PARALLEL PROGRAMMING WITH MPI

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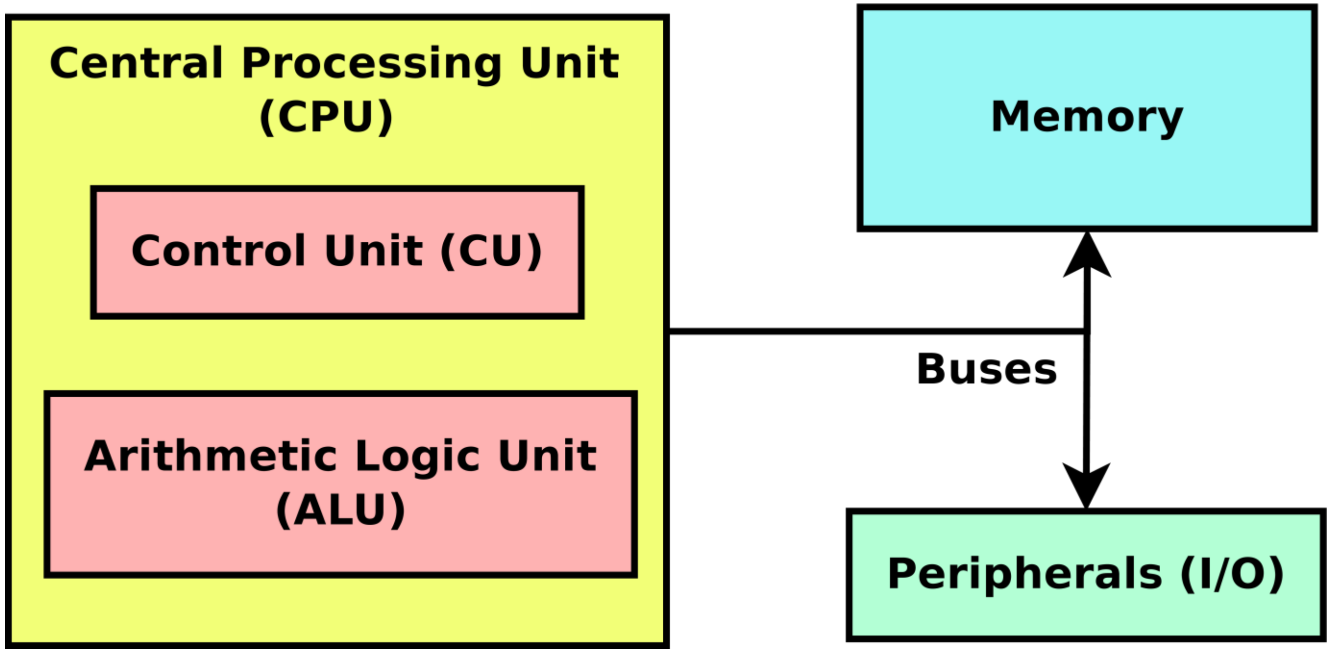
Goals

- The goal is to learn:
  - how an MPI program runs on a distributed memory system
  - how to write MPI programs
  - how to use basic point-to-point and collective MPI communication
  - how topologies can be defined
  - some useful examples for further work with MPI

Content

- MPI and distributed memory parallelism
- Structure of the library functions
- Different hands-on exercises

Recap: a computer is...



Recap: a CPU is…

Example of the MIPS architecture: control unit lines in orange, data lines in black

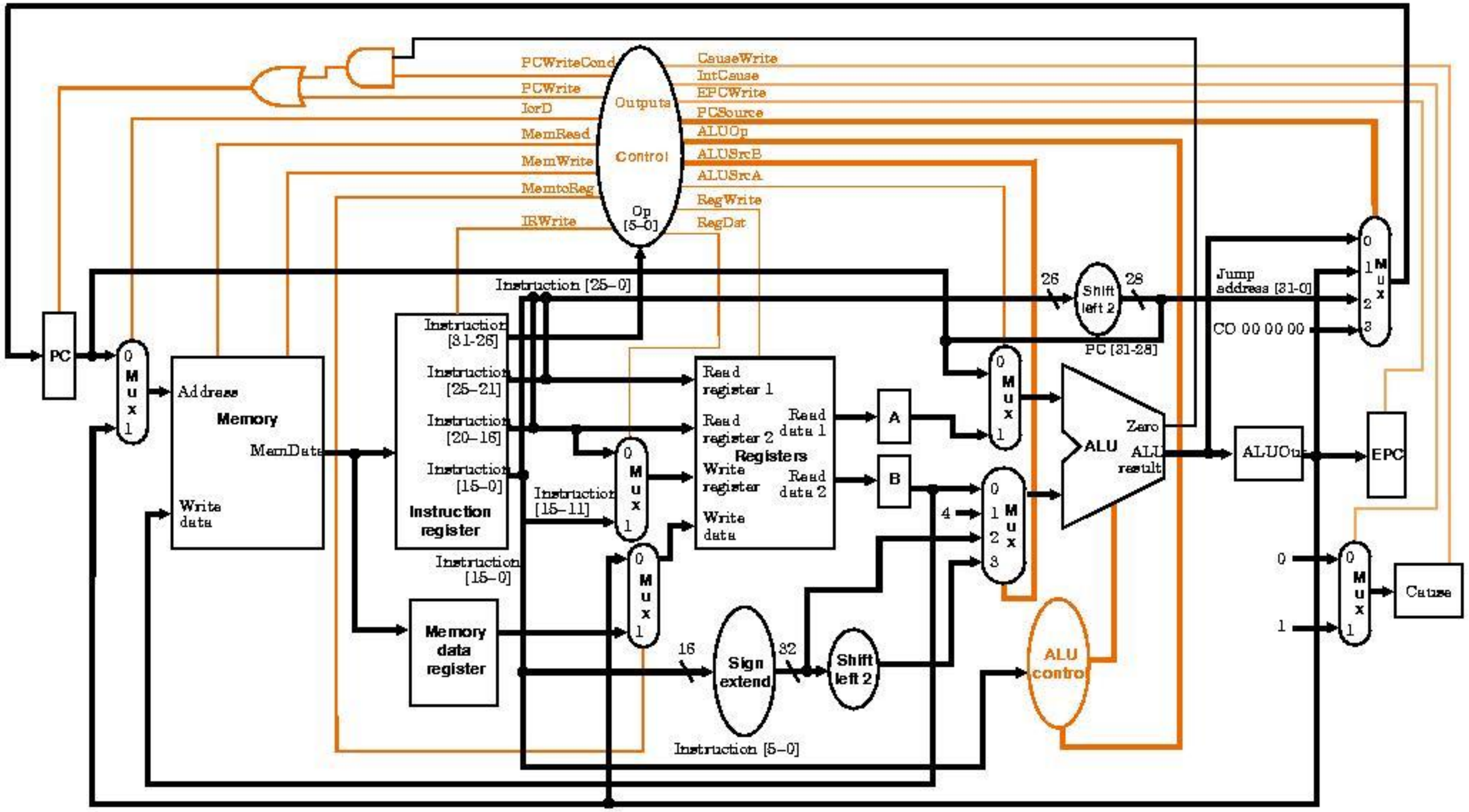


Image source: http://people.cs.pitt.edu/˜don/coe1502/current/Unit4a/Unit4a.html (last visited: 2018)

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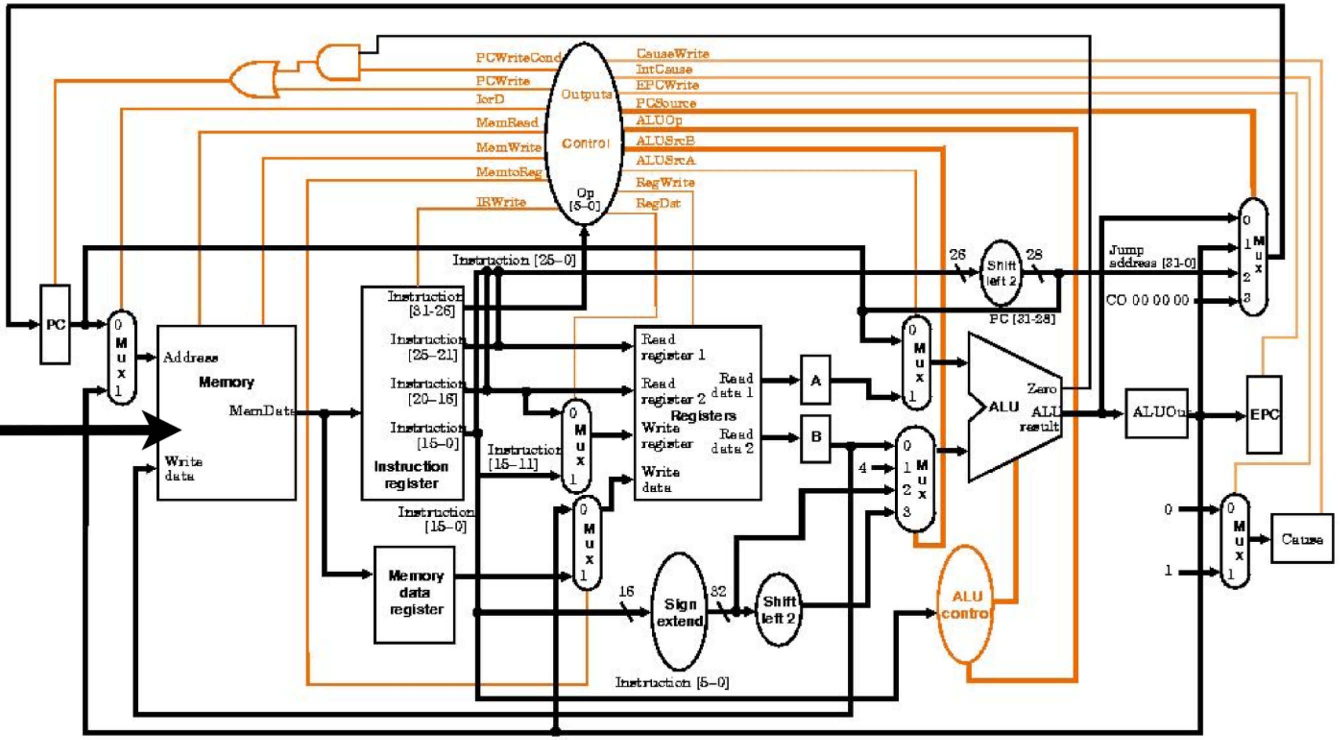
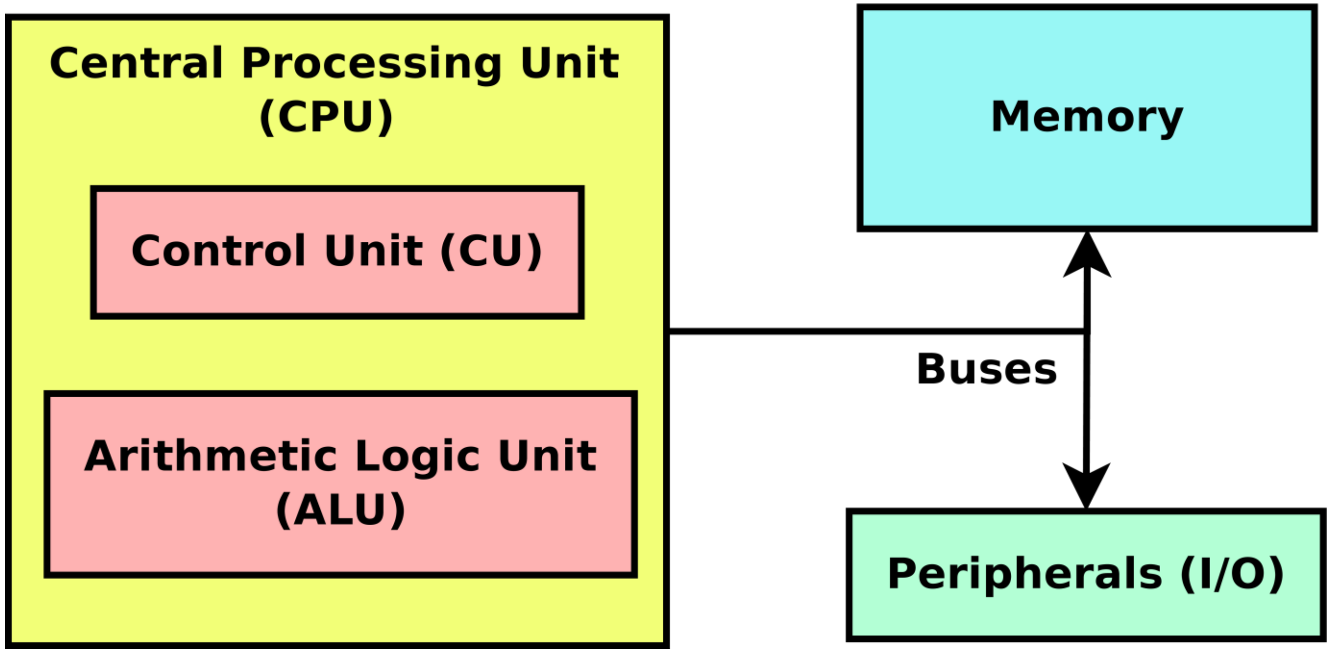
Recap: a program becomes a process…

```
00111100000000010000000000000100
00110100010000100000000000000100
00111100000000100000101110001010
00110100100001000010000000110010
...
```



Recap: different types of computer architectures



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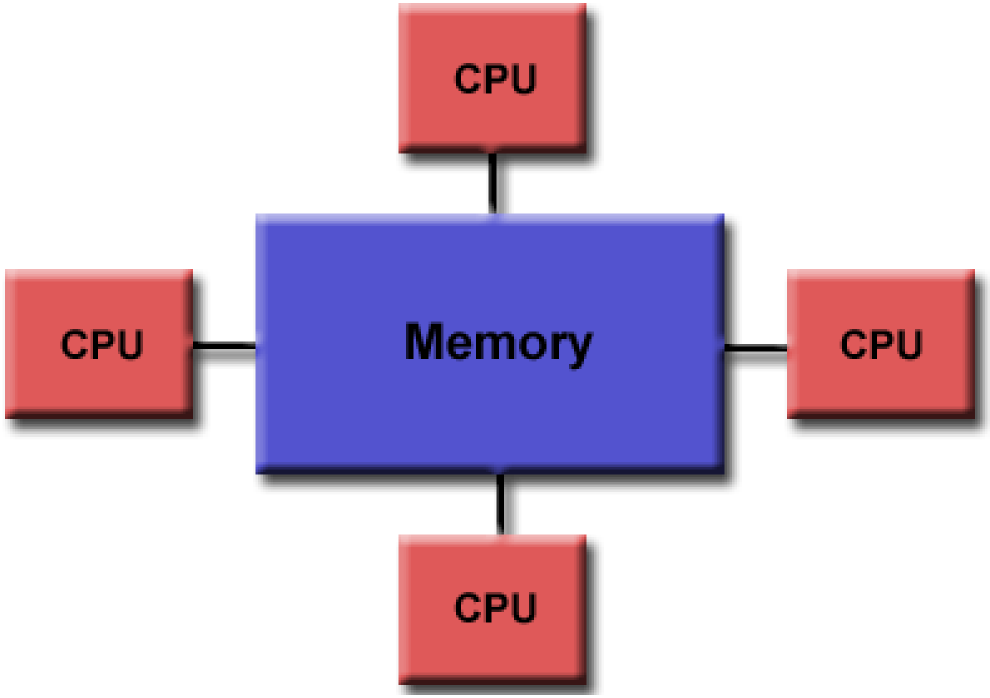

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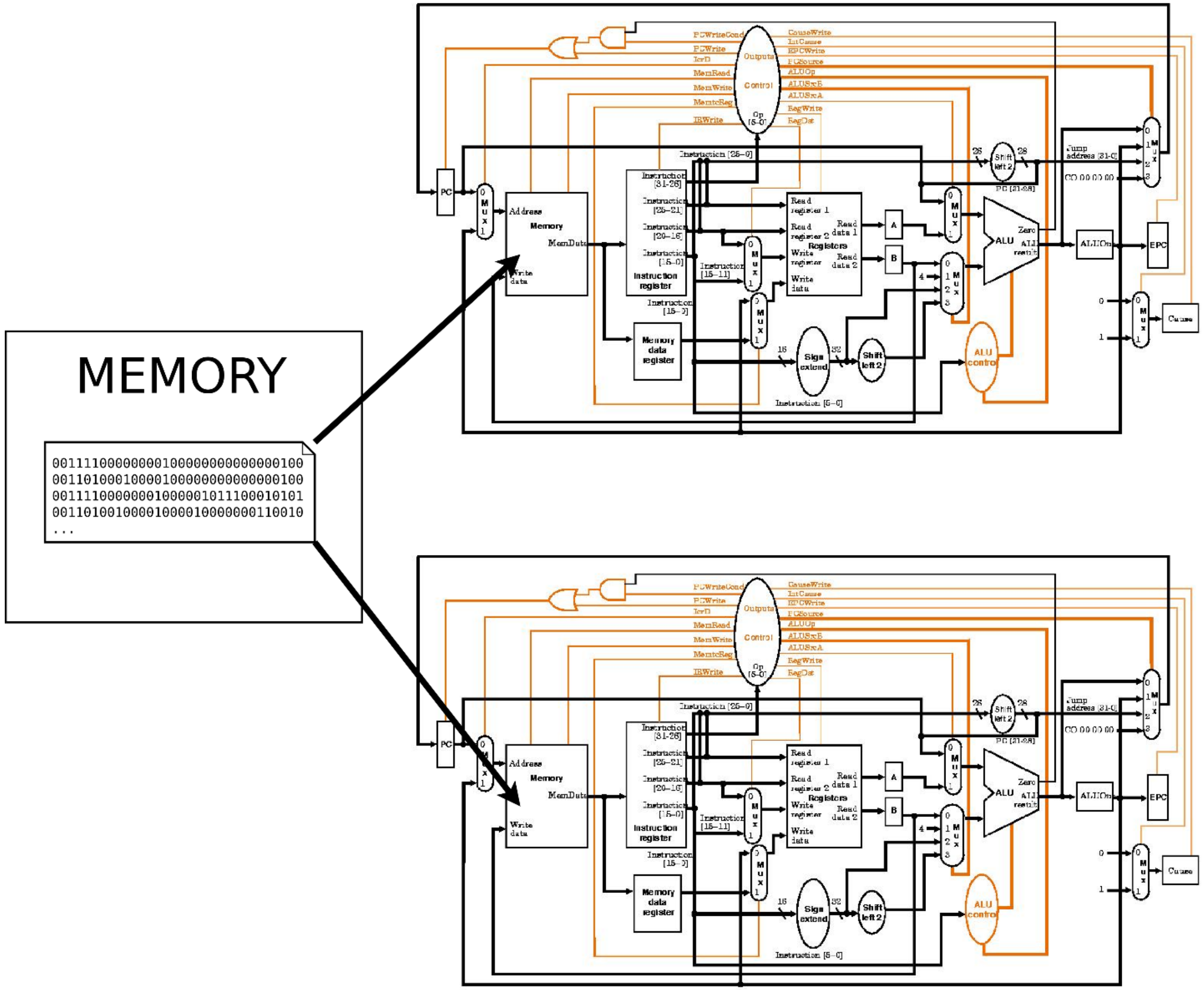
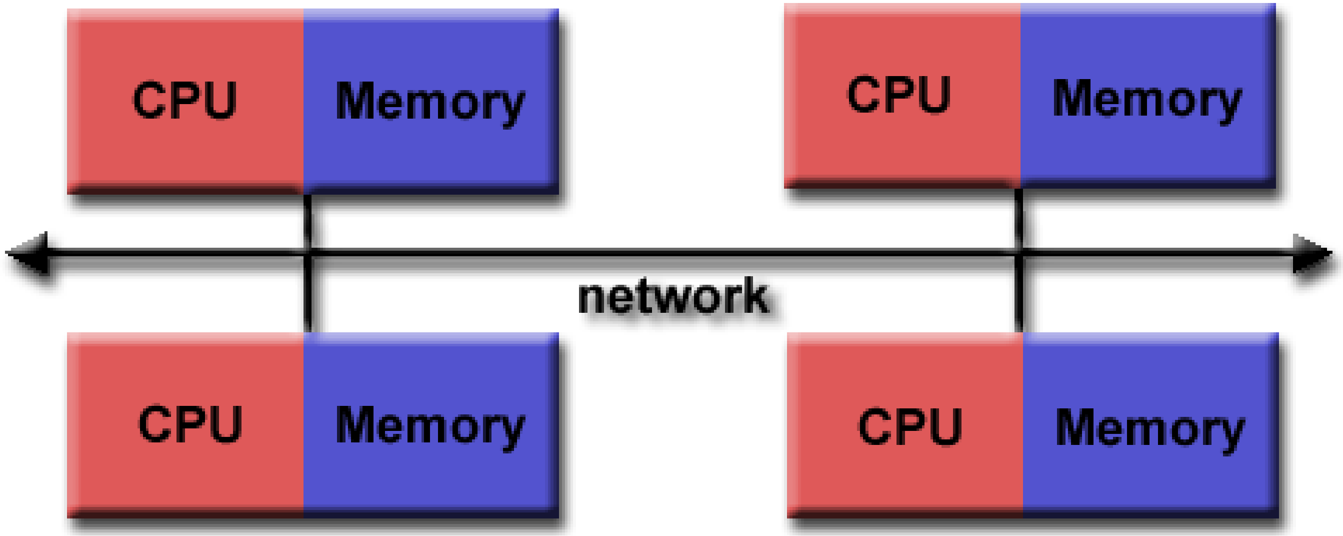


Different types of computer architectures



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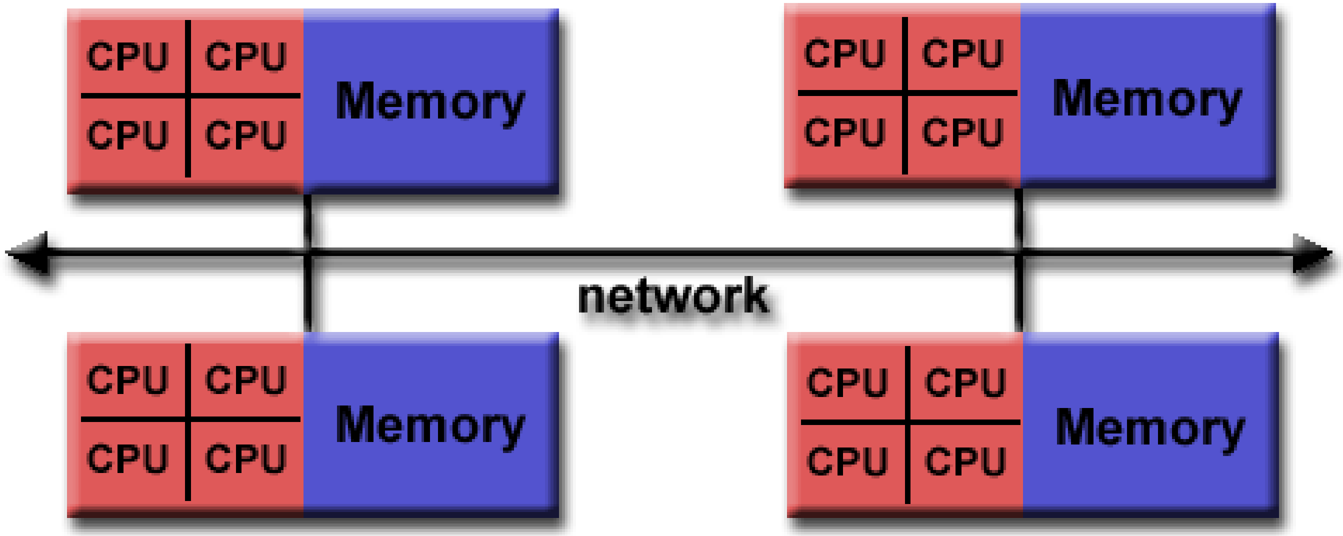
Different types of computer architectures



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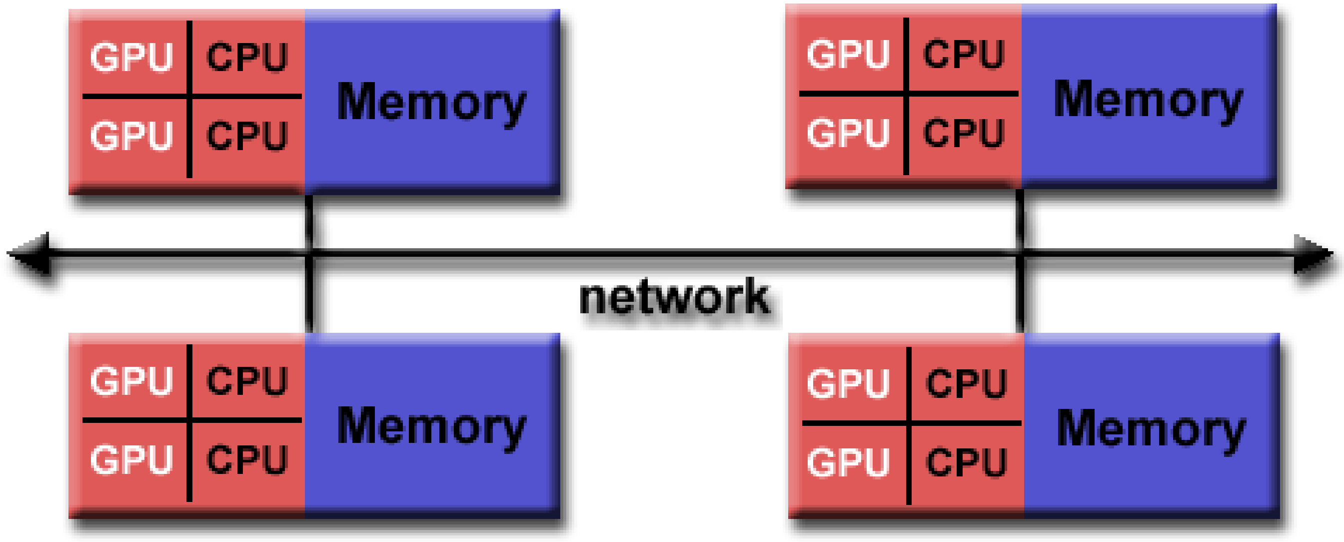
Different types of computer architectures



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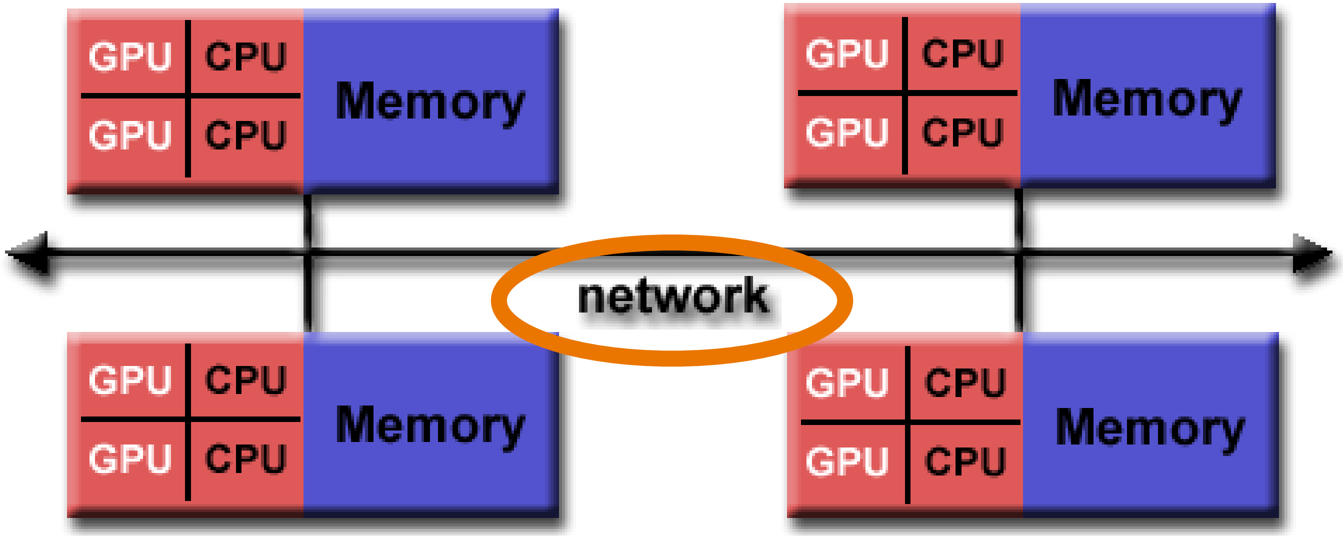
Different types of computer architectures



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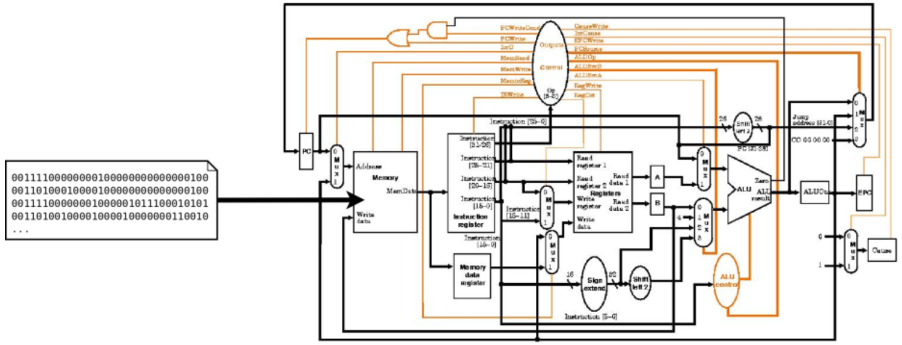
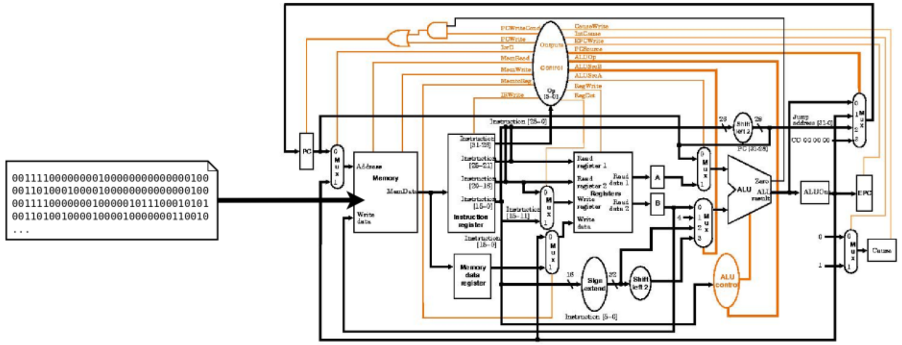
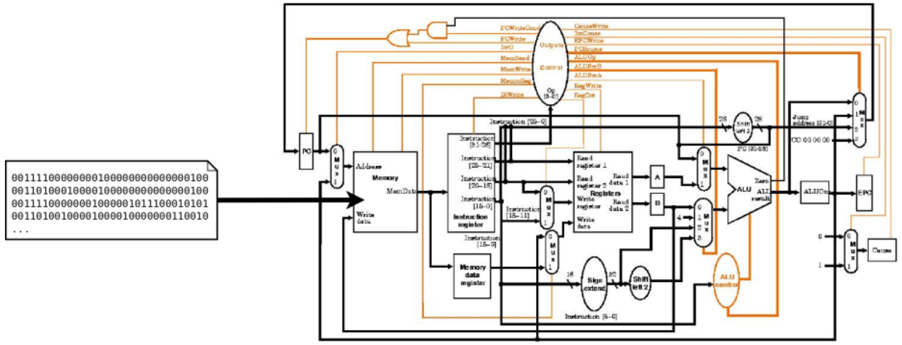
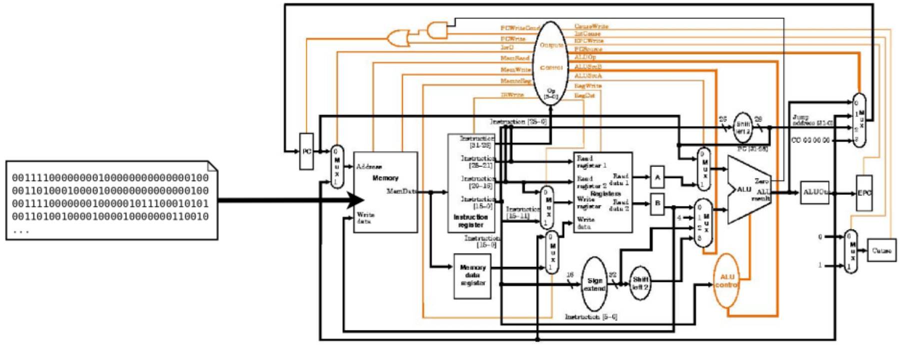
Different types of computer architectures

- Basic execution model: SPMD (Single Program, Multiple Data)
- Even MPMD (Multiple Program, Multiple Data) could be possible…



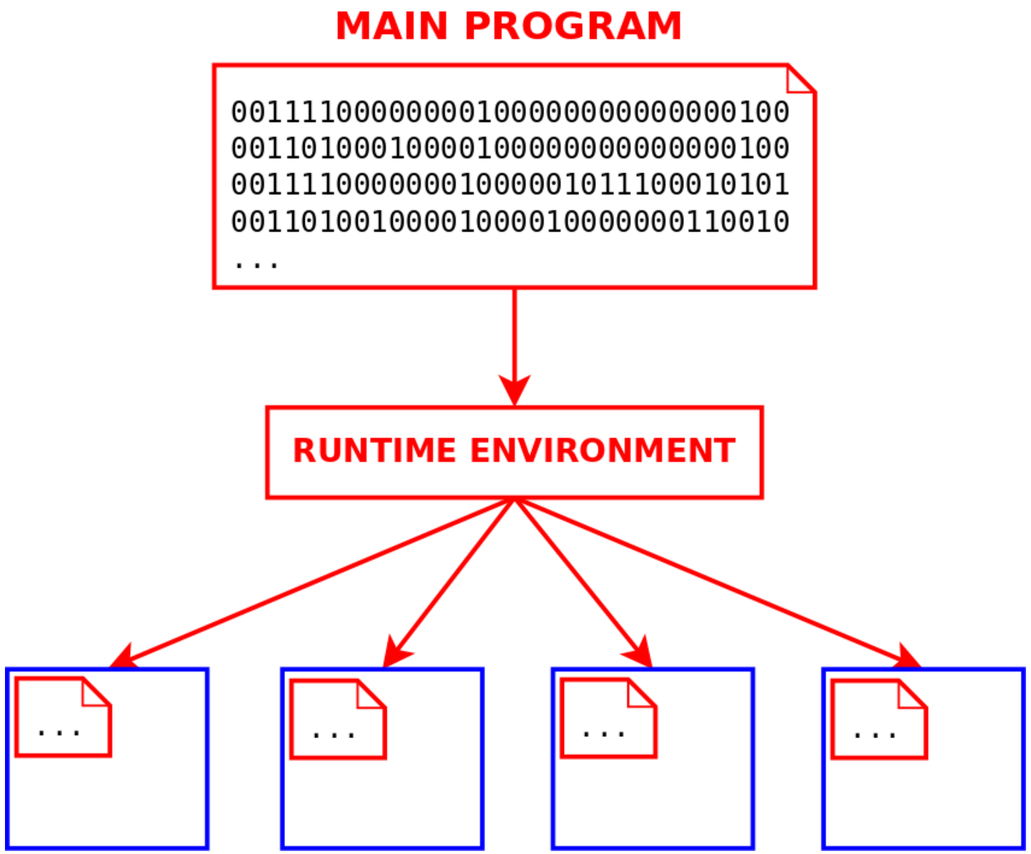






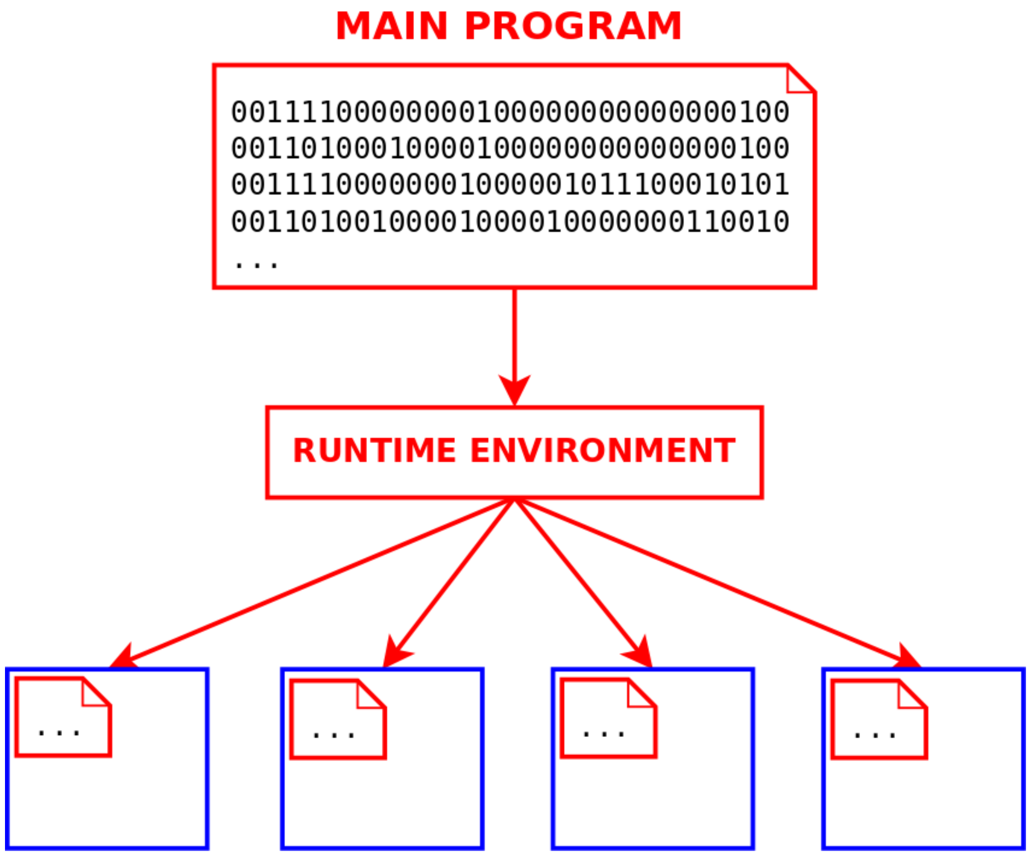
Many processes in different computers: MPI

- **MPI**: **M**essage **P**assing **I**nterface
- Different processes are created on the one or many machines (nodes)
- Each process executes the same program and has a private copy of all variables
- Inter-process communication by sending/receiving messages andsynchronizations
- Bindings for several languages, like C/C++, Fortran, Java or Python



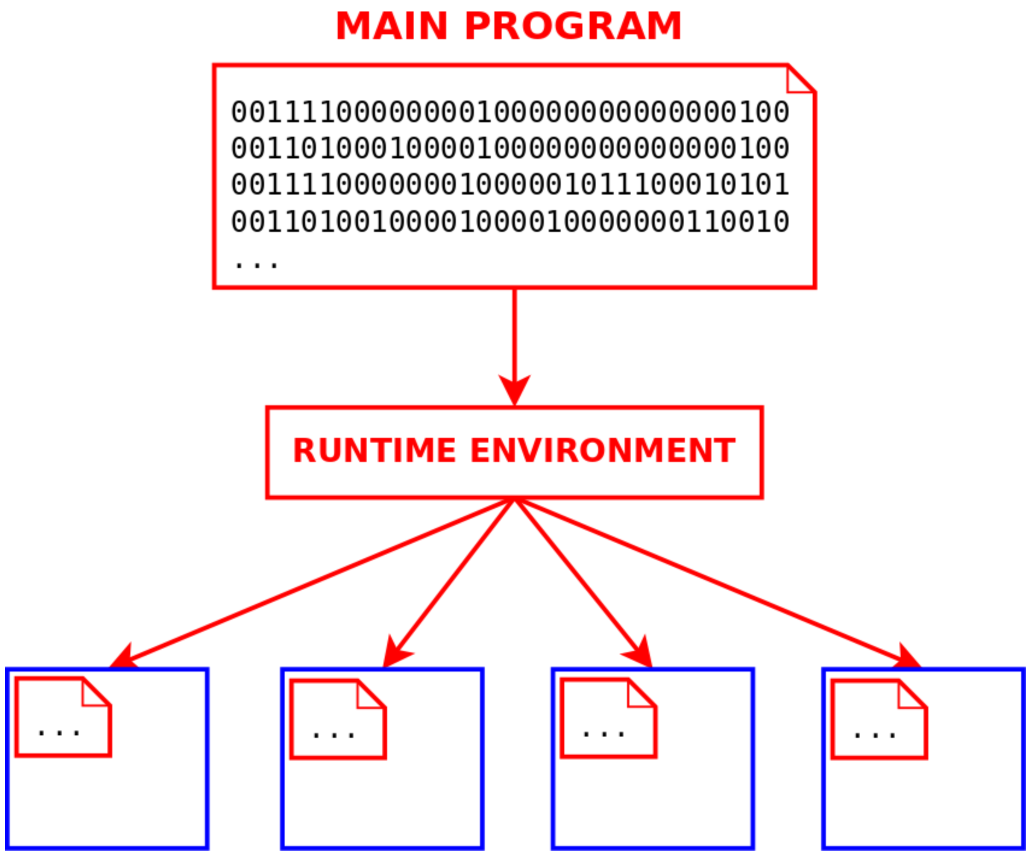
Many processes in different computers: MPI

- The interface defines the protocol and the semantic specifications of its functional parts
- Different implementations of the interface can exist
  - IntelMPI
  - OpenMPI
  - MPICH / MVAPICH
- De-facto standard for parallel programming on distributed HPC architectures



Many processes in different computers: MPI

- In general, MPI requires specific compilation (e.g. mpicc) and specific runtime environment (e.g. mpirun)
- The MPI compiler loads the necessary libraries from the selected MPI implementation
- The MPI runtime is the process that manages communications
  - Internally implemented with daemon processes



Example of multi-process execution with MPI

```
top - 11:05:19 up 41 days, 15:15,  1 user,  load average: 0,52, 0,26, 0,16
Tasks: 473 total,   5 running, 468 sleeping,   0 stopped,   0 zombie
%Cpu(s):  0,0 us,  0,1 sy, 16,7 ni, 83,2 id,  0,0 wa,  0,0 hi,  0,0 si,  0,0 st
KiB Mem : 49284800 total, 35059112 free,   784368 used, 13441320 buff/cache
KiB Swap: 25165820 total, 25136612 free,    29208 used. 46491000 avail Mem

  PID USER      PR  NI    VIRT    RES    SHR S  %CPU %MEM     TIME+ COMMAND
28875 caspar1   39  19  419216   6880   4240 R 100,0  0,0   0:04.27 my_mpi_prog
28876 caspar1   39  19  419220   6876   4236 R 100,0  0,0   0:04.27 my_mpi_prog
28877 caspar1   39  19  419220   6868   4240 R 100,0  0,0   0:04.26 my_mpi_prog
28878 caspar1   39  19  419216   6876   4236 R 100,0  0,0   0:04.26 my_mpi_prog
 3356 root      20   0   15944   1820    956 S   1,7  0,0  53:35.03 pim
  477 root      20   0       0      0      0 S   1,3  0,0  59:26.22 xfsaild/sda3
```

4 processes, each using a single CPU core

Example of multi-process execution with MPI

- Note the difference:
  - OpenMP: 1 process, 4 threads per process

```
  PID USER      PR  NI    VIRT    RES    SHR S  %CPU %MEM     TIME+  COMMAND
31648 caspar1   39  19  228816   1656   1180 R 400,0  0,0   0:22.37 my_omp_prog
   84 root      rt   0       0      0      0 S   0,3  0,0   0:08.41 migration/15
  477 root      20   0       0      0      0 S   0,3  0,0  59:26.57 xfsaild/sda3
```

  - MPI: 4 processes, 1 thread per process

```
  PID USER      PR  NI    VIRT    RES    SHR S  %CPU %MEM     TIME+  COMMAND
28875 caspar1   39  19  419216   6880   4240 R 100,0  0,0   0:04.27 my_mpi_prog
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  477 root      20   0       0      0      0 S   0,3  0,0  59:26.22 xfsaild/sda3
```

- … and you may even combine MPI + OpenMP…

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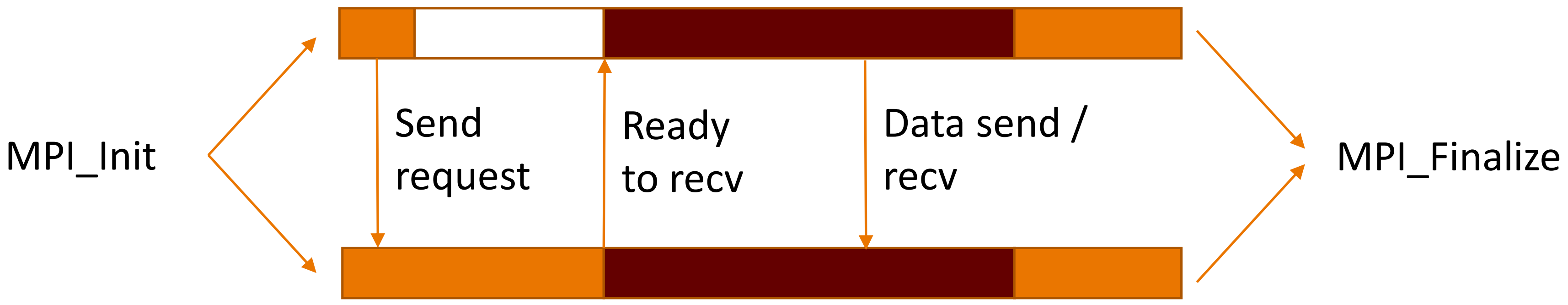
Many processes in different computers: MPI

- The use of MPI requires some programming efforts to manage all processes coordinately
- In the beginning the MPI environment is initialized, and also finalized at the end of the parallel code
- The basic element is the communicator, which defines
  - communication context
  - set of processes that can communicate between each other inside that context



Many processes in different computers: MPI

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	MPI_COMM_WORLD	My_communicator
Process 0	Rank 0	
Process 1	Rank 1	Rank 0
Process 2	Rank 2	Rank 1

General references for MPI

- Specification documents in the web page of the MPI Forum
- Current specification document: version 3.1
- Revisions and discussions for the elaboration of the MPI standard 4.0 are ongoing

Basic MPI structure and predefined handles

- MPI functions are used inside the code and require including a file or module
  - C/C++: #include <mpi.h>
  - Fortran: use mpi (with Fortran 2008, definitely do “use mpi_f08”)
- Essential structure for MPI routines
  - C/C++: error = MPI_Routine(arg0, arg1, ...);

    (the error output may be ignored, but it is very useful for debugging)
  - Fortran: call MPI_ROUTINE(arg1, arg2, …, ierror)

    (the error output is always the last argument: VERY IMPORTANT!!!)
- Global communicator: predefined handle
  - C/C++ AND Fortran: MPI_COMM_WORLD (type “MPI_Comm” or “integer”)

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Basic MPI structure and predefined handles

- Every MPI code begins with an initialization of the enviroment
  - C/C++: int MPI_Init(int *argc, char ***argv)

    typical call: MPI_Init(&argc, &argv);

    argc and *argv* are taken from the main program, NULL is possible too
  - Fortran: subroutine MPI_INIT(ierr) integer :: ierr

    typical call: call MPI_Init(ierr)
- Every MPI code ends with a finalize statement that stops the environment
  - C/C++: int MPI_Finalize()
  - Fortran: subroutine MPI_FINALIZE(ierr) integer :: ierr

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Basic MPI structure and predefined handles

- MPI has different handles that identify specific objects
- Most common handle: predefined constants
  - Defined in mpi.h (C/C++) or in the mpi/mpi_f08 modules (Fortran)
  - E.g. global communicator MPI_COMM_WORLD
- Other handles: type definitions for MPI specific variables or error return codes
  - E.g. communicator types
    - C/C++: MPI_Comm my_communicator
    - Fortran: integer :: my_communicator

      \- with mpi_f08: TYPE(MPI_Comm)

Basic MPI structure and predefined handles

- Every MPI process is identified with a number, called “rank”
  - C/C++: int MPI_Comm_rank(MPI_Comm comm, int *rank)

MPI Communicator

Output argument with size value

  - Fortran: subroutine MPI_COMM_RANK(comm, rank, ierr)

ierr argument… NEVER FORGET when using the mpi module!!!

“use mpi”: integer :: comm, rank, ierr

“use mpi_f08”: TYPE(MPI_Comm) :: comm

integer :: rank; integer, optional :: ierr

ierr argument is optional with the module mpi_f08.
Try to use this module when possible!

Basic MPI structure and predefined handles

- The number of processes in a communicator can be obtained with another routine
  - C/C++: int MPI_Comm_size(MPI_Comm comm, int *size)

MPI Communicator

Output argument with size value

  - Fortran: subroutine MPI_COMM_SIZE(comm, size, ierr)

    “use mpi”: integer :: comm, rank, ierr

    “use mpi_f08”: TYPE(MPI_Comm) :: comm

    integer :: rank; integer, optional :: ierr

ierr argument… NEVER FORGET when using the mpi module!!!

ierr argument is optional with the module mpi_f08.
Try to use this module when possible!

Ready for a first hands-on exercise?

- Go to the GitHub web page of the course

  https://github.com/sara-nl/PRACE-MPI-OpenMP

- Try to write your first MPI code!
  - C/C++: mpi_hello_world.c
  - Fortran: mpi_hello_world.f

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Some ideas about MPI execution model

- The execution environment (e.g. mpirun, srun…) creates the requested processes
- After executing MPI_Init, the processes are located in the same communication environment: MPI_COMM_WORLD
- Before MPI_Init and after MPI_Finalize the processes still exist, but there is no possible interaction or coordination between them
- MPI follows the SPMD (Single Program, Multiple Data) execution model
  - All processes execute exactly the same program
  - The programmer has the responsibility of making processes cooperate
- General way of cooperation between processes
  - Manual distribution of data and/or tasks
  - Message exchanges (send / receive)

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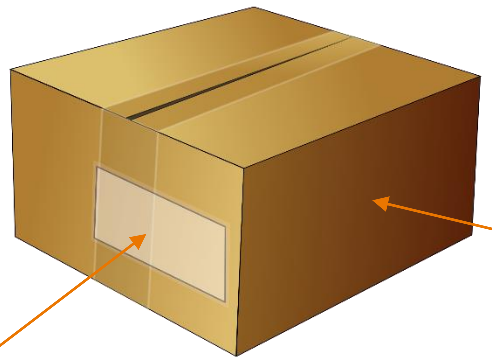
MPI point-to-point communication: messages

- MPI_Send() and MPI_Recv()
  - In order to send and receive it is necessary to create a “parcel”
  - Need for different information: mostly contents and “address label”



1. Variable(s) to send/receive
2. How many variables to send
3. The size of one variable

1. Source/Destination address
2. Tag
3. Communicator (MPI_COMM_WORLD)

MPI point-to-point communication: messages

- A message is any type of data that is communicated from one MPI process to another (or many) process(es)
- MPI datatypes can be *basic* or *derived*
  - Basic types are integer, float, double precision, etc.
  - Derived types are usually sets of basic datatypes and/or other derived datatypes
- The naming of datatypes varies with the programming language

MPI point-to-point communication: messages

- Routine to send a message
  - C/C++:

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

  - Fortran:

```
MPI_SEND(buffer, count, datatype, dest, tag, comm, ierr)
    <datatype> buffer(*)
    integer :: count, datatype, dest, tag, comm, ierr
```

MPI point-to-point communication: messages

- Routine to receive a message
  - C/C++: int MPI_Recv(void *buffer, int count, MPI_Datatype datatype,
    int dest, int tag, MPI_Comm comm, MPI_Status status);
  - Fortran: MPI_RECV(buffer, count, datatype, src, tag, comm, status, ierr)
    <datatype> buffer(*)
    integer :: count, datatype, src, tag, comm
    integer :: status(MPI_STATUS_SIZE), ierr

MPI point-to-point communication: messages

- Send / receive: C example

Rank 0

```
int send_val = 10;
MPI_Send(&send_val, 1, MPI_INT, 1, 10, MPI_COMM_WORLD)
```

Variable to send

MPI point-to-point communication: messages

- Send / receive: C example

Rank 0

```
int send_val = 10;
MPI_Send(&send_val, 1, MPI_INT, 1, 10, MPI_COMM_WORLD)
```

#Variables to send

MPI point-to-point communication: messages

- Send / receive: C example

Rank 0

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```

Datatype of the variable to send

MPI point-to-point communication: messages

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```

Datatype of the variable to send

MPI point-to-point communication: messages

- Send / receive: C example

Rank 0

```
int send_val = 10;
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```

Destination rank

MPI point-to-point communication: messages

- Send / receive: C example

Rank 0

```
int send_val = 10;
MPI_Send(&send_val, 1, MPI_INT, 1, 10, MPI_COMM_WORLD)
```

Tag of the package

MPI point-to-point communication: messages

- Send / receive: C example

Rank 0

```
int send_val = 10;
MPI_Send(&send_val, 1, MPI_INT, 1, 10, MPI_COMM_WORLD)
```

MPI Communicator

MPI point-to-point communication: messages

- Send / receive: C example

Rank 0

```
int send_val = 10;
MPI_Send(&send_val, 1, MPI_INT, 1, 10, MPI_COMM_WORLD)
```

Contains info about message & sender

Rank 1

```
int rec_val;
MPI_Recv(&rec_val, 1, MPI_INT, 0, 10, MPI_COMM_WORLD, &status)
```

Expects message of size 1 MPI_INT from rank 0 with tag 10

MPI point-to-point communication: messages

- Send / receive: Fortran example (just a couple differences)

Rank 0

```
integer :: send_val = 10;
call MPI_SEND(send_val, 1, MPI_INTEGER, 1, 10, MPI_COMM_WORLD, ierr)
```

“call” needed for Fortran subroutines… a different datatype… and of course the ierror parameter!

Rank 1

```
integer :: rec_val;
call MPI_RECV(rec_val, 1, MPI_INTEGER, 0, 10, MPI_COMM_WORLD, status, ierr)
```

MPI point-to-point communication: messages

C Data Types		Fortran Data Types	
MPI_CHAR	char	**MPI_CHARACTER**	character(1)
MPI_WCHAR	wchar_t - wide character		
MPI_SHORT	signed short int		
MPI_INT	signed int	**MPI_INTEGER** **MPI_INTEGER1** **MPI_INTEGER2** **MPI_INTEGER4**	integer integer*1 integer*2 integer*4
MPI_LONG	signed long int		
MPI_UNSIGNED	unsigned int		
MPI_FLOAT	float	**MPI_REAL** **MPI_REAL2** **MPI_REAL4** **MPI_REAL8**	real real*2 real*4 real*8
MPI_DOUBLE	double	**MPI_DOUBLE_PRECISION**	double precision
MPI_LONG_DOUBLE	long double		
MPI_C_COMPLEX **MPI_C_FLOAT_COMPLEX**	float _Complex	**MPI_COMPLEX**	complex
MPI_C_DOUBLE_COMPLEX	double _Complex	**MPI_DOUBLE_COMPLEX**	double complex
MPI_C_BOOL	_Bool	**MPI_LOGICAL**	logical
MPI_BYTE	8 binary digits	**MPI_BYTE**	8 binary digits
MPI_PACKED	data packed or unpacked with MPI_Pack()/ MPI_Unpack	**MPI_PACKED**	data packed or unpacked with MPI_Pack()/ MPI_Unpack

MPI point-to-point communication: messages

- Matching communication
  - Correct source and destination ranks inside the same communicator
  - Matching tags
  - Matching datatypes
  - … and a sufficiently large buffer on the receiver's side
- If there are many matching communications, the order is always preserved in time
  - First come, first served
- Some status information is stored in the receiving side
  - It may be ignored by using the constant MPI_STATUS_IGNORE as an argument
  - … but there is some valuable information inside

MPI point-to-point communication: messages

- Contents of status
  - C/C++: MPI_Status status

    status.MPI_SOURCE

    status.MPI_TAG
  - Fortran: integer status(MPI_STATUS_SIZE)

    status(MPI_SOURCE)

    status(MPI_TAG)

MPI point-to-point communication: messages

- Contents of status: getting the message count
  - C/C++: int MPI_Get_count(MPI_Status *status,
    MPI_Datatype datatype, int *count)
  - Fortran: MPI_GET_COUNT(status, datatype, count, ierror)
    integer :: status(MPI_STATUS_SIZE)
    integer :: datatype, count, ierror
- The "get_count" functions will be very useful in some cases, in order to allocate the receive buffer in advance with enough data for a given message

Hands-on (very quick)

- Try the code on point-to-point communication
  - C/C++: mpi_pnt2pnt.c
  - Fortran: mpi_pnt2pnt.f
- Put the correct source and destination, and the necessary tags

Different modes for sending data

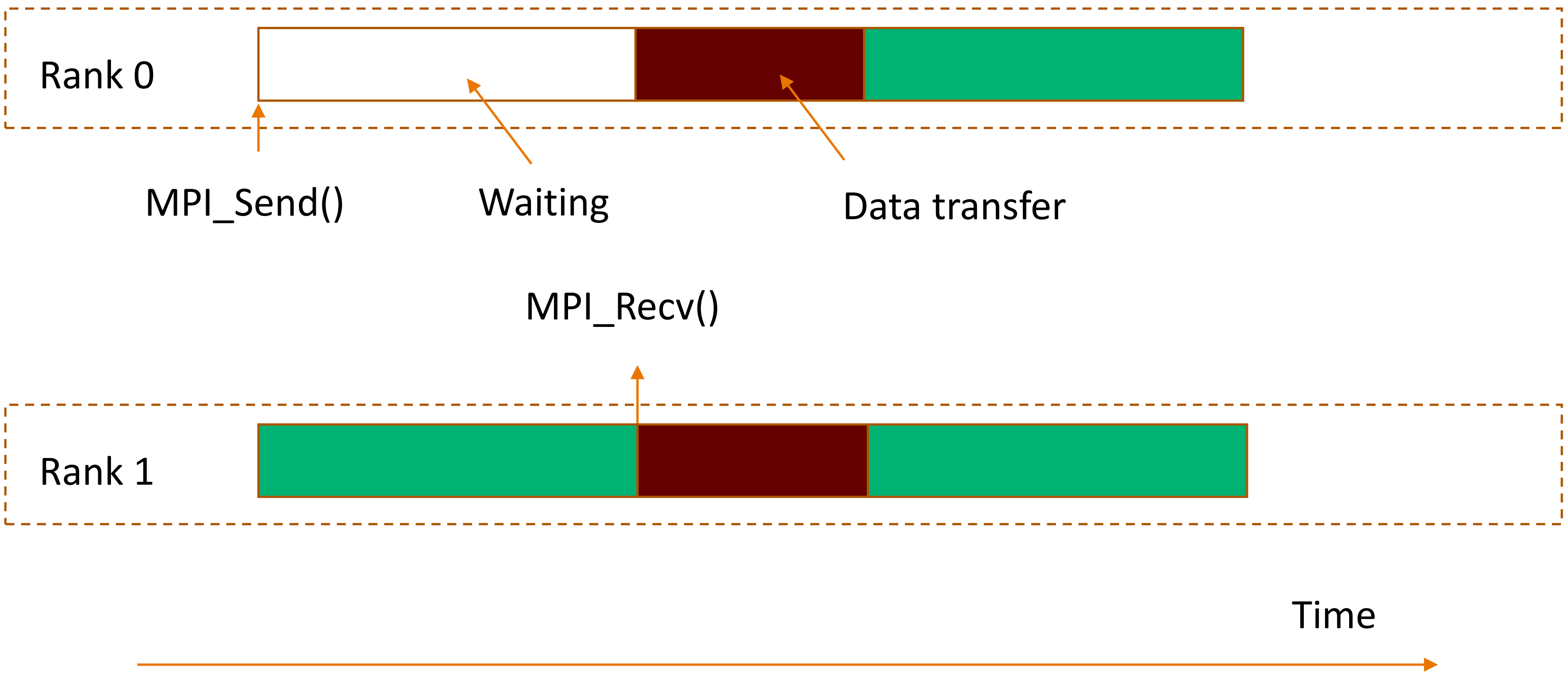
- Synchronous send (MPI_SSEND)
  - Requires synchronization between sender and receiver processes
  - It succeeds when a matching receive call is started
- Buffered send (MPI_BSEND)
  - Asynchronous: the send is always completed, even without a matching receive
  - It requires a buffer declared with MPI_BUFFER_ATTACH
- Generic send (MPI_SEND)
  - It may be either synchronous or buffered send: decision left to the MPI library
- Ready send (MPI_RSEND)
  - Performs an immediate send without checking the receiver side (better avoid…)

Only one mode for receiving data

- Generic receive (MPI_RECV)
  - Matches all possible send modes
  - It waits until a matching send is posted

MPI point-to-point communication: messages

- MPI_Send (in general) and MPI_Recv are blocking functions

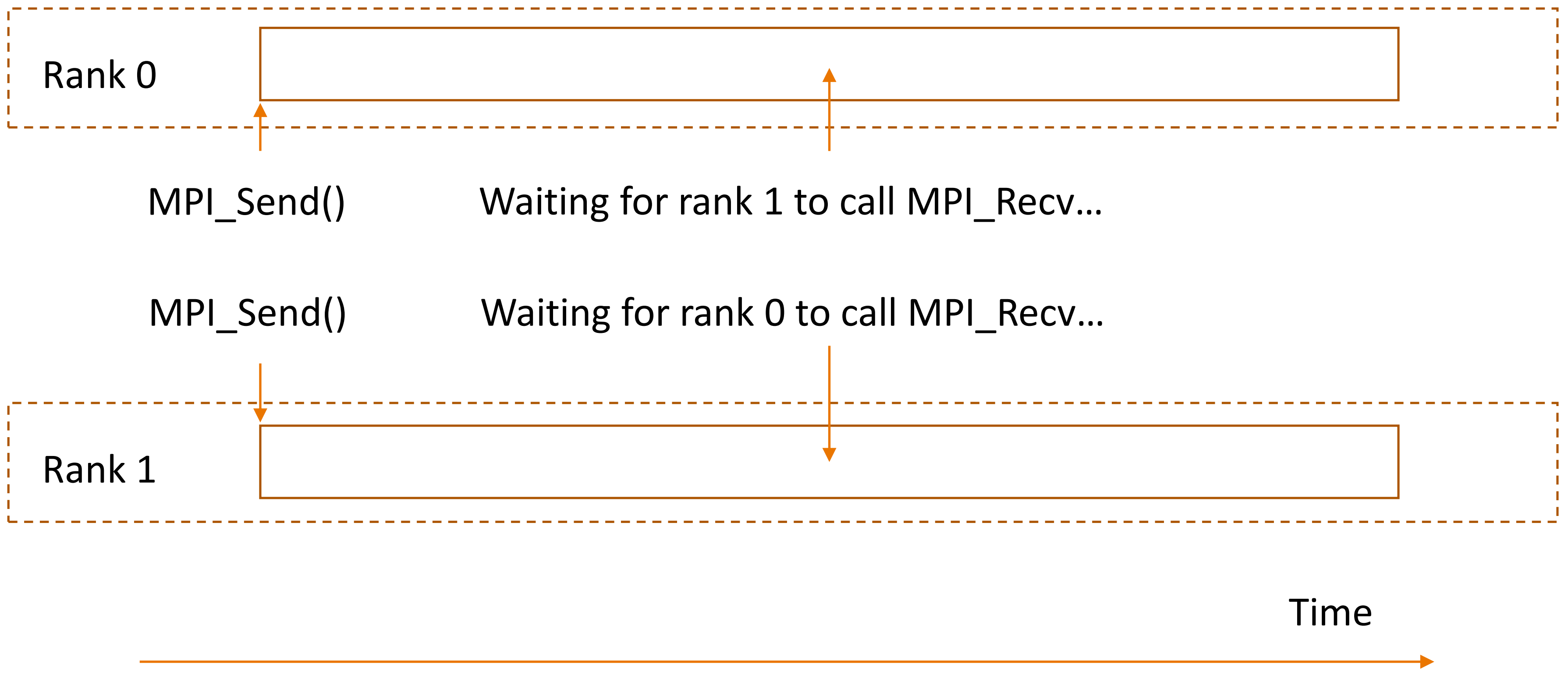


Hands-on

- Try the code of the ping-pong communication
    - C/C++: mpi_pingpong.c
    - Fortran: mpi_pingpong.f
- Have a look at the code and see how it is working
- What can be wrong?

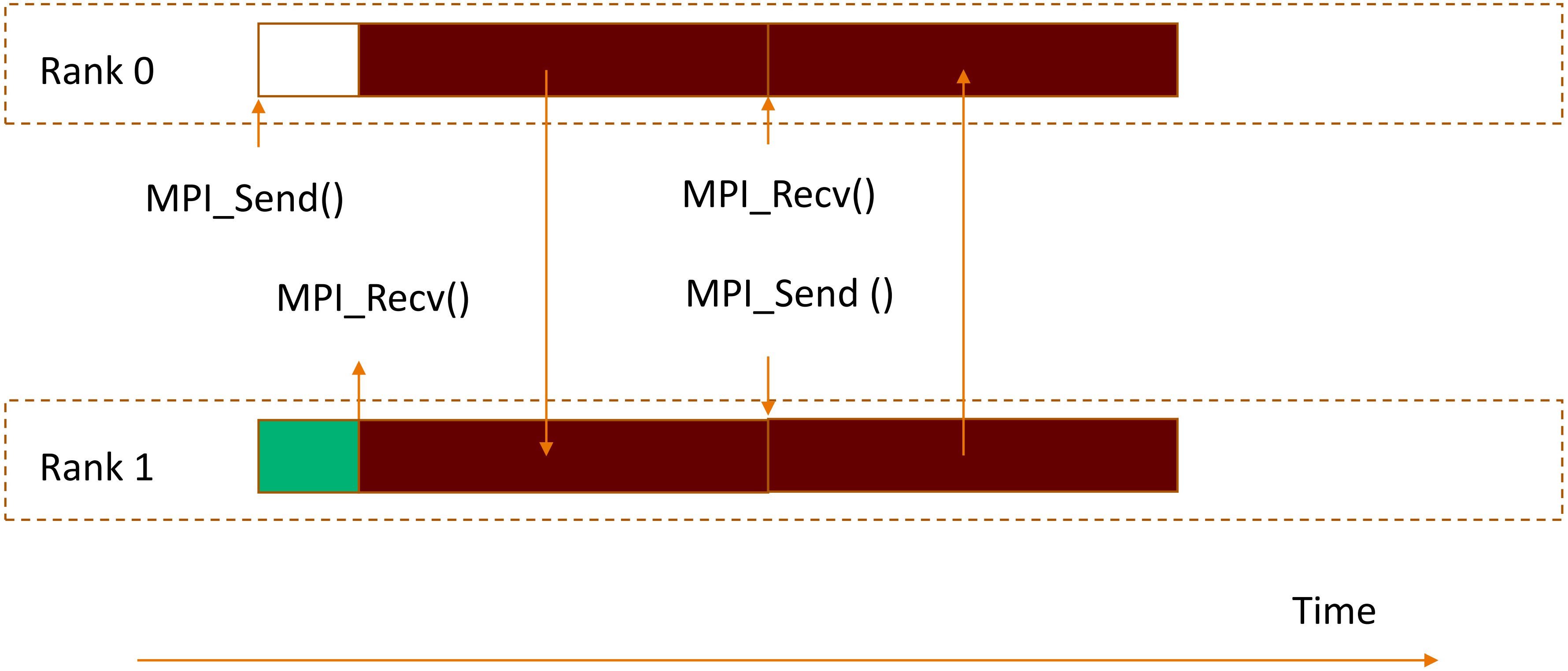
MPI point-to-point communication: messages

- MPI_Send and MPI_Recv are blocking functions: a deadlock may occur!!!



MPI point-to-point communication: messages

- Solution: reverse the order of MPI_Send and MPI_Recv for one of the communications



General problems with blocking communication

- If the MPI library implementation uses synchronous sends, a programmer may find
  - Deadlocks: complete block of the communication, in which two processes try to send at the same time
  - Serialization: inefficient communication because of a bad scheduling of communications

General problems with blocking communication

- If the MPI library implementation uses synchronous sends, a programmer may find
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  - Serialization: inefficient communication because of a bad scheduling of communications
- Solution: non-blocking communications

Non-blocking communication

- It is possible to split the communication process (both send and recv) in two steps
- First step: post a communication request
  - Immediate return of the call and obtain an identifier for the MPI request
  - The effective communication will be done by the MPI library in the background
- Second step: wait for the communication to be completed
  - This will happen after the whole send buffer has been processed and the receive buffer contains all the necessary information

Non-blocking communication

- General routine to immediately send a message

  - C/C++: int MPI_Isend(void *buffer, int count, MPI_Datatype datatype,
    int dest, int tag, MPI_Comm comm, MPI_Request request);

  - Fortran: MPI_ISEND(buffer, count, datatype, dest, tag, comm, request, ierr)
    <datatype> buffer(*)
    integer :: count, datatype, dest, tag, comm, request, ierr

Non-blocking communication

- General routine to immediately receive a message
  - C/C++: int MPI_Irecv(void *buffer, int count, MPI_Datatype datatype,
    int src, int tag, MPI_Comm comm, MPI_Request request);
  - Fortran: MPI_IRECV(buffer, count, datatype, src, tag, comm, request, ierr)
    <datatype> buffer(*)
    integer :: count, datatype, src, tag, comm, request, ierr

Non-blocking communication

- General routine wait for a communication to complete
  - C/C++: int MPI_Wait(MPI_Request request, MPI_Status status);
  - Fortran: MPI_WAIT(request, status, ierr)

    integer :: request, status(MPI_STATUS_SIZE), ierr

Non-blocking communication

- In a practical way, a call to the wait routine right after an immediate send or receive is analogous to a call to the blocking send or receive, respectively
- In any case, the request obtained from the isend or irecv should be matched in wait
- Between the two steps (immediate communication and wait) a process is allowed to perform additional operations that are unrelated to the communication
- This means the following:
  - The sending process is not allowed to access or reuse the sending buffer or any of the request information
  - The completeness of the operation is only ensured after calling the wait function
  - ……. at least for C/C++

Non-blocking communication (Fortran only)

- There is a special issue with Fortran: it is an optimizing language, so a call to the wait routine may not imply that the send or recv buffers are ready for use again
- After MPI 3.0, an additional line of code is required In order to avoid any problem with buffer synchronization in Fortran
- Necessary steps:
  - Use the module mpi_f08 and declare the isend or irecv buffer as asynchronous

```
<datatype>, asynchronous :: buffer
```

  - Execute the following line of code always immediately after MPI_WAIT

```
  IF (.NOT. MPI_ASYNC_PROTECTS_NONBLOCKING)
&                CALL MPI_F_SYNC_REG( buf )
```

Reference: MPI: A Message-Passing Interface Standard Version 3.1, Chapter 17, page 644, section “Calling MPI_F_SYNC_REG”

Non-blocking communication

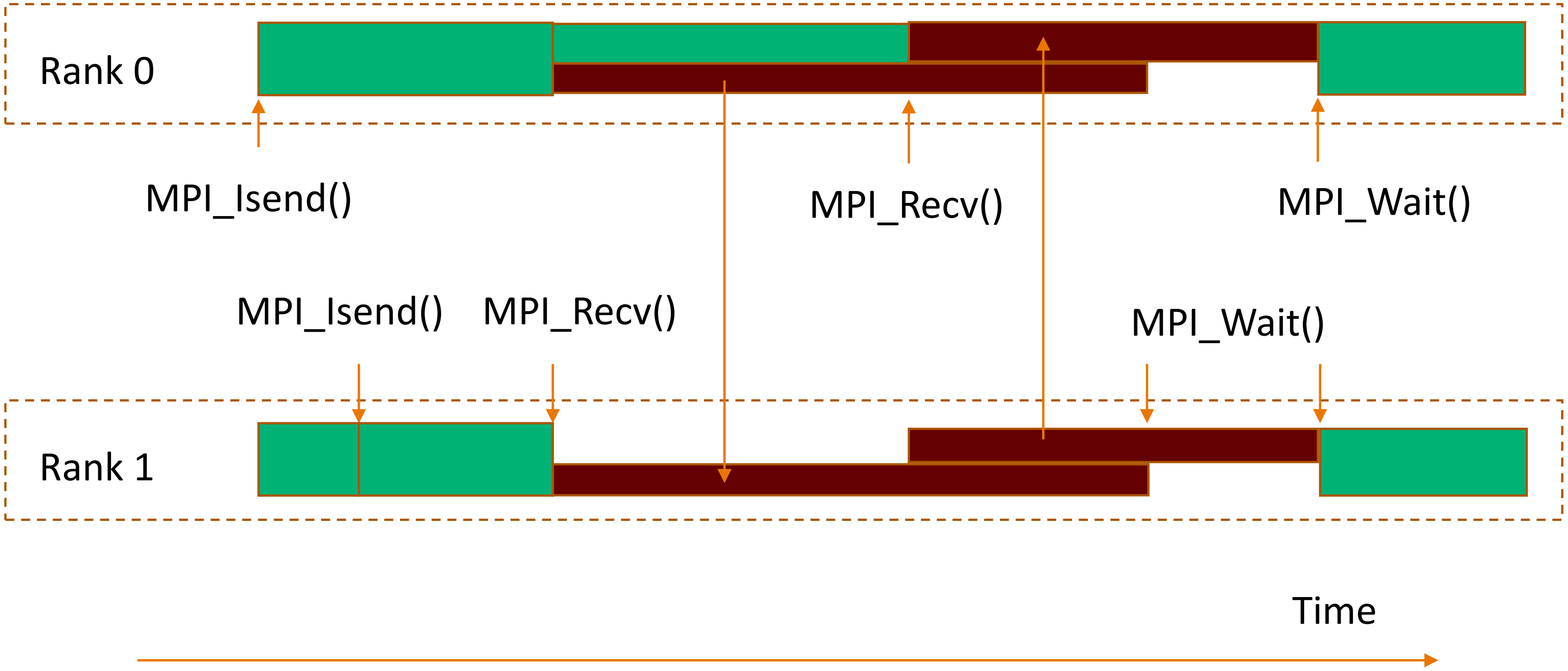
- It is also possible to perform a wait in a different way using the test routine
- The use of test requires a loop until the request is fulfilled
  - flag == 1 in C or flag == .TRUE. in Fortran
  - Fortran: this is equivalent to wait, so the asynchronous buffer should also be protected using MPI_F_SYNC_REG as indicated
- Test function
  - C/C++: int MPI_Test(MPI_Request request, int flag, MPI_Status status);
  - Fortran: MPI_TEST(request, flag, status, ierr)

    integer :: request, status(MPI_STATUS_SIZE), ierr

    logical :: flag

Non-blocking communication example

- The processing of two MPI_Isend() and MPI_Recv() calls may be overlapped
- Deadlocks are gone, and it provides a way to avoid serialization!



Hands-on

- Work with the following code:
  - C/C++: mpi_pingpong_nonblocking.c
  - Fortran: mpi_pingpong_nonblocking.f
- Adapt the code to be really non-blocking
- Use MPI_Isend and/or MPI_Irecv conveniently
- Check the performance of the code compared to the blocking version
  - C/C++: mpi_pingpong_blocking.c
  - Fortran: mpi_pingpong_blocking.f
- Which is the fastest version, and how much fast is it?
- There is another function called MPI_SENDRECV… Can you check the standard specification and see if it would be possible to use it here?

Collective communication

- Sometimes it is necessary to use many point-to-point communications at a time, with specific coordination and synchronization between processes
- Collective functions provide optimized implementations for some common communication patterns
- Different types of collectives
  - Data movement
  - Computation
  - Synchronization

Collective communication

- One-to-all

P0	A	B	C	D
P1				
P2				
P3				

Collective communication

- One-to-all

P0	A	B	C	D
P1				
P2				
P3				

$\xrightarrow{\text{Broadcast}}$

P0	A			
P1	A			
P2	A			
P3	A			

Collective communication

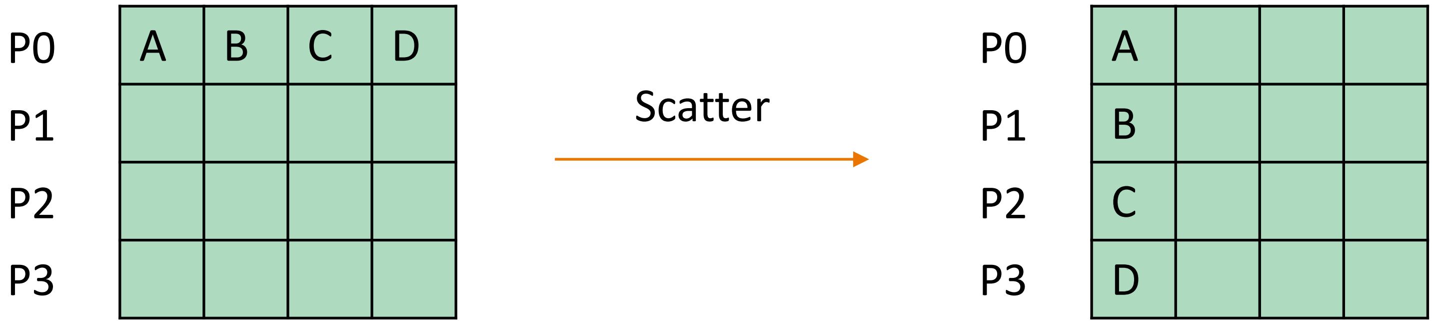
- Broadcast
  - C/C++: int MPI_Bcast(void *buffer, int count, MPI_Datatype datatype, int root, MPI_Comm comm);
  - Fortran: MPI_BCAST(buffer, count, datatype, root, comm, ierr)

    <datatype> buffer(*)

    integer :: count, datatype, root, comm, ierr

Collective communication

- One-to-all



Collective communication

- Scatter (with the option of defining MPI_IN_PLACE as sendbuffer)
  - C/C++: int MPI_Scatter(

```
void *sendbuffer, int sendcount, MPI_Datatype senddatatype,
void *recvbuffer, int recvcount, MPI_Datatype recvdatatype,
int root, MPI_Comm comm);
```

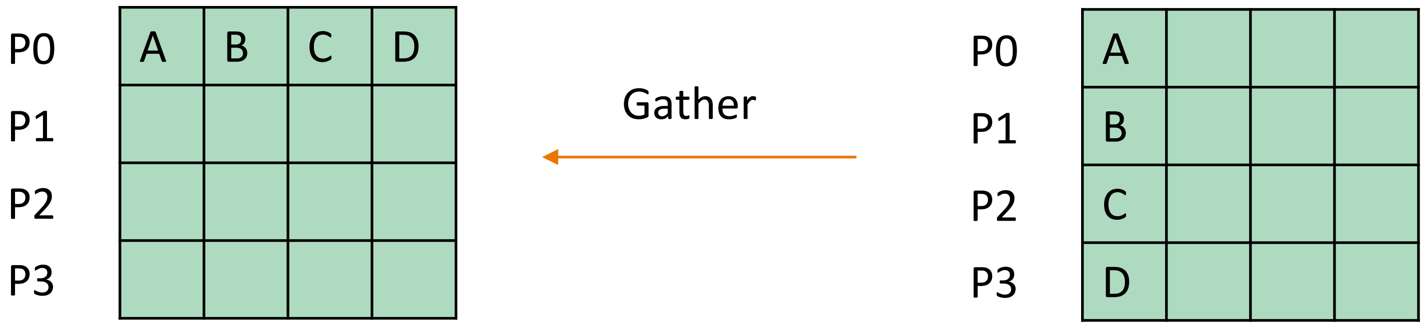
  - Fortran: MPI_SCATTER(sendbuffer, sendcount, senddatatype,

```
recvbuffer, recvcount, recvdatatype,
root, comm, ierr)
```

```
<datatype> sendbuffer(*), recvbuffer(*)
integer :: sendcount, senddatatype, recvcount, recvdatatype, root, comm, ierr
```

Collective communication

- All-to-one



Collective communication

- Gather (with the option of defining MPI_IN_PLACE as sendbuffer)
  - C/C++:

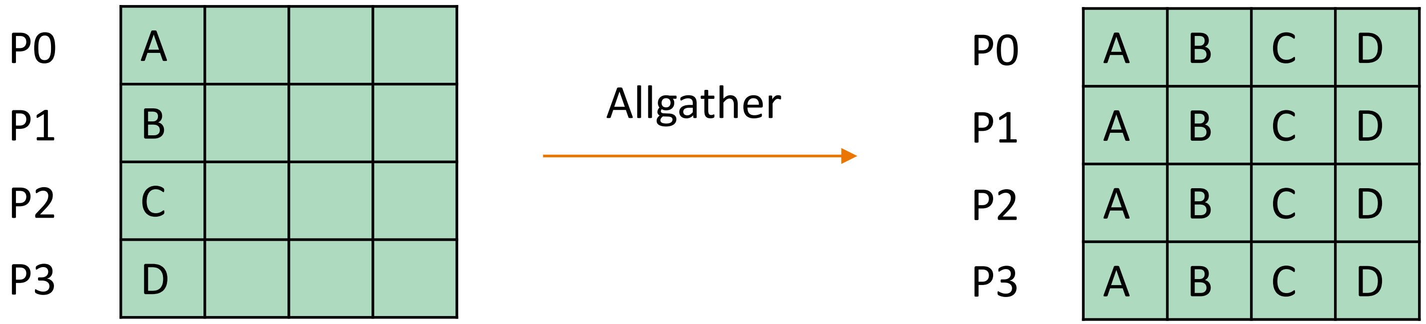
```
int MPI_Gather(
    void *sendbuffer, int sendcount, MPI_Datatype senddatatype,
    void *recvbuffer, int recvcount, MPI_Datatype recvdatatype,
    int root, MPI_Comm comm);
```

  - Fortran:

```
MPI_GATHER(sendbuffer, sendcount, senddatatype,
           recvbuffer, recvcount, recvdatatype,
           root, comm, ierr)
<datatype> sendbuffer(*), recvbuffer(*)
integer :: sendcount, senddatatype, recvcount, recvdatatype, root, comm, ierr
```

Collective communication

- All-to-all



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Collective communication

- Allgather
  - C/C++: int MPI_Allgather(

```
int MPI_Allgather(
    void *sendbuffer, int sendcount, MPI_Datatype senddatatype,
    void *recvbuffer, int recvcount, MPI_Datatype recvdatatype,
    MPI_Comm comm);
```

  - Fortran:

```
MPI_ALLGATHER(sendbuffer, sendcount, senddatatype,
              recvbuffer, recvcount, recvdatatype,
              comm, ierr)

<datatype> sendbuffer(*), recvbuffer(*)

integer :: sendcount, senddatatype, recvcount, recvdatatype, comm, ierr
```

Collective communication

- All-to-all

P0	A	A	A	A
P1	B	B	B	B
P2	C	C	C	C
P3	D	D	D	D

$\xrightarrow{\text{Alltoall}}$

P0	A	B	C	D
P1	A	B	C	D
P2	A	B	C	D
P3	A	B	C	D

Collective communication

- Alltoall
  - C/C++:

```
int MPI_Alltoall(
    void *sendbuffer, int sendcount, MPI_Datatype senddatatype,
    void *recvbuffer, int recvcount, MPI_Datatype recvdatatype,
    MPI_Comm comm);
```

  - Fortran:

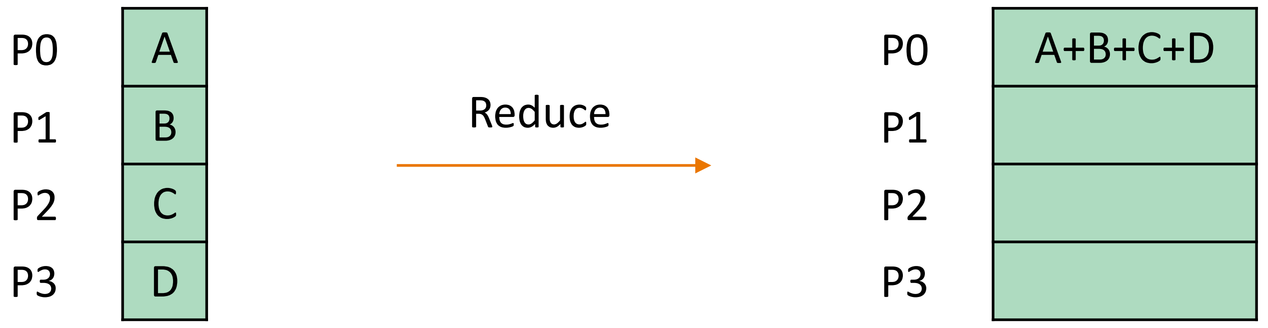
```
MPI_ALLTOALL(sendbuffer, sendcount, senddatatype,
             recvbuffer, recvcount, recvdatatype,
             comm, ierr)

<datatype> sendbuffer(*), recvbuffer(*)

integer :: sendcount, senddatatype, recvcount, recvdatatype, comm, ierr
```

Collective communication

- Computational operations are also possible
  - Most common one: reduce



Collective communication

- Reduce
  - C/C++: int MPI_Reduce(

```
void *sendbuffer, void *recvbuffer, int count,
MPI_Datatype datatype, MPI_Op op, int root,
MPI_Comm comm);
```

  - Fortran: MPI_REDUCE(sendbuffer, recvcount, count, datatype

```
op, root, comm, ierr)
```

```
<datatype> sendbuffer(*), recvbuffer(*)
integer :: count, datatype, op, comm, ierr
```

Collective communication: reduction operations

- There are different predefined operations for reduce
  - MPI_MIN, MPI_MAX, MPI_SUM, MPI_PROD
- Another option: custom definition of the operation
  - C/C++:

```
int MPI_Op_create(MPI_User_function *function,
                  int commute, MPI_Op *op);
```

  - Fortran:

```
MPI_OP_CREATE(function, commute, op, ierr)
                  external :: function
                  logical :: commute
                  integer :: op, ierr
```

Collective communication

- Other collective operation: synchronization barrier
  - C/C++: `int MPI_Barrier(MPI_Comm comm);`
  - Fortran: `MPI_BARRIER(comm, ierr)`

```
integer :: comm, ierr
```

Hands-on (1)

- Try to solve the exercise on collective functions proposed in this directory

  https://github.com/sara-nl/PRACE-MPI-OpenMP/tree/master/MPI/collectives

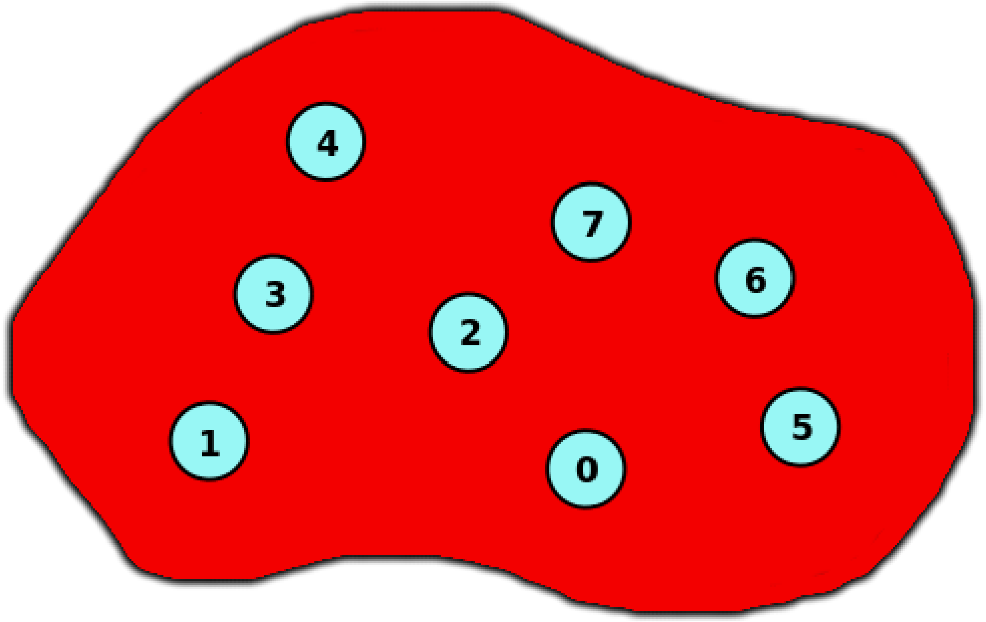
- The original codes are stored in the PRACE CodeVault

Hands-on (2)

- … we’ve already come a long way here. Time for a parallelization from scratch!
- Try to parallelize the computation of pi
  - C/C++: mpi_pi.c
  - Fortran: mpi_pi.f
- Three main tasks need to be performed
  - Distribution of the different iterations between processes
  - Getting the final complete result from all processes
  - Checking that there is scalability with a significant amount of threads

Communicators and virtual topologies

- Well known initial communicator: MPI_COMM_WORLD
- Main representation: pool of processes



Communicators and virtual topologies

- Possible definition of specific connections between processes to obtain a more structured view of a communicator
- Reasons to obtain this?

Communicators and virtual topologies

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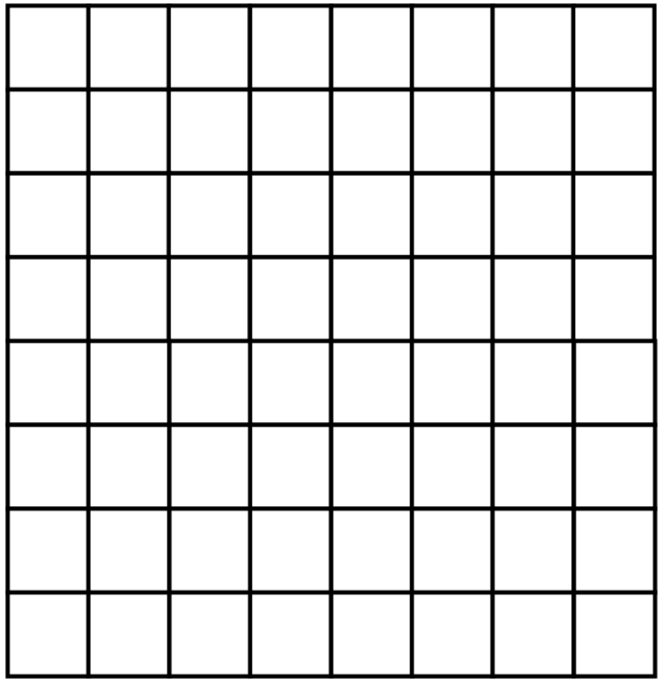
- Mimic the structure of the data that we are working on!



Communicators and virtual topologies

- Possible definition of specific connections between processes to obtain a more structured view of a communicator
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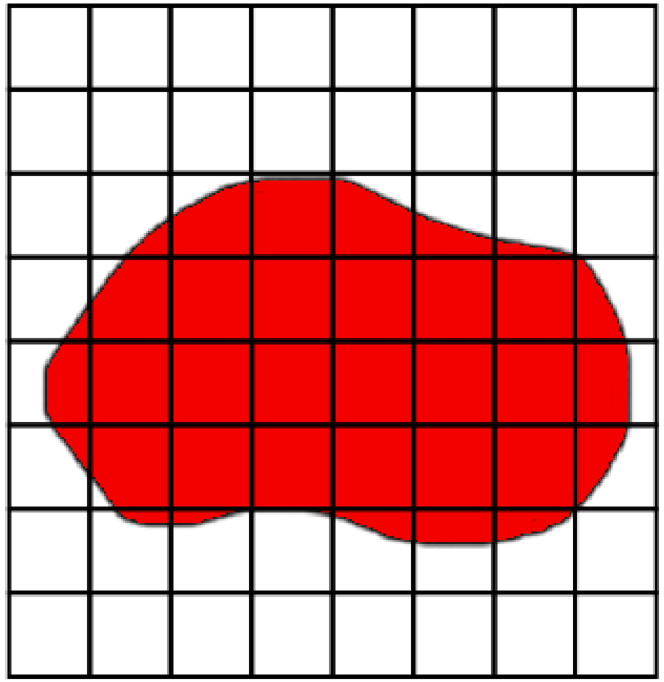


Communicators and virtual topologies

- MPI provides virtual topologies to organize processes
- Easy access to neighbor processes for communication
- Most common case: cartesian topology
  - C/C++:
    ```
    int MPI_Cart_create(MPI_Comm comm_old, int ndims,
                        int dims[], int periods[], int reorder,
                        MPI_Comm *comm_cart);
    ```
  - Fortran:
    ```
    MPI_CART_CREATE(comm_old, ndims, dims, periods, reorder,
                    comm_cart, ierr)
        integer :: comm_old, ndims, dims(*), comm_cart, ierr
        logical :: periods(*), reorder
    ```

Communicators and virtual topologies

- Connections between processes in cartesian topologies are established by their given coordinates: easy to calculate and to convert to/from rank

  - C/C++: int MPI_Cart_coords(MPI_Comm comm, int rank, int maxdims, int coords[]);
  - Fortran: MPI_CART_COORDS(comm, rank, maxdims, coords, ierr) integer :: comm, rank, maxdims, coords(*), ierr

Communicators and virtual topologies

- Connections between processes in cartesian topologies are established by their given coordinates: easy to calculate and to convert to/from rank

  - C/C++: `int MPI_Cart_rank(MPI_Comm comm, int coords[], int *rank);`
  - Fortran: `MPI_CART_RANK(comm, coords, rank, ierr)`

    `integer :: comm, coords(*), rank, ierr`

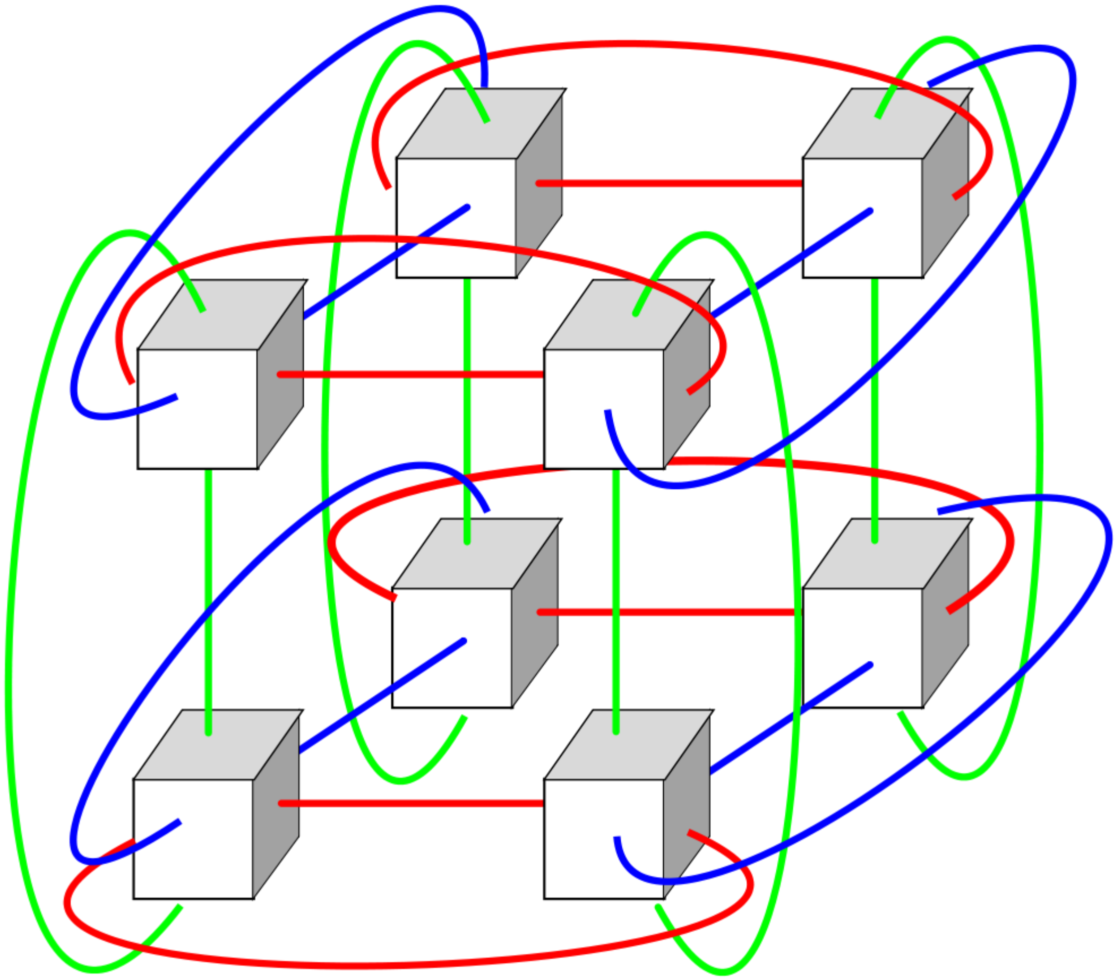
Communicators and virtual topologies

- Cartesian topologies may also be subdivided in their different dimensions

  - C/C++:
    ```
    int MPI_Cart_sub(MPI_Comm comm, int remain_dims[],
                     MPI_Comm *comm_new);
    ```
  - Fortran:
    ```
    MPI_CART_SUB(comm, remain_dims, comm_new, ierr)
        integer :: comm, comm_new, ierr
        logical :: remain_dims(*)
    ```

Hands-on

- Just do this:
  - C/C++: mpi_torus.c
  - Fortran: mpi_torus.f



Communicators and virtual topologies

- Communicators also have maximum flexibility to be created with a custom amount of threads, and later reorganized
- It is necessary to operate at the level of groups of processes to define a completely custom communicator

  - C/C++: int MPI_Comm_split(MPI_Comm comm, int color, int key,
    MPI_Comm *newcomm);
  - Fortran: MPI_COMM_SPLIT(comm, color, key, newcomm,ierr)
    integer :: comm, color, key, newcomm, ierr

Communicators and virtual topologies

- Communicators also have maximum flexibility to be created with a custom amount of threads, and later reorganized
- It is necessary to operate at the level of groups of processes to define a completely custom communicator

  - C/C++: `int MPI_Comm_group(MPI_Comm comm, MPI_Group *group);`
  - Fortran: `MPI_COMM_GROUP(comm, group, ierr)`

    `integer :: comm, group, ierr`

Communicators and virtual topologies

- Communicators also have maximum flexibility to be created with a custom amount of threads, and later reorganized
- It is necessary to operate at the level of groups of processes to define a completely custom communicator

  - C/C++: int MPI_Group_incl(MPI_Group group, int nranks, int ranks[],
    MPI_Group *newgroup);
  - Fortran: MPI_GROUP_INCL(group,nranks,ranks,newgroup, ierr)
    integer :: group, nranks, ranks(*), newgroup, ierr

Communicators and virtual topologies

- Communicators also have maximum flexibility to be created with a custom amount of threads, and later reorganized
- It is necessary to operate at the level of groups of processes to define a completely custom communicator

  - C/C++:

    ```
    int MPI_Comm_create(MPI_Comm comm, MPI_Group group,
                        MPI_Comm *newcomm);
    ```

  - Fortran:

    ```
    MPI_COMM_CREATE(comm, group, newcomm, ierr)
        integer :: comm, group, newcomm, ierr
    ```

Hands-on

- Take the previous example of the 3D torus
- Create communicators for each dimension of it
- Check the values of the ranks for every communicator

General comments (1)

- MPI is based on processes, but also provides threading possibilities
  - MPI_InitThread(int *argc, char ** argv[], int thr_requested, int thr_provided);
  - Varying level of support by the different MPI implementations
- MPI provides a quite complete I/O library with plenty of functionality
  - Recommended: use of high-level libraries that use it with wrappers
  - E.g. PnetCDF, SIONlib
- Derived data types can be defined and may be useful, but relatively cumbersome
  - Try to check if it is possible to codify relatively complex communication using basic data types
  - Use the general type MPI_PACKED and different routines (MPI_Pack and MPI_Unpack to put different data types in the same stream

General comments (& 2)

- MPI also supports one-sided and shared memory communication
  - MPI_Get / MPI_Put / MPI_Win_create …
  - Efficient way of performing data movements without explicit "handshake"
  - More info in a forthcoming PRACE MOOC on FutureLearn
- MPI has lots of further possibilities
  - Keep checking the standard documentation
  - Keep practising and be challenged!

PARALLEL PROGRAMMING WITH MPI

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