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; hightly portable.
- Multiple Implementation:
 - Available implementations include OpenMPI, MPICH, and Intel MPI, etc.
- Difficalt 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

2.1.1 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
```

2.1.2 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 <<</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
```

2.1.3 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
```

2.1.4 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	aplicit C syntax Almost same as C call and subroutine base	
Compiler	r mpicc mpicxx or mpic++ mpif90 or	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.

2.2.1 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.

2.2.2 Communicator Image

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

```
- Eaxmple:
- 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
```

2.2.3 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.

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

```
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
```

• 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
);
```

Many MPI functions have the following signature

```
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

3. Collective Coommunication

3.1 syncronization

- Collective communication is a communication method that involves all processes in a communicator.
- In collective communication, syncronization 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 processed, 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
```

- 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.

. . .

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

3.4.1 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.

- 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 == 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
```

3.4.2 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.

- 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.

```
#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,
            O, 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
```

3.4.3 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 processed 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.

```
#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
```

3.5.1 MPI_Reduce

- 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 distribulted 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
```

3.5.2 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.

```
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. 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