

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 **SIMD**

1.2 Parallel Programming Classification

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

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	Free version included
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

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

2. Basic Learning of MPI

2.1 Minimum MPI Program

2.1.1 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
```

2.1 Minimum MPI Program

2.1.2 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 <<
std::endl;
    std::cout << "My Rank      : " << my_rank << std::endl;

    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      : 2
```

2.1 Minimum MPI Program

2.1.3 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
```

2.1 Minimum MPI Program

2.1.4 MPI Language Differences

	C	C++ (※)	Fortran
MPI Header	<code>#include <mpi.h></code>	<code>#include <mpi.h></code>	<code>use mpi</code> or <code>include 'mpif.h'</code>
Official MPI support	○	▲	○
Syntax intuitiveness	Explicit C syntax	Almost same as C	<code>call</code> and subroutine based
Compiler	<code>mpicc</code>	<code>mpicxx</code> or <code>mpic++</code>	<code>mpif90</code> or <code>mpifort</code>
Scientific computing	○	▲	◎

- 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.

2.2 Important Terms of MPI

2.2.1 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`.

2.2 Important Terms of MPI

2.2.2 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
```

```
Communicator: MPI_COMM_WORLD  
Group: [P0, P1, P2, P3]  
Rank:  0    1    2    3
```

2.2 Important Terms of MPI

2.2.3 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.

2.2 Important Terms of MPI

- **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);
```

2.2 Important Terms of MPI

- **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 0 => Group 0, New Rank 0 of 3
```

2.2 Important Terms of MPI

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

2.3 Point-to-Point Communication

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);
```

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");
```

2.3 Point-to-Point Communication

```
$ 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 ]
```

2.3 Point-to-Point Communication

- 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");
}
```


2.3 Point-to-Point Communication

```
$ 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
```

2.3 Point-to-Point Communication

- many MPI functions have the following signature:

```
MPI_Send(  
    void* data,  
    int count,  
    MPI_Datatype datatype,  
    int destination,  
    int tag,  
    MPI_Comm communicator  
);
```

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

2.3 Point-to-Point Communication

- Many MPI functions have the following signature

```
MPI_Send(  
    void* data,           // data buffer address  
    int count,            // number of elements in the buffer  
    MPI_Datatype datatype, // data type of the elements  
    int destination,      // destination process rank  
    int tag,              // message tag (for filtering)  
    MPI_Comm communicator // communicator  
);
```

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

2.3 Point-to-Point Communication

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

3. Collective Coommunication

3.1 sincronization

- Collective communication is a communication method that involves all processes in a communicator.
- 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 to 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

```
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 2: after barrier
```


3.3 MPI_Bcast

- **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.

```
MPI_Bcast(  
    void* data,           // data buffer address  
    int count,           // number of elements in the buffer  
    MPI_Datatype datatype, // data type of the elements  
    int root,            // rank of the root process  
    MPI_Comm communicator // communicator  
);
```

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

3.3 MPI_Bcast

```
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 ]
```

3.3 MPI_Bcast

- 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++) {
            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?

3.3 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.
- ...

3.3 MPI_Bcast

- 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

3.4 MPI_Scatter, MPI_Gather, MPI_Allgather

3.4.1 MPI_Scatter

- **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.

```
MPI_Scatter(  
    void* send_data,           // data buffer address to send  
    int send_count,           // number of elements to send to each process  
    MPI_Datatype send_datatype, // data type of the elements to send  
    void* recv_data,          // data buffer address to receive  
    int recv_count,           // number of elements to receive  
    MPI_Datatype recv_datatype, // data type of the elements to receive  
    int root,                 // rank of the root process  
    MPI_Comm communicator.    // communicator  
);
```

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

3.4 MPI_Scatter, MPI_Gather, MPI_Allgather

```
#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 == 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
```

3.4 MPI_Scatter, MPI_Gather, MPI_Allgather

3.4.2 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.

```
MPI_Gather(  
    void* send_data,           // data buffer address to send  
    int send_count,           // number of elements to send from each process  
    MPI_Datatype send_datatype, // data type of the elements to send  
    void* recv_data,          // data buffer address to receive  
    int recv_count,           // number of elements to receive from each process  
    MPI_Datatype recv_datatype, // data type of the elements to receive  
    int root,                 // rank of the root process  
    MPI_Comm communicator     // communicator  
);
```

- 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.

3.4 MPI_Scatter, MPI_Gather, 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 * 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;
        i++)
        printf("%d ", recv_data[i]);
    printf("\n");
}
```

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

3.4 MPI_Scatter, MPI_Gather, MPI_Allgather

3.4.3 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(  
    void* send_data,           // data buffer address to send  
    int send_count,           // number of elements to send from each process  
    MPI_Datatype send_datatype, // data type of the elements to send  
    void* recv_data,          // data buffer address to receive  
    int recv_count,           // number of elements to receive from each process  
    MPI_Datatype recv_datatype, // data type of the elements to receive  
    MPI_Comm communicator     // communicator  
);
```

- MPI_Allgather does not have a root process parameter.

3.4 MPI_Scatter, MPI_Gather, 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++)
    printf(" %d", recv_data[i]);
printf("\n");
```

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

4. References

4.1 MPI Reference

- [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](#)