Parallel Computing

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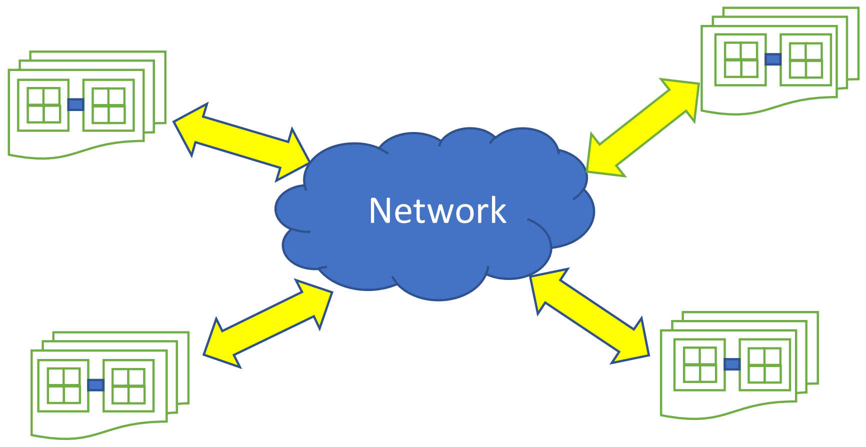
Lecture 10:

- ❑ Distributed-Memory Programming with MPI

Distributed-Memory Architectures

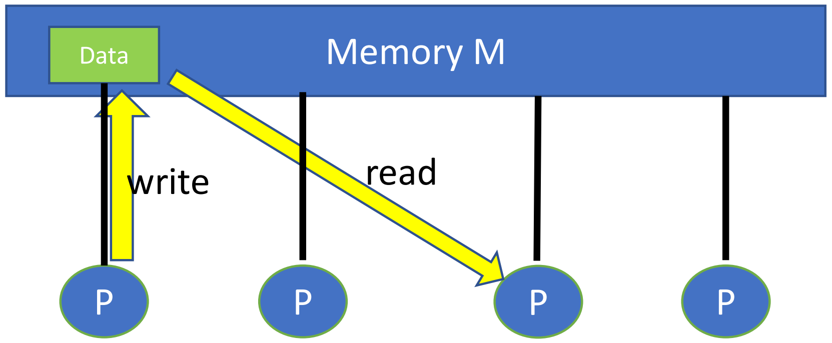
A **HPC cluster** consists of compute nodes

- each node has **no direct access to other nodes' memory**
- each node runs a separate copy of OS



Shared-Memory Programming Model

All processing elements **P** have direct access to memory **M**.

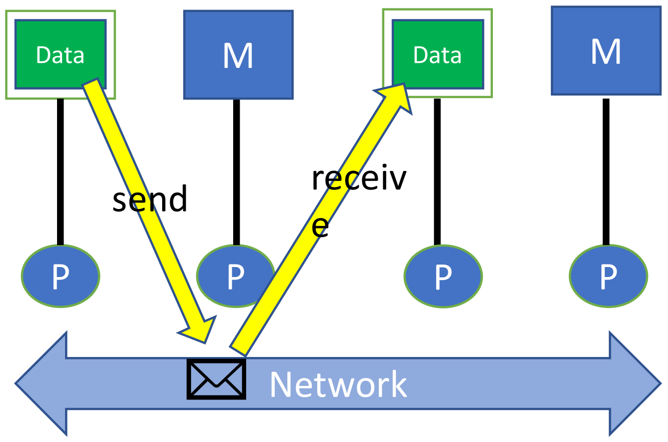


Data exchange is achieved through **read/write operations on shared variables** located in the **physical global address space**.

- Pthreads
- OpenMP

Distributed-Memory Programming Model

Each processing element **P** has its own memory module **M**.



Data exchange is achieved through **send/received operations** via a **message passing** mechanism over the network.

- Two distinct copies of the data are at the sender and the receiver because the two processing elements do not share the same physical address space.

Distributed-Memory Programming Model

Each processing element works on a separate memory module **M.**

Data exchange is achieved through **message passing**.

- Message Passing = Send/Receive operations.
- No shared variables are involved because the processing elements do not share a common virtual global address space.
- Synchronization is done implicitly via send/receive operations.

Single Program Multiple Data

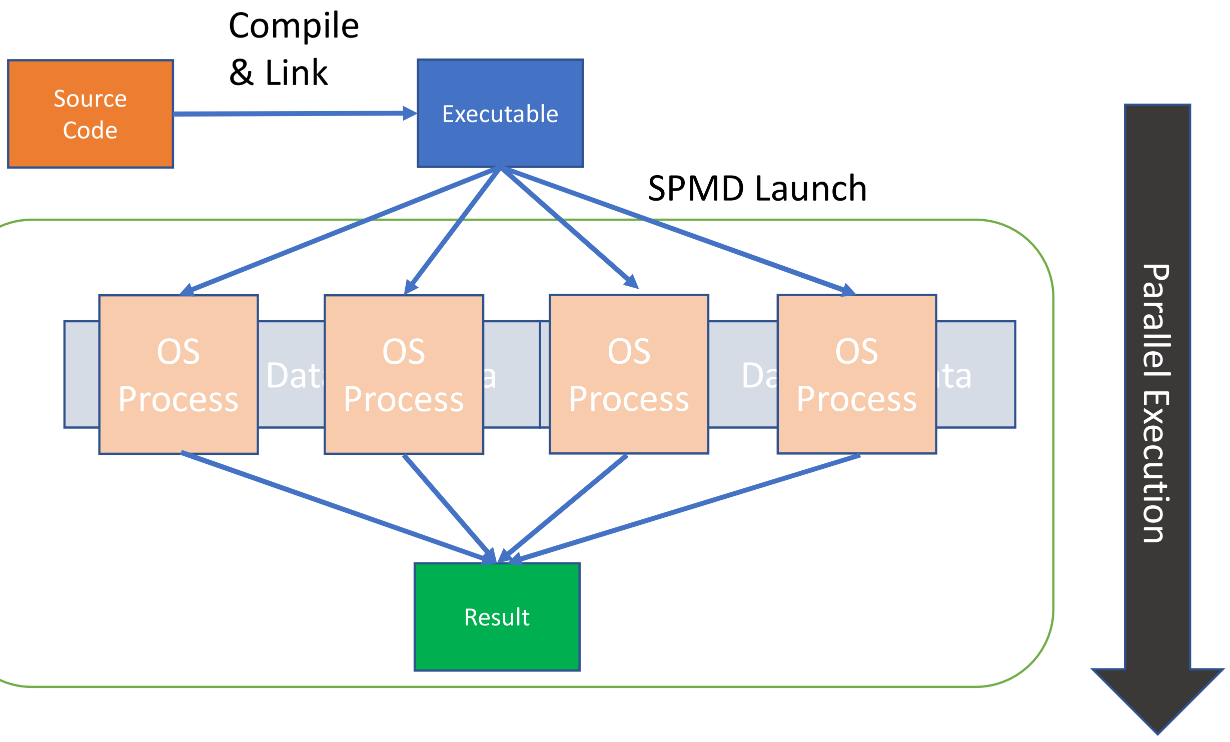
Single Program Multiple Data (**SPMD**)

- Single Binary Executable
- Multiple (different parts of) Data
- Each process identifies itself using a unique ID.

In an application that employs the distributed-memory programming model, each processing element has an OS process:

- Each runs the same binary executable.
- Each has its own virtual address space separated from those running on the other processing elements.
- Process use their unique IDs to steer control flow of the individual processes.

Single Program Multiple Data



Single Program Multiple Data

Requirements for SPMD environments

- Dynamic unique identification of processes
- Robust mechanisms for data exchange
    - Identity of sender and receiver
    - Amount of data
    - Type of data
    - Arrival of data
- Synchronization and communication mechanisms
    - Point-to-point communication
    - Collective communication
    - One-sided communication
- Process Launch and control mechanisms
- Portability across different platforms

Message Passing Interface (MPI)

Message Passing Interface

- The de-facto standard API for explicit message passing
- Maintained by the non-profit **Message Passing Interface Forum**
  - **https://www.mpi-forum.org**
- A number of implementations of the standard API by different vendors
  - MPICH, Intel MPI, Open MPI etc.
- Standard Bindings include
  - C and Fortran
  - Non-standard bindings for other languages also exist
    - C++, Python and Java

Message Passing Interface (MPI)

MPI is implemented as a runtime library, not a language/compiler extension.

Initialization Mechanism:

To use MPI in a program, the programmer needs to initialize the MPI runtime.

Classical MPI (pre-MPI 4.0)

- MPI_Init (with a **single thread**)
- MPI_Init_thread (with **multiple threads**)

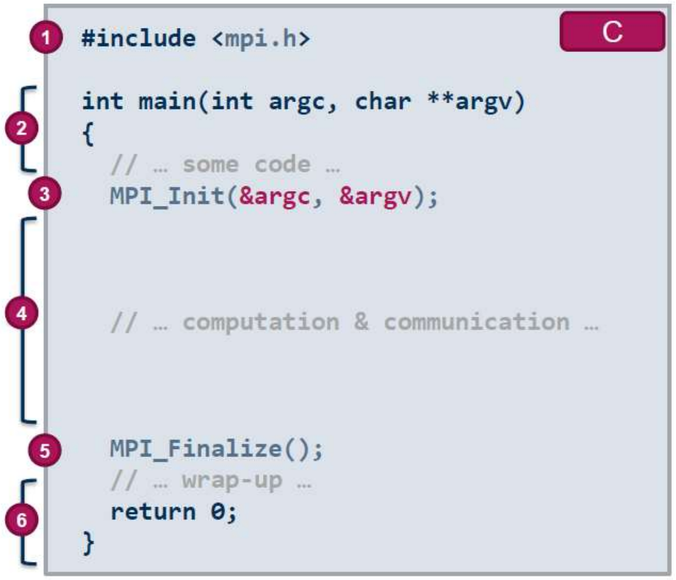
New MPI (MPI 4.0)

- MPI_Session_init

MPI: Initialization & Finalization

Initialization and Finalization:

1. inclusion of the header file
2. Pre-initialization
   1. No MPI function calls are allowed with a few exceptions.
3. Initialization of the MPI environment
4. Parallel Computation and Communication
5. Finalization of the MPI environment
6. Post-finalization
   - No MPI function calls are allowed with a few exceptions.



```
#include <mpi.h>

int main(int argc, char **argv)
{
  // … some code …
  MPI_Init(&argc, &argv);



  // … computation & communication …



  MPI_Finalize();
  // … wrap-up …
  return 0;
}
```

MPI: Initialization (Single-Threaded)

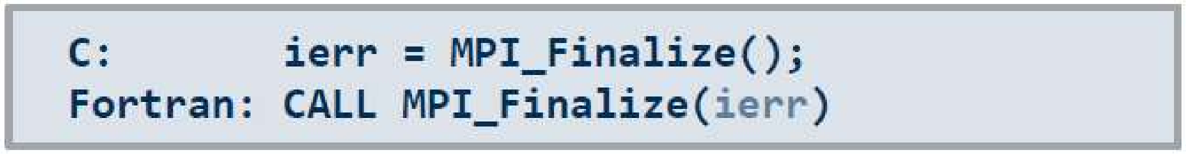
Initialization:

```
C:        ierr = MPI_Init(&argc, &argv);
Fortran: CALL MPI_Init(ierr)
```

- **MPI_Init** initializes the **MPI runtime environment** and makes the calling process a member of MPI_COMM_WORLD.
    - Both arguments can be NULL.
    - An error code is returned (for the C binding)
- **MPI_Init** must be called once during the program execution.

MPI: Finalization

Finalization:



```
C:         ierr = MPI_Finalize();
Fortran:  CALL MPI_Finalize(ierr)
```

- **MPI_Finalize** cleans up and terminates the **MPI runtime environment**.
- **MPI_Finalize** must be called once before the process terminates.
  - It is not recommended to have other code after the call.

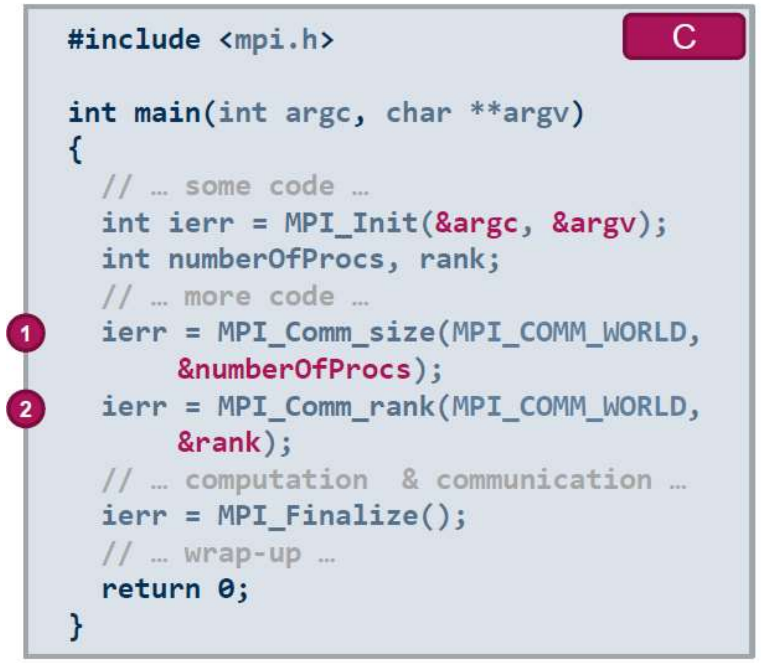
MPI: General Structure of an MPI Program

How many MPI processes are there?

- The calling process can find out how many processes there are in the MPI program with **MPI_Comm_size**.

Who am I?

- The calling process can find out its identity or **rank** with **MPI_Comm_rank**.
- Ranks are numbered **starting from zero**.



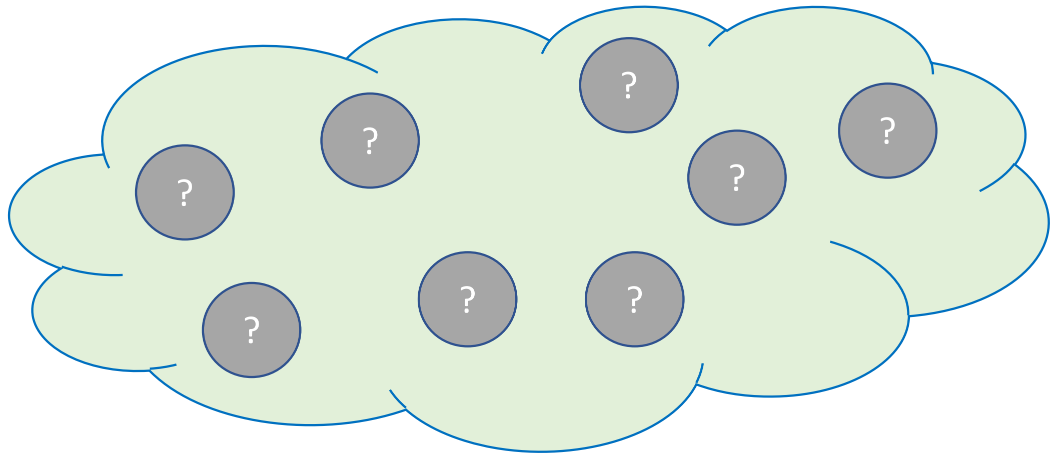
```c
#include <mpi.h>

int main(int argc, char **argv)
{
  // … some code …
  int ierr = MPI_Init(&argc, &argv);
  int numberOfProcs, rank;
  // … more code …
  ierr = MPI_Comm_size(MPI_COMM_WORLD,
       &numberOfProcs);
  ierr = MPI_Comm_rank(MPI_COMM_WORLD,
       &rank);
  // … computation  & communication …
  ierr = MPI_Finalize();
  // … wrap-up …
  return 0;
}
```

MPI: Rank

The processes in an MPI program are initially indistinguishable.

MPI assigns each process a unique identity (**rank**) in a communication context (**communicator**).

- The **initial communication context** is **MPI_COMM_WORLD**, which contains all the MPI processes within the MPI program.



MPI: Rank

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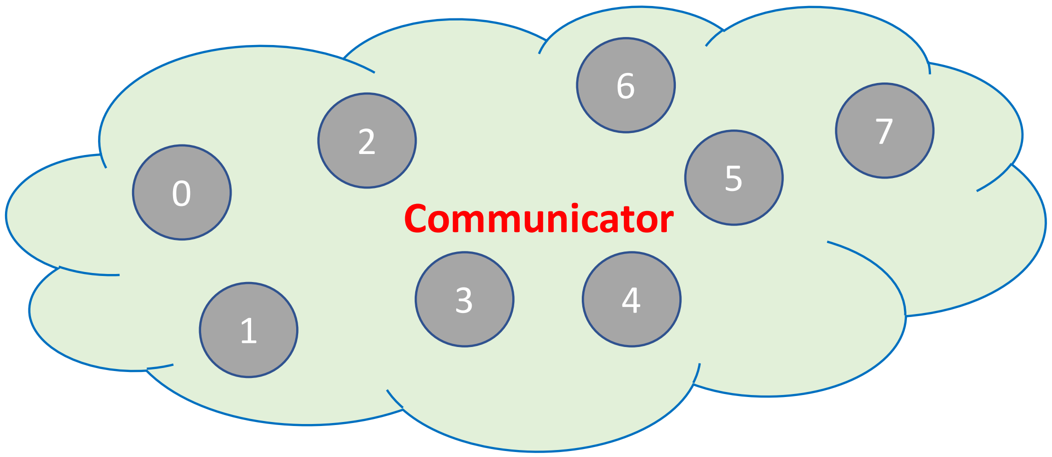


MPI: Rank and Communicator

Rank:

- Ranks range from 0 to n-1.
  where n is the number of MPI processes in the communication context (communicator).
- MPI processes within an MPI program can have **different ranks in different communicators**.

Communicator:

- A communicator is **a logical context in which communication occurs**.
  - a group of processes together with additional information.
- The initial communicator **MPI_COMM_WORLD** is implicitly available in every MPI program.
  - a group of all processes the MPI runtime environment is initially launched with at startup.

MPI: Compiling an MPI Program

- MPI is a library with C header files.
- Most MPI vendors provide compiler wrappers that the programmer can conveniently use.

$$\begin{tikzcd}
\boxed{\textbf{cc}} \arrow[r] & \boxed{\textbf{mpicc}} \\
\boxed{\textbf{c++}} \arrow[r] & \boxed{\textbf{mpic++}} \\
\boxed{\textbf{f90}} \arrow[r] & \boxed{\textbf{mpif90}}
\end{tikzcd}$$

Note that names are not standardized.

MPI: Executing an MPI Program

Most implementations provide a **special launcher program** **mpiexec**.

```
mpiexec -n nprocs … program <arg1> <arg2> <arg3> …
```

- The launcher launches **nprocs** instances of **program** with arguments **arg1**, **arg2**, **arg3** etc.

The MPI standard specifies the **mpiexec** launcher program, but does not require it.

MPI: Executing an MPI Program

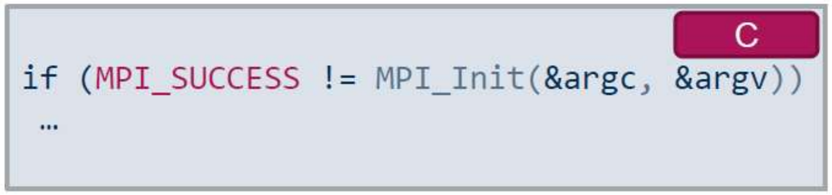
The launcher performs the following procedure at startup:

- help MPI processes find each other and establish the **MPI_COMM_WORLD** communicator
- redirect the standard output of all processes to the terminal
- redirect the terminal input to the standard input of rank 0
- forward received signals

MPI: Error Handling

Error codes indicate the success of MPI calls:

- Failure is indicated by an error code other than **MPI_SUCCESS**.



```
if (MPI_SUCCESS != MPI_Init(&argc, &argv))
 …
```

- An MPI error handler is called first before the call returns.
    - The default error handler for **non-IO calls** abort the entire MPI program.

- The values of error codes are **implementation-dependent**.
    - **MPI_Error_string** can be used decode error codes into human-reader information

MPI: Handles to MPI Opaque Objects

MPI objects such as communicators are referenced through **handles**.

- Process-local values cannot be passed from one process to another.
- Objects are referenced by handles are **opaques**.
  - Implementation-dependent
  - Blackbox to the user

Examples of handles in MPI are **MPI_Comm**, **MPI_Datatype**, **MPI_Request** etc.

MPI: Datatype Handle

MPI cannot automatically deduce the data types of supplied buffers at runtime.

- The program must provide additional information on the data types.

MPI datatype handles tell the MPI runtime environment how to:

- read binary values from the receive buffer
- write binary values into the send buffer
- correctly apply value alignments
- convert values between different machine representations in heterogeneous environments

MPI: Datatype Handle

MPI datatypes are **handles**.

- They cannot be used to declare variables of a specific language type.
- **sizeof(MPI_INT)** returns the size of the datatype handle, **not** the size of an int in the C programming language.

Basic datatypes corresponds to **native datatypes** in the programming language.

MPI data type	C native data type
MPI_CHAR	char
MPI_SHORT	short
MPI_INT	int
MPI_FLOAT	float
MPI_DOUBLE	double
MPI_UNSIGNED_INT	unsigned int
…	…
MPI_BYTE	

No binary conversion is used for untyped data.

MPI: Local and Non-Local Operations

A **Local** operation requires

- no communication with another MPI process.
- Its completion depends only on the local operations.

A **Non-local** operation requires

- some specific, semantically MPI-related procedure to be called on another MPI process.
- Such an operation requires communication with another MPI process.

MPI: MPI Operations

MPI defines several operations that are **a sequence of steps** performed by the MPI runtime environment to establish and enable

- data transfer
- data synchronization

Four stages:

1. Initialization:
   - Resources (e.g. buffer address, arguments) are passed to the MPI runtime environment.
2. Starting:
   - The operation takes over control of the resources (e.g., buffer contents).
3. Completion:
   - The operation returns control of the resources (e.g., buffer contents).
4. Freeing:
   - The operation returns control of the remaining resources.

MPI: Blocking and Non-Blocking

A **blocking** procedure can return only when the associated operation completes locally.

- Upon completion, any supplied input arguments (e.g., supplied buffer) can be safely reused or deallocated.
  - For example, a blocking send operation **does not mean** the message must have been successfully delivered to the destination before the send operation can complete. (We will see more about this)

A **non-blocking** procedure may return before the associated operation completes locally.

- One or more additional MPI calls are required to complete the operation.
- The supplied input arguments are not allowed to be reused or deallocated until the operation completes.

MPI: Synchronous and Asynchronous

A **synchronous** procedure blocks the calling process until the operation completes.

- A synchronous procedure completes locally only with specific remote intervention.
  - In the case of a send-and-receive communication, both the sender and the receiver complete when the receiver has started to receive the message.

An **asynchronous** procedure may complete locally without remote intervention.

Note that synchronous/asynchronous implies blocking/non-blocking, but not vice versa.

References

[1] *William Gropp, Ewing Lusk, and Anthony Skjellum. 2014. Using MPI: Portable Parallel Programming with the Message-Passing Interface. The MIT Press.*

[2] M*arc-Andre Hermanns. 2021. MPI in Small Bites. PPCES 2021.*