

# Parallel Algorithms and Programming

## MPI

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# Agenda

Message Passing Systems

Introduction to MPI

Point-to-point communication

Collective communication

Other features

# Agenda

## Message Passing Systems

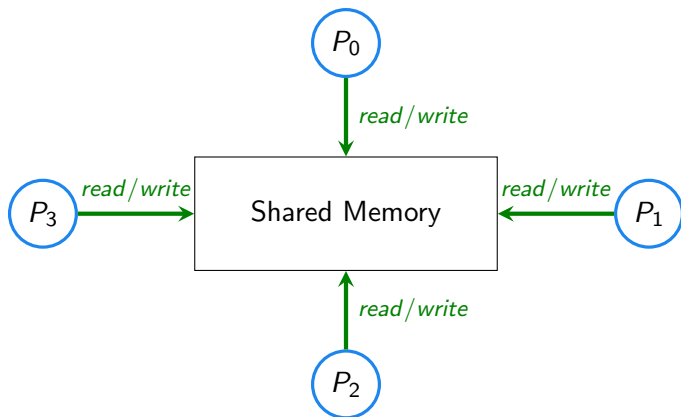
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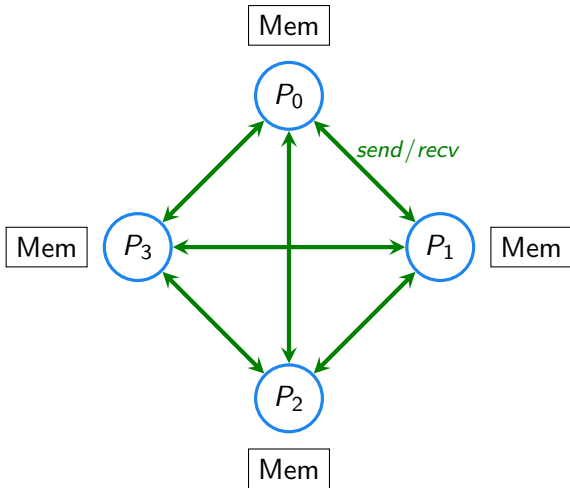
## Shared memory model



- Processes have access to a shared address space
- Processes communicate by reading and writing into the shared address space

# Distributed memory model

## Message passing



- Each process has its own private memory
- Processes communicate by sending and receiving messages

# Applying the models

## Natural fit

- The **distributed memory model** corresponds to processes executing on servers interconnected through a network

## However

- The distributed memory model can be implemented on top of shared memory
  - ▶ Send/Recv operations can be implemented on top of shared memory

# In large-scale parallel systems

And more generally in any cluster of machines

A large number of servers:

- Interconnected through a high-performance network
- Equipped with multicore multi-processors and accelerators

## What programming model to use?

- Hybrid solution
  - ▶ Message passing for inter-node communication
  - ▶ Shared memory inside a node
- Message passing everywhere
  - ▶ Communication inside the nodes are implemented with message passing on top of the shared memory
  - ▶ Less and less used as the number of cores per node increases

# Message Passing Programming Model

## Differences with the shared memory model

- Communication is explicit
  - ▶ The user is in charge of managing communication
  - ▶ The programming effort is bigger
- No good automatic techniques to parallelize code
- More efficient when running on a distributed setup
  - ▶ Better control on the data movements



# The Message Passing Interface (MPI)

<http://mpi-forum.org/>

MPI is the most commonly used solution to program message passing applications in the HPC context.

## What is MPI?

- MPI is a standard
  - ▶ It defines a set of operations to program message passing applications.
  - ▶ The standard defines the semantic of the operations (not how they are implemented)
  - ▶ Current version is 4.0 (<https://www.mpi-forum.org/docs/mpi-4.0/mpi40-report.pdf>)
- Several implementations of the standard exist (libraries)
  - ▶ Open MPI and MPICH are the two main open source implementations (provide C and Fortran bindings)

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# My first MPI program

```
#include <stdio.h>
#include <string.h>
#include <mpi.h>

int main(int argc, char *argv[])
{
    char msg[20];
    int my_rank;
    MPI_Status status;

    MPI_Init(&argc, &argv);

    MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);

    if (my_rank == 0) {
        strcpy(msg, "Hello !");
        MPI_Send(msg, strlen(msg), MPI_CHAR, 1, 99, MPI_COMM_WORLD);
    }
    else {
        MPI_Recv(msg, 20, MPI_CHAR, 0, 99, MPI_COMM_WORLD, &status);
        printf("I received %s!\n", msg);
    }
    MPI_Finalize();
}
```

# SPMD application

MPI programs follow the SPMD execution model:

- SPMD = Single Program Multiple Data
- Each process executes the same program at independent points
- Only the data differ from one process to the others
  - ▶ At least the logical identifier (rank) of each process is different
- Different actions may be taken based on the rank of the process

# Compiling and executing

## Compiling

- Use `mpicc` instead of `gcc` (`mpicxx`, `mpif77`, `mpif90`)

```
mpicc -o hello_world hello_world.c
```

## Executing

```
mpirun -n 2 -hostfile machine_file ./hello_world
```

- Creates 2 MPI processes that will run on the 2 first machines listed in the `machine_file` (the allocation policy is implementation dependent)
- If no `machine_file` is provided, the processes are created on the local machine

# The execution of the `hello_world` program

## About the created processes

- Each process created by `mpirun` has a unique identifier called its `rank`.
- Each process executes the same program but will execute different branches of the code depending on its rank.

## Result of our program

- In the `hello_world` program, the process with rank 0 sends a string to the process with rank 1 that receives it.
- Note that the program hangs if it is run with more than 2 processes:
  - ▶ If a process with rank 2 is created, it will also try to receive a message from rank 0 but it will never receive one.

# Analyzing our example

## Mandatory calls (by every process)

- `MPI_Init()`: Initialize the MPI execution environment
  - ▶ No other MPI calls can be done before `Init()`.
- `MPI_Finalize()`: Terminates MPI execution environment
  - ▶ To be called before terminating the program

Note that all MPI functions are prefixed with `MPI_`

# Communicators and ranks

## Communicators

- A communicator defines a **group** of processes that can communicate in a communication **context**.
- Inside a group, processes have a unique rank
- Ranks go from 0 to  $p - 1$  in a group of size  $p$
- At the beginning of the application, a default communicator including all application processes is created:  
**MPI\_COMM\_WORLD**
- Any communication occurs in the context of a communicator
- Processes may belong to multiple communicators and have a different rank in different communicators



## Communicators and ranks: Retrieving basic information

- `MPI_Comm_rank(MPI_COMM_WORLD, &rank)`: Get rank of the process in `MPI_COMM_WORLD`.
- `MPI_Comm_size(MPI_COMM_WORLD, &size)`: Get the number of processes belonging to the group associated with `MPI_COMM_WORLD`.

```
#include <mpi.h>

int main(int argc, char **argv)
{
    int size, rank;
    char name[256];

    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    MPI_Comm_size(MPI_COMM_WORLD, &size);

    gethostname(name, 256);
    printf("Hello from %d on %s (out of %d procs.)\n", rank, name, size);

    MPI_Finalize();
}
```

# MPI Messages

A MPI message includes a payload (the data) and metadata (called the envelope).

## Metadata

- Processes rank (sender and receiver)
- A Communicator (the context of the communication)
- A message tag (can be used to distinguish between messages inside a communicator)

## Payload

The payload is described with the following information:

- Address of the beginning of the buffer
- Number of elements
- Type of the elements

## Signature of send/recv functions

```
int MPI_Send(const void *buf,  
             int count, MPI_Datatype datatype,  
             int dest, int tag, MPI_Comm comm);
```

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

## Elementary datatypes in C

MPI datatype	C datatype
MPI_CHAR	signed char
MPI_SHORT	signed short int
MPI_INT	signed int
MPI_LONG	signed long int
MPI_UNSIGNED_CHAR	unsigned char
MPI_UNSIGNED_SHORT	unsigned short int
MPI_UNSIGNED	unsigned int
MPI_UNSIGNED_LONG	unsigned long int
MPI_FLOAT	float
MPI_DOUBLE	double
MPI_LONG_DOUBLE	long double
MPI_BYTE	1 Byte
MPI_PACKED	see MPI_Pack()

## A few more things

### The status object

Contains information about the communication (3 fields):

- `MPI_SOURCE`: the id of the sender.
- `MPI_TAG`: the tag of the message.
- `MPI_ERROR`: the error code

The status object has to be allocated by the user.

- But its value is assigned by the `MPI_Recv()` function.

### Wildcards for receptions

- `MPI_ANY_SOURCE`: receive from any source
- `MPI_ANY_TAG`: receive with any tag

## About wildcards

- Wildcards should be avoided when they are not strictly needed
  - ▶ Specifying explicitly the message that is supposed to be received allows avoiding/detecting bugs.
- There are some cases where wildcards can be useful:
  - ▶ The programmer is unable to determine before execution time from which rank a process is going to receive data
  - ▶ A process is supposed to receive data with different tags without a predefined order.

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## Blocking communication

`MPI_Send()` and `MPI_Recv()` are blocking communication primitives.

- `MPI_Send()` corresponds to the **standard** communication mode<sup>1</sup>

What does blocking means in this context?

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<sup>1</sup>See additional slides for the description of other modes



# Blocking communication

`MPI_Send()` and `MPI_Recv()` are blocking communication primitives.

- `MPI_Send()` corresponds to the **standard** communication mode<sup>1</sup>

What does blocking means in this context?

- **Blocking send:** When the call returns, it is safe to reuse the buffer containing the data to send.
  - ▶ It does not mean that the data has been transferred to the receiver.
  - ▶ It might only be that a local copy of the data has been made
  - ▶ It may complete before the corresponding receive has been posted
- **Blocking recv:** When the call returns, the received data are available in the buffer.

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<sup>1</sup>See additional slides for the description of other modes

# Protocols for standard mode

## A taste of the implementation

MPI libraries implement several protocols for point-to-point communication

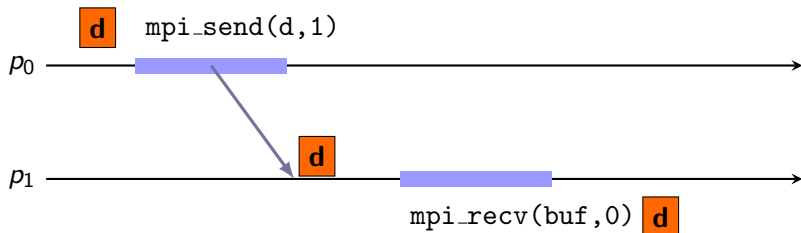
- The protocol used for each communication is chosen based on different parameters
  - ▶ The main parameter is the message size

Two of the main protocols are:

- The **Eager** protocol (for small messages)
- The **Rendezvous** protocol (for large messages)

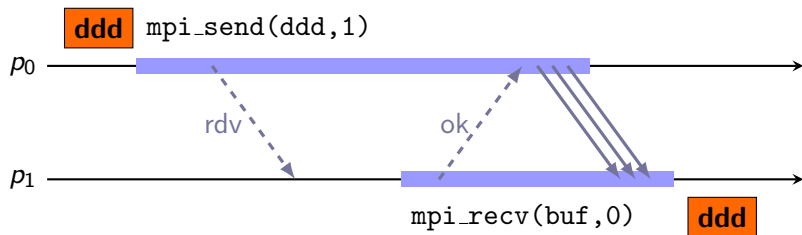
## Eager protocol

- Data sent assuming receiver can store it
- The receiver may not have posted the corresponding reception
- This solution is used only for small messages (typically < 64kB)
  - ▶ This solution has low synchronization delays
  - ▶ It may require an extra message copy on destination side



# Rendezvous protocol

- Message is not sent until the receiver is ready
- Protocol used for *large messages*
  - ▶ Higher synchronization cost
  - ▶ If the message is big, it should be buffered on sender side.



# Non blocking communication

Basic idea: dividing communication into two logical steps

- Posting a request: Informing the library of an operation to be performed
- Checking for completion: Verifying whether the action corresponding to the request is done

## Posting a request

- Non-blocking send: `MPI_Isend()`
- Non-blocking recv: `MPI_Irecv()`
- They return a `MPI_Request` to be used to check for completion

# Non blocking communication

## Checking request completion

- Testing if the request is completed : `MPI_Test()`
  - ▶ Returns true or false depending if the request is completed
- Other versions to test several requests at once (suffix `_any`, `_some`, `_all`)

## Waiting for request completion

- Waiting until the request is completed : `MPI_Wait()`
- Other versions to wait for several requests at once (suffix `_any`, `_some`, `_all`)

## Overlapping communication and computation

Non-blocking communication primitives allow trying to overlap communication and computation

- Better performance if the two occur in parallel

```
MPI_Isend(..., req);  
...  
/* run some computation */  
...  
MPI_Wait(req);
```

However, things are not that simple:

- MPI libraries are not multi-threaded (by default)
  - ▶ The only thread is the application thread (no progress thread)
- The only way to get overlapping is through specialized hardware
  - ▶ The network card has to be able to manage the data transfer alone

## Matching incoming messages and reception requests

MPI communication channels are *First-in-First-out* (FIFO)

- Note however that a communication channel is defined in the context of a communicator

### Matching rules

- When the reception request is named (source and tag defined), it is matched with the next arriving message from the source with correct tag.
- When the reception request is anonymous (`MPI_ANY_SOURCE`), it is matched with next message from any process in the communicator
  - ▶ Note that the matching is done when the envelope of the message arrives.
  - ▶ The message size is not taken into account for the matching



# Discussion about performance of P2P communication

Things to have in mind to get good communication performance:

- Avoid extra copies of messages (notion of *zero-copy*)
  - ▶ Reception requests should be posted before corresponding send requests
  - ▶ Using *non-blocking recv* can help
- Reduce synchronization delays
  - ▶ Same solution as before
- Take into account the topology of the underlying network
  - ▶ Contention can have a dramatic impact on performance
  - ▶ Beyond the scope of this lecture

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## Collective communication

A collective operation involves all the processes of a communicator.

All the classic operations are defined in MPI:

- Barrier (global synchronization)
- Broadcast (one-to-all)
- Scatter/ gather
- Allgather (gather + all members receive the result)
- AllToAll
- Reduce, AllReduce (Example of op: sum, max, min)
- etc.

There are **v** versions of some collectives (Gatherv, Scatterv, Allgatherv, Alltoallv):

- They allow using a vector of send or recv buffers.

# Example with broadcast

## Signature

```
int MPI_Bcast( void *buffer,
               int count, MPI_Datatype datatype,
               int root, MPI_Comm comm );
```

## Broadcast Hello

```
#include <mpi.h>
int main(int argc, char *argv[])
{
    char msg[20];
    int my_rank;
    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);

    if (my_rank == 0)
        strcpy(msg, "Hello from 0!");
    MPI_Bcast(msg, 20, MPI_CHAR, 0, MPI_COMM_WORLD);
    printf("rank_%d: I received %s\n", my_rank, msg);
    MPI_Finalize();
}
```

# About collectives and synchronization

## What the standard says

A collective communication call may, or may not, have the effect of synchronizing all calling processes.

- It cannot be assumed that collectives synchronize processes
  - ▶ Synchronizing here means that no process would complete the collective operation until the last one entered the collective
  - ▶ `MPI_Barrier()` still synchronize the processes in all cases
- Why is synchronization useful?
  - ▶ Ensure correct message matching when using anonymous receptions
  - ▶ Avoid too many *unexpected* messages (where the reception request is not yet posted)

# About collectives and synchronization

## What about real life?

- In most libraries, collectives imply a synchronization
  - ▶ Because implementing a version without synchronization is costlier
- A user program that assumes no synchronization is erroneous

## Incorrect code (High risk of deadlock)

```
if(my_rank == 1)
    MPI_Recv(0);
```

```
MPI_Bcast(...);
```

```
if(my_rank == 0)
    MPI_Send(1);
```

# Implementation of collectives

- MPI libraries implement several algorithms for each collective operation
- Different criteria are used to select the best one for a call, taking into account:
  - ▶ The number of processes involved
  - ▶ The size of the message
- A supercomputer may have its own custom MPI library
  - ▶ Take into account the physical network to optimize collectives

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## Derived datatypes

We have already introduced the basic datatypes defined by MPI

- They allow sending contiguous blocks of data of one type

Sometimes one will want to:

- Send non-contiguous data (a sub-block of a matrix)
- Buffers containing different datatypes (an integer count, followed by a sequence of real numbers)

One can defined derived datatypes

# Derived datatypes

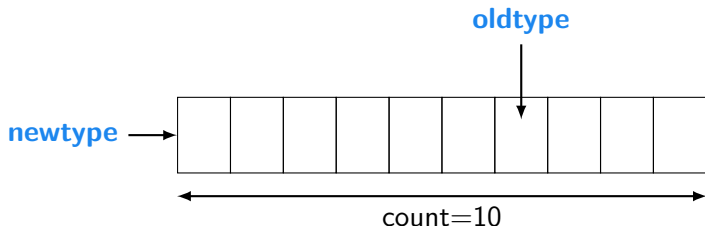
- A derived datatype is defined based on a type-map
  - ▶ A type-map is a sequence of pairs {dtype, displacement}
  - ▶ The displacement is an address shift relative to the basic address

## Committing types

- `MPI_Type_commit()`
  - ▶ Commits the definition of the new datatype
  - ▶ A datatype has to be committed before it can be used in a communication
- `MPI_Type_free()`
  - ▶ Mark the datatype object for de-allocation

## Data type: Contiguous

- `int MPI_Type_contiguous(int count, MPI_Datatype oldtype, MPI_Datatype *newtype)`
  - ▶ `count` is the number of elements concatenated to build the new type.

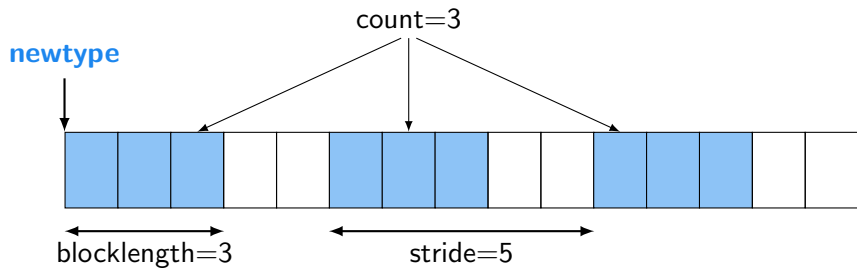


## Data type: Vector

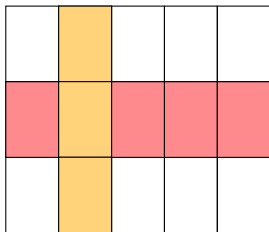
The vector type allows defining a set of blocks containing multiple elements with an equal distance between the blocks.

- `int MPI_Type_vector(int count, int blocklength, int stride, MPI_Datatype oldtype, MPI_Datatype *newtype)`
  - ▶ `count` is the number of blocks.
  - ▶ `blocklength` is the number of elements in one block
  - ▶ `stride` is the number of elements between the start of each block

## Data type: Vector



## Exercise



Define the datatype that corresponds to a row and to a column:

- `nb_col`: the number of columns
- `nb_row`: the number of rows
- Matrix allocation:

```
int *matrix= malloc(nb_col * nb_row * sizeof(int));
```

Matrix stored in a row-contiguous manner.

## Exercise

```
MPI_Datatype Col_Type, Row_Type;

MPI_Type_contiguous(nb_col, MPI_INT, &Row_Type);
MPI_Type_vector(nb_row, 1, nb_col, MPI_INT, &Col_Type);

MPI_Type_commit(&Row_Type);
MPI_Type_commit(&Col_Type);

...

MPI_Type_free(&Row_Type);
MPI_Type_free(&Col_Type);
```

## Performance with derived datatypes

Derived datatypes should be used carefully:

- By default, the data are copied into a contiguous buffer before being sent (no zero-copy)
- Special hardware support is required to avoid this extra copy



# Operations on communicators

New communicators can be created by the user:

- Duplicating a communicator (`MPI_Comm_dup()`)
  - ▶ Same group of processes as the original communicator
  - ▶ New communication context

```
int MPI_Comm_dup(MPI_Comm comm, MPI_Comm *newcomm);
```

- Splitting a communicator (`MPI_Comm_split()`)

```
int MPI_Comm_split(MPI_Comm comm, int color, int key,  
                  MPI_Comm *newcomm);
```

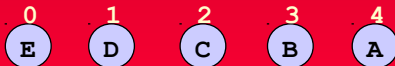
- ▶ Partitions the group associated with `comm` into disjoint subgroups, one for each value of `color`.
- ▶ Each subgroup contains all processes of the same `color`.
- ▶ Within each subgroup, the processes are ranked in the order defined by the value of the argument `key`.
- ▶ Useful when defining hierarchy of computation



MPI\_COMM\_WORLD

```
MPI_Comm_rank(MPI_COMM_WORLD, rank);
MPI_Comm_size(MPI_COMM_WORLD, size);
color = 2*rank/size;
key = size - rank - 1
```

```
MPI_Comm_split(MPI_COMM_WORLD, color, key, n_comm)
```



N\_COMM\_1



N\_COMM\_2

# Warning

The goal of this presentation is only to provide an overview of the MPI interface.

Many more features are available, including:

- One-sided communication
- Non-blocking collectives
- Process management
- Inter-communicators
- etc.

MPI 3.1 standard is a 836-page document

# References

- Many resources available on the Internet
- The man-pages
- The specification documents are available at:  
<http://mpi-forum.org/docs/>

Additional slides

# Communication Mode ()

- **Standard (MPI\_Send())**
  - ▶ The send may buffer the message locally or wait until a corresponding reception is posted.
- **Buffered (MPI\_BSend())**
  - ▶ Force buffering if no matching reception has been posted.
- **Synchronous (MPI\_SSend())**
  - ▶ The send cannot complete until a matching receive has been posted (the operation is not local)
- **Ready (MPI\_RSend())**
  - ▶ The operation fails if the corresponding reception has not been posted.
  - ▶ Still, send may complete before reception is complete

**In a vast majority of cases the standard MPI\_Send() is used.**