the entries indicate the probability of moving from that node to others
- The Page Rank vector is updated iteratively until convergence.

$$\begin{split} x^{\{(1)\}} &= dM x^{\{(0)\}} + (1-d)v \\ x^{\{(2)\}} &= dM x^{\{(1)\}} + (1-d)v \\ x^{\{(3)\}} &= dM x^{\{(2)\}} + (1-d)v \end{split}$$

• • •

How to cunduct Page Rank calculation in parallel?

- Split the link matrix M into submatrices, each assigned to a process.
- Each process calculates the Page Rank for its submatrix.
- Use MPI_Allreduce to combine the results from all processes.
- Repeat until convergence.
- The following code is a simple example of Page Rank calculation using MPI.

Run Step:

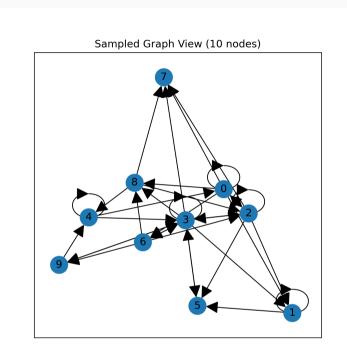
- 1. Generate a graph data file.
- 2. (option) Visualize the graph data.
- 3. Run the Page Rank calculation.

```
$ cd tutorial/pagerank/

// graph data generation
$ ./create_venv.sh
$ python3 preprocess/generate_graph.py
$ ls data/

// graph data visualization
$ python3 preprocess/visualize.py

// Page Rank calculation
$ cd tutorial/pagerank/naive
$ ./run.sh
```



```
$ ./run.sh

Final PageRank:
     0    1    2    3    4    5    6    7    8    9
PR: 0.0490 0.0817 0.0678 0.1453 0.0616 0.0748 0.0374 0.0598 0.0453 0.0384
```

- We divide the M matrix into submatrices, each assigned to a process.
- Each process only have a submatrix of M and a subvector of $x_k(*x)$, but the whole vector of $x_{k+1}(*new_x_full)$.

```
typedef struct {
    int n nodes;
    int n edges;
    int *out degree;
    double **M;
} Graph;
Graph g;
int n = g.n nodes;
// Data partitioning (row-wise)
int rows per proc = n / size;
int remainder = n % size;
int my rows = rows per proc + (rank < remainder ?</pre>
1:0):
int my start = rank * rows per proc + (rank <</pre>
remainder ? rank : remainder):
```

```
double *x = malloc(n * sizeof(double));
double *new x local = malloc(my rows *
sizeof(double));
for (int i = 0; i < n; i++) x[i] = 1.0 / n;
for (int i = 0; i < size; i++) {
    recvcounts[i] = rows per proc + (i <</pre>
remainder ? 1 : 0);
    displs[i] = i * rows per proc + (i <</pre>
remainder ? i : remainder);
double *new x full = malloc(n * sizeof(double));
```

• MPI_Allgatherv is different from MPI_Allgather in that it allows each process to send a different number of elements.

```
for (int iter = 0; iter < MAX ITER; iter++) {</pre>
    for (int i = 0; i < my rows; i++) {
        int global i = my start + i;
        new x local[i] = 0.0;
        for (int j = 0; j < n; j++) {
            new x local[i] += q.M[qlobal i][i] *
x[j];
        new x local[i] = DAMPING * new x local[i]
+ (1.0 - DAMPING) / n;
    MPI_Allgatherv(new_x_local, my rows,
MPI DOUBLE,
                    new x full, recvcounts,
displs, MPI DOUBLE, MPI COMM WORLD);
```

```
// チェック用: rank 0 が diff を計算
   double diff = 0.0:
   if (rank == 0) {
       for (int i = 0; i < n; i++) {
           diff += fabs(new x full[i] - x[i]);
   // 全rankにdiffをブロードキャスト(終了判定共有)
   MPI Bcast(&diff, 1, MPI DOUBLE, 0,
MPI COMM WORLD);
   if (diff < TOL) break;</pre>
   // x を更新
   for (int i = 0; i < n; i++)
       x[i] = new x full[i];
```

5. References

5. References

- Referenced in this tutorial:
 - ▶ MPI「超」入門(C言語編)- 東京大学情報基盤センター
 - ▶ 並列プログラミング入門
 - MPI Tutorial
- For Advanced Users:
- ・ 行列-行列積(2) 非同期通信 東京大学情報基盤センター
- Open MPI GitHub Repository

6. Appendix

6.1 How to use Page Rank when requested a search query

- Page Rank is just a algorithm to rank web pages.
- The requested search query is just a string, so we cannot use Page Rank directly.
- One approach is:
 - 1. we get related web pages according to DF-IDF or BM25 algorithm
 - 2. then we apply Page Rank to rerank the related web pages.

```
graph_loader.h
```

```
#ifndef GRAPH LOADER H
#define GRAPH LOADER H
typedef struct {
    int n nodes;
    int n edges;
    int *out degree;
    double **M;
} Graph;
int read graph(const char *filename, Graph *g);
void free graph(Graph *q);
#endif
```

graph_loader.c

```
#include "graph loader.h"
#include <stdio.h>
#include <stdlib.h>
int read graph(const char *filename, Graph *g) {
    FILE *fp = fopen(filename, "r");
    if (!fp) {
        perror("fopen");
        return -1;
    if (fscanf(fp, "%d", &g->n nodes) != 1) {
        fprintf(stderr, "Failed to read node
count\n");
        return -1;
```

```
g->out degree = calloc(g->n nodes,
sizeof(int));
    g->M = malloc(g->n nodes * sizeof(double
*));
    for (int i = 0; i < q -> n \text{ nodes}; i++) {
         q \rightarrow M[i] = calloc(q \rightarrow n nodes,
sizeof(double));
    int from, to;
    q - n edges = 0;
    while (fscanf(fp, "%d %d", &from, &to) == 2)
{
         g \rightarrow M[to][from] += 1.0;
         g->out degree[from]++;
         g->n edges++;
    fclose(fp);
```

```
// 正規化:M[to][from] /= out degree[from]
    for (int i = 0; i < g > n \text{ nodes}; i++) {
        for (int j = 0; j < q > n nodes; j++) {
            if (g->out degree[j] > 0) {
                 g->M[i][j] /= g->out degree[j];
    return 0:
void free graph(Graph *g) {
    for (int i = 0; i < q > n \text{ nodes}; i++) {
        free(g->M[i]);
    free(q->M);
    free(g->out degree);
```

main.c

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include <mpi.h>
#include "graph loader.h"
#define DAMPING 0.85
#define TOL 1e-6
#define MAX ITER 100
int main(int argc, char **argv) {
    MPI Init(&argc, &argv);
    int rank, size;
    MPI Comm rank(MPI COMM WORLD, &rank);
    MPI Comm size(MPI COMM WORLD, &size);
```

```
if (argc < 2) {
    if (rank == 0) {
        fprintf(stderr, "Usage: %s <n node>\n",
argv[0]);
    MPI Abort(MPI COMM WORLD, 1);
int n node = atoi(argv[1]);
char graph path[256], pagerank path[256];
snprintf(graph path, sizeof(graph path), "data/
%d/graph.txt", n node);
snprintf(pagerank path, sizeof(pagerank path),
"data/%d/pagerank.txt", n node);
Graph g;
if (read graph(graph path, &g) != 0) {
    MPI Abort(MPI COMM WORLD, 1);
```

```
int n = g.n nodes;
// データ分割(行分割)
int rows per proc = n / size;
int remainder = n % size;
int my rows = rows per proc + (rank <</pre>
remainder ? 1 : 0);
int my_start = rank * rows_per_proc + (rank <</pre>
remainder ? rank : remainder):
// PageRankベクトルxと各プロセスが担当する新しいベクトル
new x local(len(my rows)次元)を確保
double *x = malloc(n * sizeof(double));
double *new x local = malloc(my rows *
sizeof(double));
// 全プロセスで保持するの新しいPageRankベクトル
new x full(n次元)を確保
double *new x full = malloc(n * sizeof(double));
int *recvcounts = malloc(size * sizeof(int));
int *displs = malloc(size * sizeof(int));
for (int i = 0; i < n; i++) x[i] = 1.0 / n;
```

```
for (int i = 0; i < size; i++) {
    recvcounts[i] = rows per proc + (i <</pre>
remainder ? 1 : 0);
    displs[i] = i * rows per proc + (i <</pre>
remainder ? i : remainder);
if (rank == 0) {
    printf("Starting PageRank computation with
%d processes...\n", size);
printf("[Rank %d] Local rows: %d, Start index:
%d\n", rank, my rows, my start);
double t start = MPI Wtime();
for (int iter = 0; iter < MAX ITER; iter++) {</pre>
    for (int i = 0; i < my rows; i++) {
        int global i = my start + i;
        new x local[i] = 0.0;
        for (int j = 0; j < n; j++) {
            new x local[i] += g.M[global i][j] *
x[j];
        new x local[i] = DAMPING *
new x local[i] + (1.0 - DAMPING) / n;
```

```
MPI Allgatherv(new x local, my rows,
MPI DOUBLE,
                   new x full, recvcounts,
displs, MPI DOUBLE, MPI COMM WORLD);
    // チェック用: rank 0 が diff を計算
    double diff = 0.0:
    if (rank == 0) {
       for (int i = 0; i < n; i++) {
            diff += fabs(new x full[i] - x[i]);
       printf("[Iter %d] diff = %f\n", iter +
1, diff);
    // 全rankにdiffをブロードキャスト(終了判定共有)
    MPI Bcast(&diff, 1, MPI DOUBLE, 0,
MPI COMM WORLD);
    if (diff < TOL) break;</pre>
   // x を更新
    for (int i = 0; i < n; i++) x[i] =
new x full[i];
```

```
double t end = MPI Wtime();
if (rank == 0) {
    printf("Main Loop Time: %.6f seconds\n",
t end - t start);
free(new x full);
free(recvcounts);
free(displs);
// 結果表示
if (rank == 0) {
    printf("\n\nFinal PageRank:\n");
    for (int i = 0; i < n; i++) {
        printf("Node %6d: %f\n", i, x[i]);
    printf("\n");
```

```
// 結果をファイルに書き出す
if (rank == 0) {
    FILE *fp = fopen(pagerank path, "w");
    if (fp == NULL) {
       perror("Failed to open result file");
       MPI Abort(MPI COMM WORLD, 1);
    fprintf(fp, "%d\n", n);
   for (int i = 0; i < n; i++) {
       fprintf(fp, "%d %f\n", i, x[i]);
    fclose(fp);
    printf("PageRank results written to %s\n", pagerank_path);
free(x);
free(new x local);
free graph(&g);
MPI Finalize();
return 0;
```

6.3 Example code of Communication and Group

6.3 Example code of Communication and Group

• Example code of p.21 slide

```
MPI Group world group;
MPI Comm group (MPI COMM WORLD, &world group);
// === Group A: \{0,1,2,3\} ===
int ranks a[] = \{0, 1, 2, 3\};
MPI Group group a;
MPI Group incl(world group, 4, ranks a,
&group a);
MPI Comm comm a;
MPI Comm create group (MPI COMM WORLD, group a, 0,
&comm a);
// === Group B: \{0,1,2,4\} ===
int ranks b[] = \{0, 1, 2, 4\};
MPI Group group b;
MPI Group incl(world group, 4, ranks b,
&group b);
MPI Comm comm b;
MPI_Comm_create_group(MPI_COMM_WORLD, group_b, 1,
&comm b);
```

```
// Rank 0 in each comm sends a message to others
if (comm a != MPI COMM NULL) {
    int comm a rank;
    MPI Comm rank(comm a, &comm a rank);
    if (comm a rank == 0) {
        int msg = 100;
        for (int i = 1; i < 4; i++)
           MPI Send(&msg, 1, MPI INT, i, 0,
comm a);
    } else {
        int recv:
        MPI Recv(&recv, 1, MPI INT, 0, 0, comm a,
MPI STATUS IGNORE);
        printf("comm a: World Rank %d received %d
from Rank 0\n", world rank, recv);
```

6.3 Example code of Communication and Group

```
if (comm b != MPI COMM NULL) {
    int comm b rank;
    MPI Comm rank(comm b, &comm b rank);
    if (comm b rank == 0) {
        int msq = 200;
        for (int i = 1; i < 4; i++)
            MPI Send(&msg, 1, MPI INT, i, 0,
comm b);
    } else {
        int recv;
        MPI Recv(&recv, 1, MPI INT, 0, 0, comm b,
MPI STATUS IGNORE);
        printf("comm b: World Rank %d received %d
from Rank 0\n", world rank, recv);
}
```

```
// Rank 3 sends a message to Rank 4 via (failed)
if (world rank == 3) {
    int msq = 999:
    int rc = MPI Send(&msg, 1, MPI INT, 4, 99,
MPI COMM WORLD);
    printf("Rank 3 tried to send to Rank 4 via
MPI COMM WORLD (rc=%d)\n", rc);
if (world rank == 4) {
    int recv, flag;
    MPI Status status;
    MPI Iprobe(3, 99, MPI COMM WORLD, &flag,
&status):
    if (flag) {
        MPI Recv(&recv, 1, MPI INT, 3, 99,
MPI COMM WORLD, MPI STATUS IGNORE);
        printf("Rank 4 received unexpected
message from Rank 3: %d\n", recv);
    } else {
        printf("Rank 4: No message from Rank 3
(as expected)\n");
```

6.3 Example code of Communication and Group

```
// Cleanup
if (comm_a != MPI_COMM_NULL)
MPI_Comm_free(&comm_a);
if (comm_b != MPI_COMM_NULL)
MPI_Comm_free(&comm_b);
MPI_Group_free(&group_a);
MPI_Group_free(&group_b);
MPI_Group_free(&world_group);
```

```
$ mpicc comm_group.c -o comm_group
$ mpirun -np 5 ./comm_group

comm_a: World Rank 1 received 100 from Rank 0
comm_b: World Rank 1 received 200 from Rank 0
comm_a: World Rank 3 received 100 from Rank 0
Rank 3 tried to send to Rank 4 via MPI_COMM_WORLD
(rc=0)
comm_a: World Rank 2 received 100 from Rank 0
comm_b: World Rank 2 received 200 from Rank 0
comm_b: World Rank 4 received 200 from Rank 0
Rank 4: No message from Rank 3 (as expected)
```