Training @ CINES

MPI

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Summary

Clusters Architecture

OpenMP

MPI

Hybrid MPI+OpenMP

Sommaire

MPI – Message Passing Interface

1. *Introduction*
2. **MPI Environment**
3. **Point to point communications**
4. **Collective communications**
5. **Communicators**

MPI – Message Passing Interface

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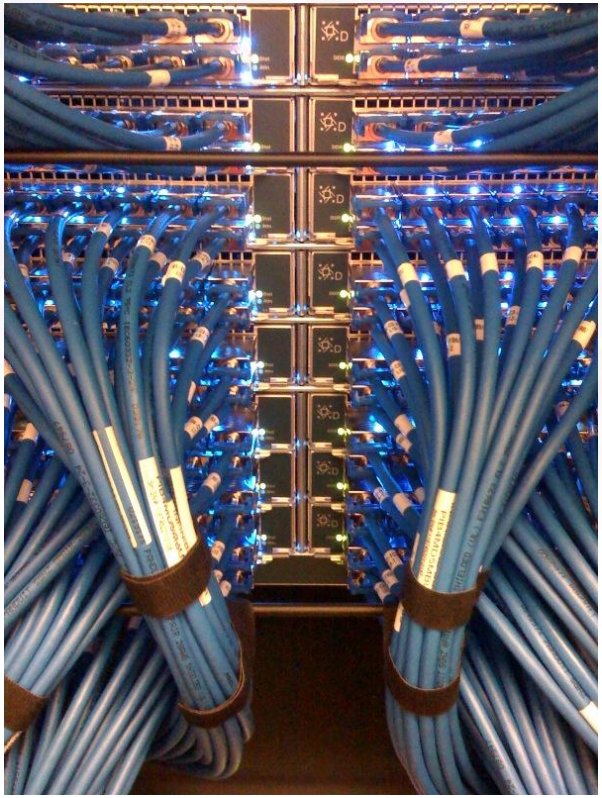
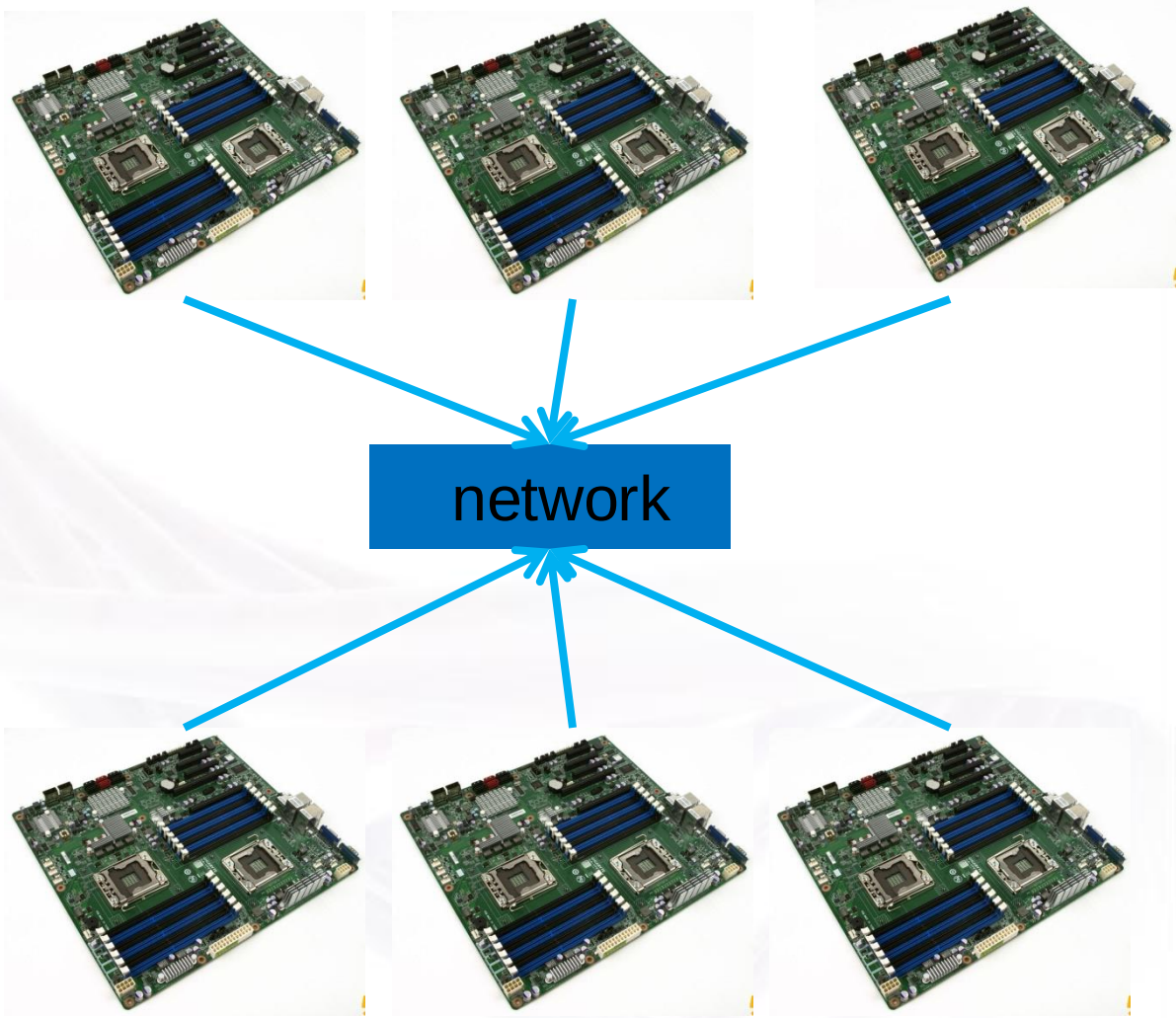
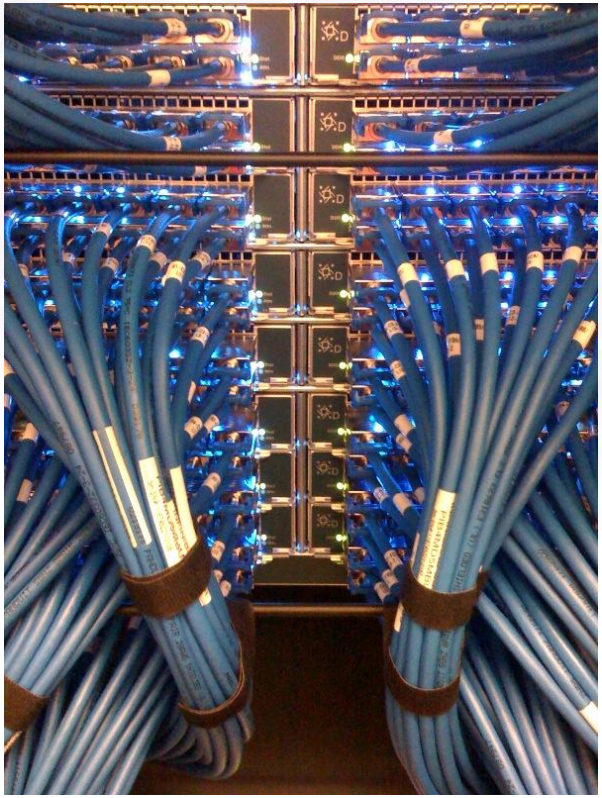
4. **Collective communications**
5. **Communicators**

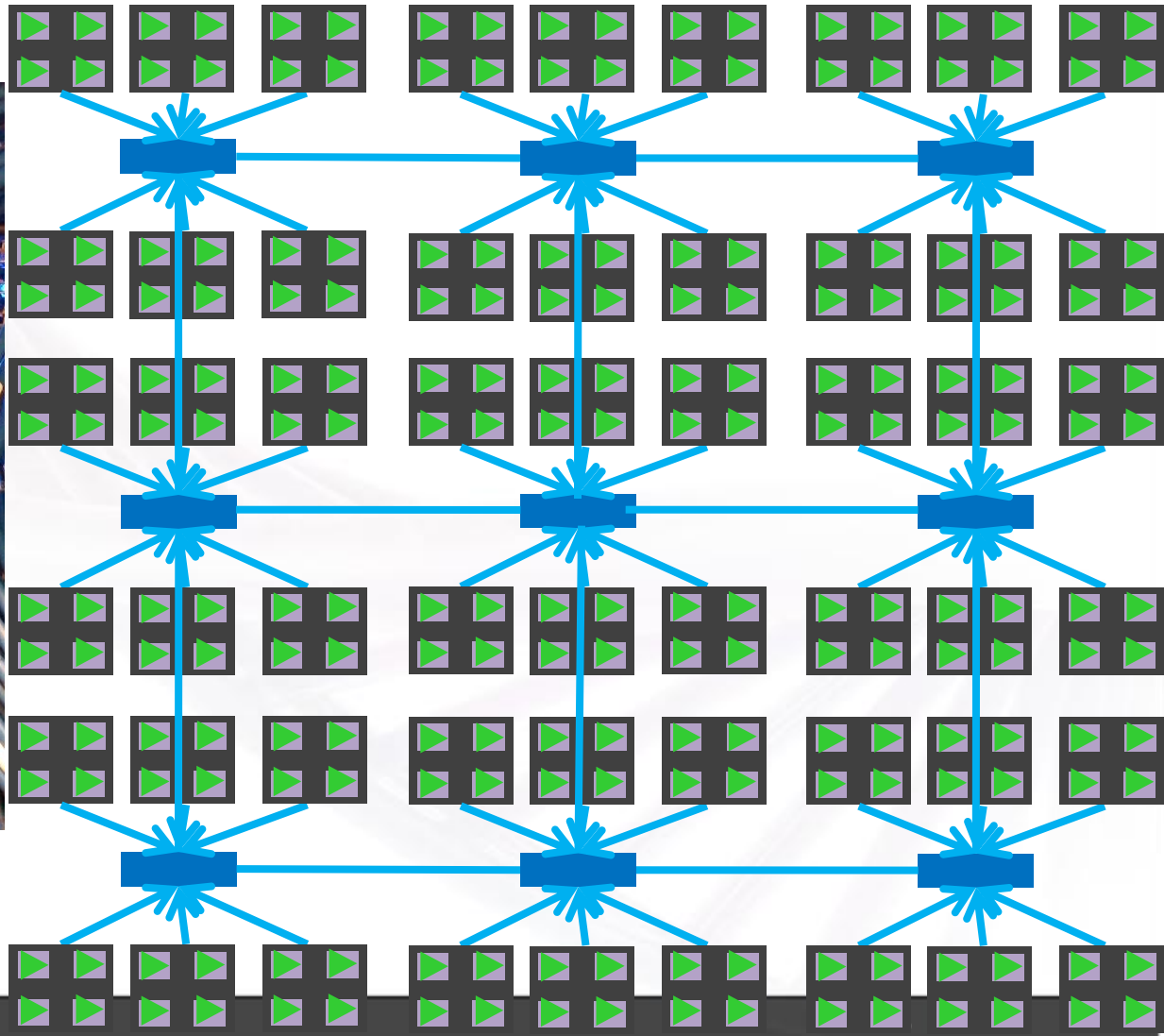
Message Passing Interface





Introduction

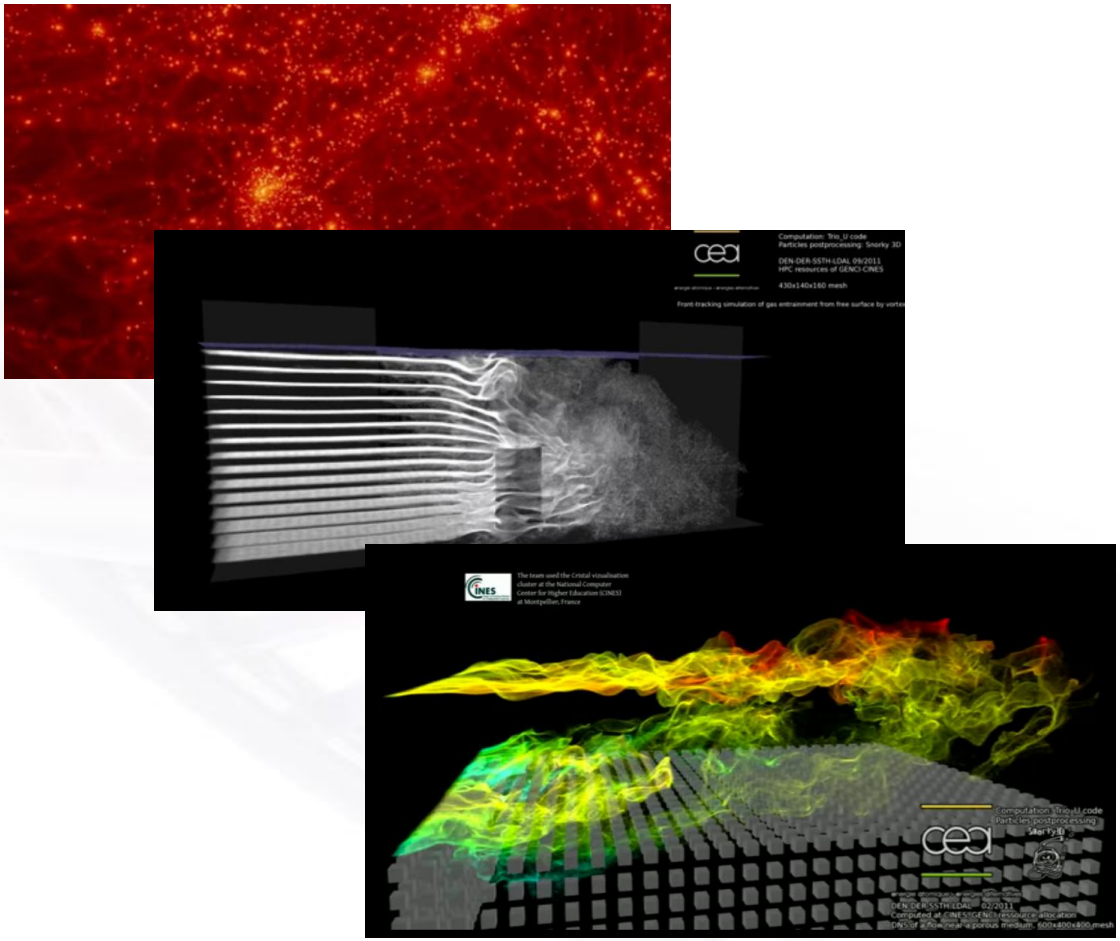




Introduction

MPI Applications :

- Astrophysics
- Fluid Dynamic
- DNA
- Mechanical Structures
- Biochemistry
- Data Mining
- Cryptanalyze
- Brute force
- Reverse engineering
- etc



Introduction

What is MPI ?

- An **API** : defined code to be used.
- A list of **headers** (include), provided by your mpi runtime package.
- A list of **libraries** (lib/lib64), provided by your mpi runtime package.
- A **Launcher** (mpirun/mpiexec), provided by your mpi runtime package and whose purpose is to manage MPI processes during calculations (based on a hostfile).

Note : as seen, mpif90/mpicc are only **wrappers** to your compiler with added mpi include and libs.

Introduction

What is MPI ?

API

```
program hello_world
 use mpi
 implicit none
 integer ::  rank, nb_mpi_processes, ierror, hostname_len
 character (len=MPI_MAX_PROCESSOR_NAME) :: hostname

 !To enhance code readability, we let MPI call or MPI native variables in capital letters in
Fortran
 call MPI_INIT(ierror) ! Init MPI (init MPI_COMM_WORLD communicator, set rank to each process,
etc)

 call MPI_COMM_SIZE(MPI_COMM_WORLD, nb_mpi_processes, ierror) ! Ask the number of MPI processes
running

 call MPI_COMM_RANK(MPI_COMM_WORLD, rank, ierror) ! Ask the rank of the current process

 call MPI_GET_PROCESSOR_NAME(hostname,hostname_len,ierror) ! Ask the name of the host the process
is running on

 print*, 'Hello world ! I am process',rank,'on',nb_mpi_processes,'processes. I am running
on',hostname ! Say hello

 call MPI_FINALIZE(ierror) ! Close MPI

end program hello_world
```

Compilation, using provided wrapper (include/lib)

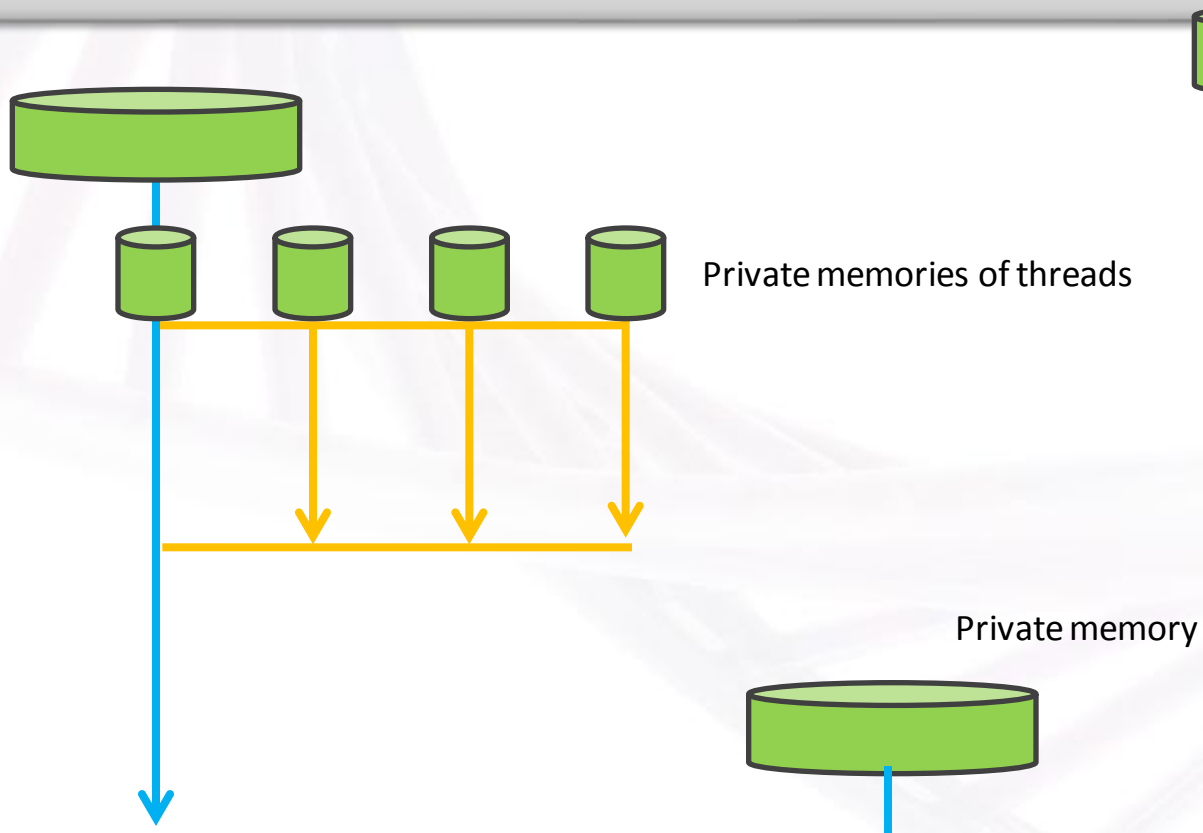
```
:~$ mpif90 hello.f90
```

Conductor and computations

```
:~$ mpirun -np 2 ./a.out
 Hello world ! I am process 1 on 2 processes. I am running on
occigen50
 Hello world ! I am process 0 on 2 processes. I am running on
occigen50
```

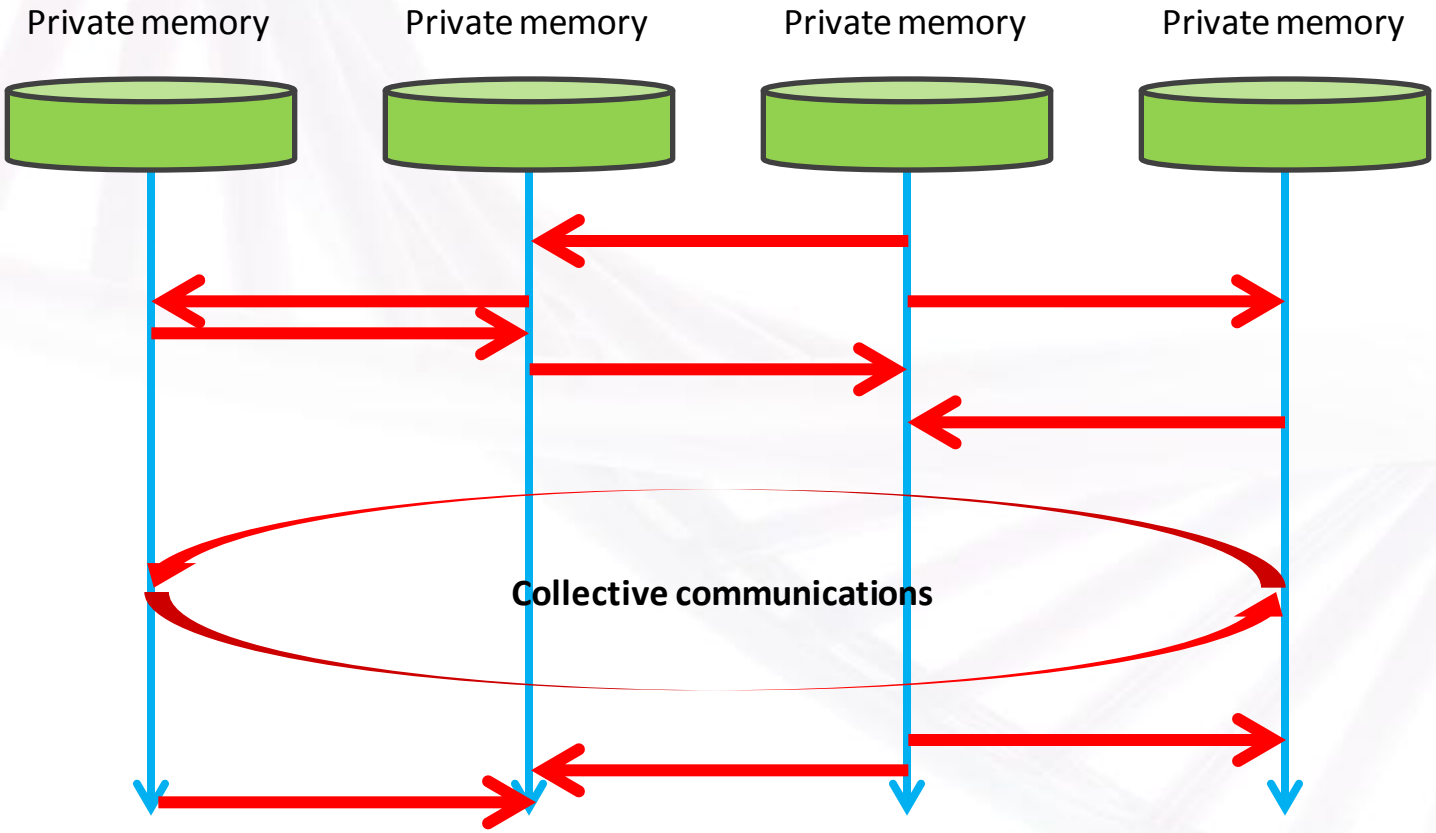
Introduction

Vocabulary : A process with sons threads

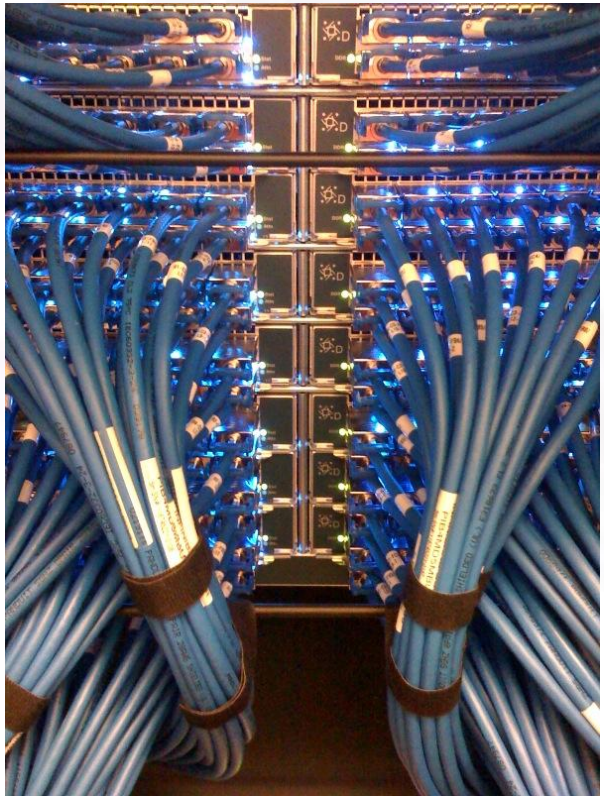


Introduction

MPI is multiple processes working together by communicating through network



Introduction



General MPI Program Structure

MPI include file

Declarations, prototypes, etc.

Program Begins

. . . *Serial code*

Initialize MPI environment *Parallel code begins*

. . .

Do work & make message passing calls

. . .

Terminate MPI environment *Parallel code ends*

. . . *Serial code*

Program Ends

Introduction

Communicate

How do you communicate using mails ?

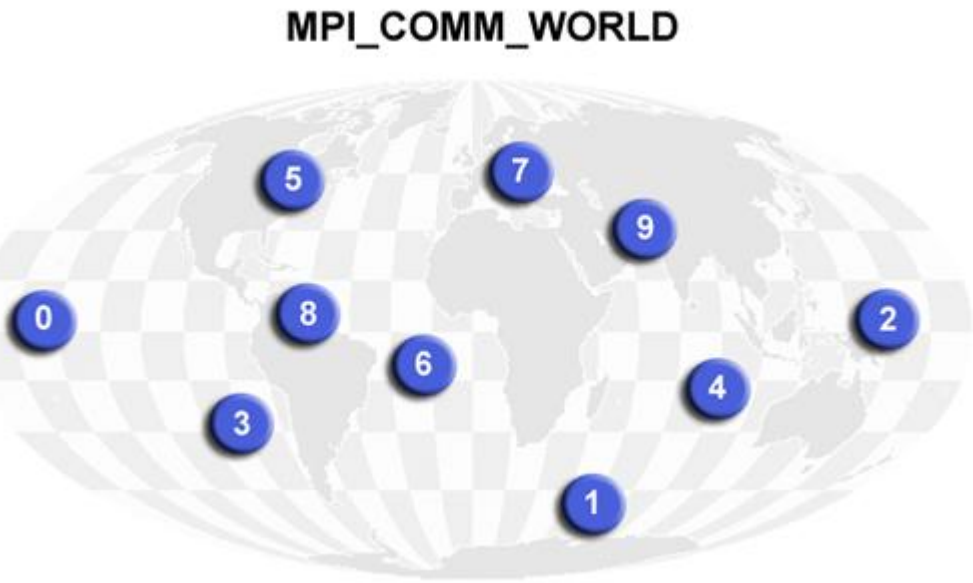
- You have a departing address (the rank)
- You specify a destination address (the rank)
- You use a letter/box adapted to the size of what you send (the size of data)
- You choose the support to use : Web, US Postal Service, UPS, La Poste, etc (the communicator)

Same with MPI, with also

- The type of what you send (integer, real/float, etc)
- A communication number (tag)
- Error return for Fortran and Status.

Introduction

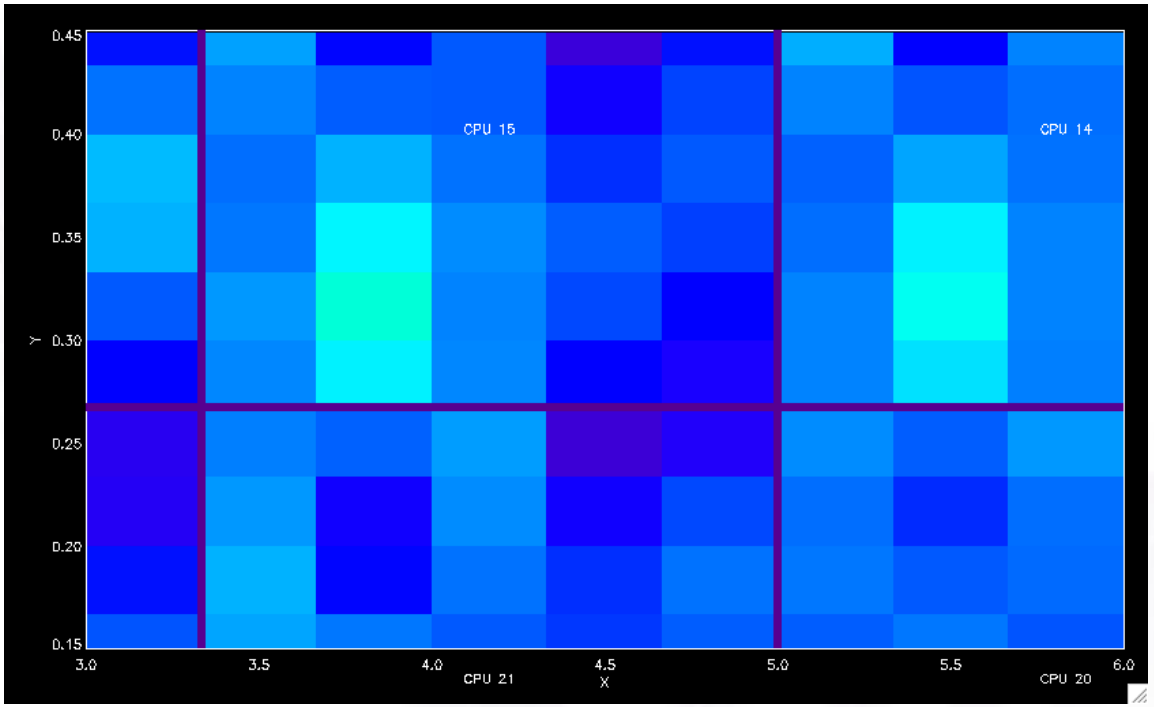
Communicator



Predefined communicator that includes all your MPI processes

Introduction

Domain decomposition



MPI – Message Passing Interface

1. *Introduction*
2. *MPI environment*
3. **Point to point communications**
4. **Collective communications**
5. **Communicators**

MPI Environment

```
program hello_world
 use mpi
 implicit none
 integer ::  rank, nb_mpi_processes, ierror, hostname_len
 character (len=MPI_MAX_PROCESSOR_NAME) :: hostname

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letters in Fortran
 call MPI_INIT(ierror) ! Init MPI (init MPI_COMM_WORLD communicator, set rank to each
process, etc)

 call MPI_COMM_SIZE(MPI_COMM_WORLD, nb_mpi_processes, ierror) ! Ask the number of MPI
processes running

 call MPI_COMM_RANK(MPI_COMM_WORLD, rank, ierror) ! Ask the rank of the current
process

 call MPI_GET_PROCESSOR_NAME(hostname,hostname_len,ierror) ! Ask the name of the host
the process is running on

 print*, 'Hello world ! I am process',rank,'on',nb_mpi_processes,'processes. I am
running on',hostname ! Say hello

 call MPI_FINALIZE(ierror

end program hello_world
```

```
:~$ mpiMPI hello world
f90 hello.f90
:~$ mpirun -np 2 ./a.out
 Hello world ! I am process 1 on 2 processes. I am running on
service2
 Hello world ! I am process 0 on 2 processes. I am running on
service2
```

MPI Environment

MPI basic code

Load headers or modules

Fortran : use mpi

C : #include<mpi.h>

Initialize the MPI execution environment

Fortran : call MPI_INIT(ierror)

C : MPI_Init(NULL, NULL);

MPI Environment

MPI basic code

Get the rank of the current process

Fortran : call MPI_COMM_RANK(MPI_COMM_WORLD, rank, ierror)

C : MPI_Comm_rank(MPI_COMM_WORLD, &rank);

Get the total number of processes currently working together

Fortran : call MPI_COMM_SIZE(MPI_COMM_WORLD, nb_mpi_processes, ierror)

C : MPI_Comm_size(MPI_COMM_WORLD, &nb_mpi_processes);

MPI Environment

MPI basic code

Get the name of the computer/node your process is running on

Fortran : call MPI_GET_PROCESSOR_NAME(hostname,hostname_len,ierror)

C : MPI_Get_hostname(hostname,&hostname_len);

Finalize MPI context

Fortran : call MPI_FINALIZE(ierror)

C : MPI_Finalize();

MPI Environment

Exercises 1.1, 1.2

MPI – Message Passing Interface

1. *Introduction*
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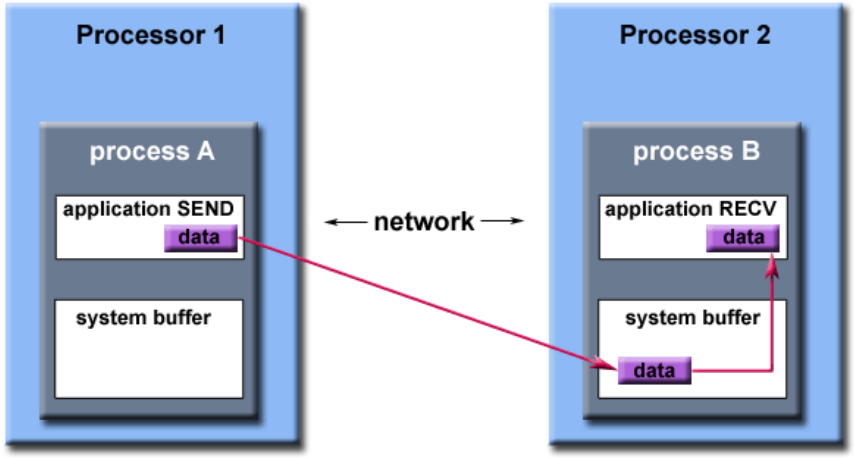
Point to point communications

Types of point-to-point operations

Two different MPI tasks : one send a message, the other perform a matching receive

- Synchronous send
- Blocking send / blocking receive
- Non_blocking send/non-blocking receive
- Buffered send
- Combined send/receive…

Buffering



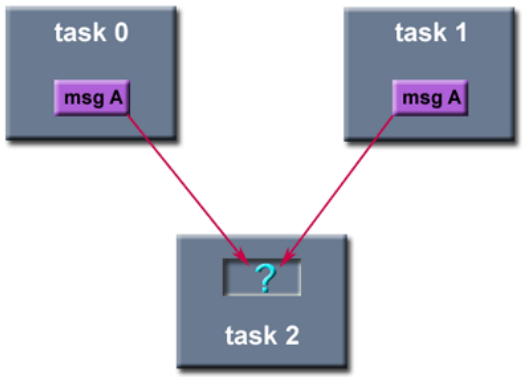
Path of a message buffered at the receiving process

Point to point communications

Blocking or non-blocking communications

Blocking send/receive : easiest, but might waste time..
Non-blocking send/receive : might be able to overlap wait with other stuff
need the use of MPI_WAIT and/or MPI_TEST

Fairness

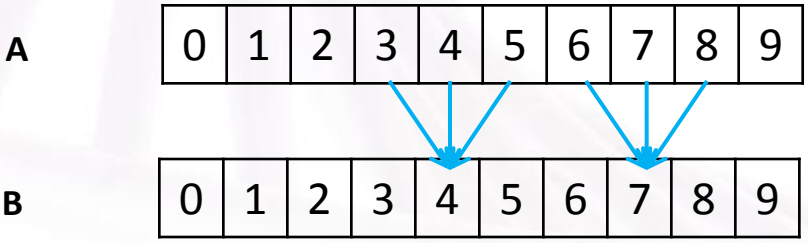


Point to point communications

Sending data to another process

Example, 1D blur : A(i-1) + A(i) + A(i+1) -> B(i)

Sequential or OpenMP :



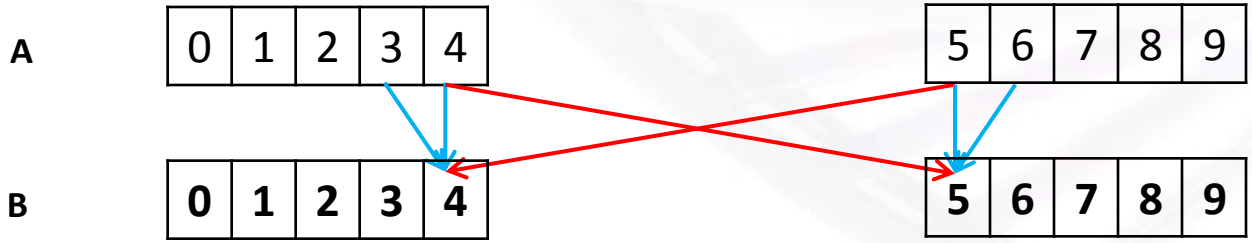
MPI ? Need to share work, and so to share memory

Point to point communications

Sending data to another process

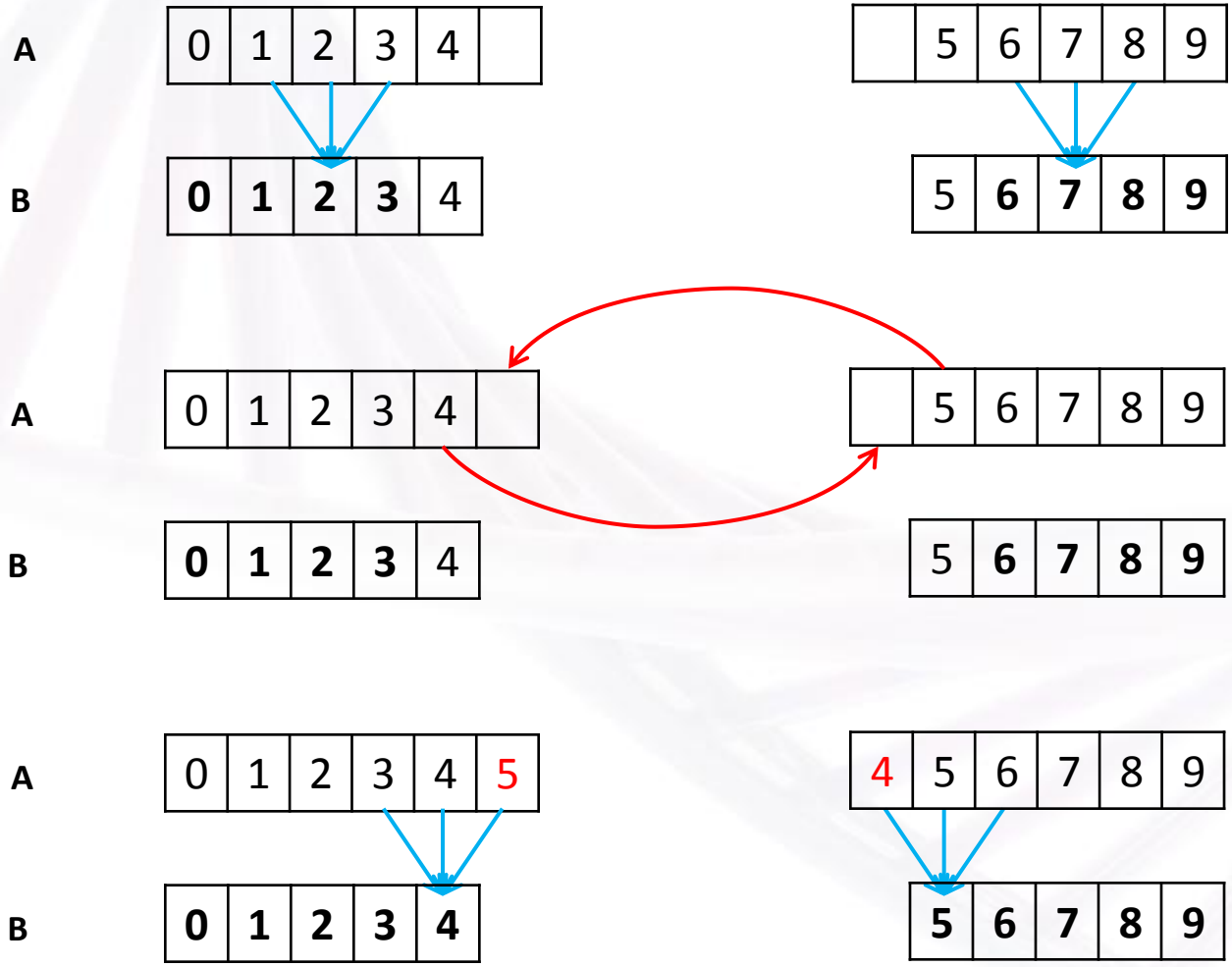
MPI ? Need to share work, and so to share memory :

Need to communicate to know neighbor's data :



Point to point communications

Sending data to another process : use “ghosts” cells



Point to point communications

Synchronous Send data

Fortran :

call MPI_SEND (ball , 1 , MPI_INTEGER , 1 , tag , MPI_COMM_WORLD, ierror)

C : MPI_Send (&ball , 1 , MPI_INTEGER , 1 , tag , MPI_COMM_WORLD);

- Ball : data to be sent
- 1 : int, number of items of this data to be sent
- MPI_INTEGER : int, type of the data
- 1 : int, rank of destination
- MPI_COMM_WORLD : int, communicator to use
- ierror : int

Point to point communications

Synchronous Receive data

Fortran :

```
call MPI_RECV ( ball , 1 , MPI_INTEGER , 0 , tag , MPI_COMM_WORLD , status , ierror )
```

C :

```
MPI_Recv ( &ball , 1 , MPI_INTEGER , 0 , tag , MPI_COMM_WORLD, MPI_STATUS_IGNORE);
```

Point to point communications

Synchronous Send or Receive data

Synchronous Send/Receive data :

Theses communications are synchronous.

The process will wait here until data is sent or received.

In order to make it work, you have to choose an order : a process send it's data while the receiver waits it. When its done, reverse : the first one waits for the data and the second one send it.

This is laborious, we will see some bypass after.

```
program ping_pong
 use mpi
 implicit none
 integer :: rank, nb_mpi_processes, ie
 integer :: niter = 6
 call MPI_INIT( ierror )
 call MPI_COMM_SIZE( MPI_COMM_WORLD , n
 call MPI_COMM_RANK( MPI_COMM_WORLD , i

 if(nb_mpi_processes /= 2) stop 'This p

 ball = 0
 do n=1,niter
    if(rank==0) then
       call MPI_SEND ( ball , 1 , MPI_INTEGER , 1 , tag , MPI_COMM_WORLD , ierror )
       ! 0 send ball to 1, and wait for transfer to be finished
       call MPI_RECV ( ball , 1 , MPI_INTEGER , 1 , tag , MPI_COMM_WORLD , MPI_STATUS_IGNORE
, ierror )
       ! 0 receive ball from 1, and wait for transfer to be finished
       ball = ball + 2
    end if

    if(rank==1) then
       call MPI_RECV ( ball , 1 , MPI_INTEGER , 0 , tag , MPI_COMM_WORLD , MPI_STATUS_IGNORE
, ierror )
       ball = ball + 1
       call MPI_SEND ( ball , 1 , MPI_INTEGER , 0 , tag , MPI_COMM_WORLD , ierror )
    end if

    print*, 'Process',rank,'iter',n,'ball value is :',ball

    call MPI_BARRIER(MPI_COMM_WORLD,ierror) ! A barrier. processes stop here, and can pass it
only if ALL processes are here. Useful for debug, can impact performances

 end do

 call MPI_FINALIZE ( ierror ) ! Close MPI
```

```
:~$ mpirun -np 2 ./a.out
 Process           0 iter           1 ball value is :
3
 Process           0 iter           2 ball value is :
6
 Process           0 iter           3 ball value is :
9
 Process           0 iter           4 ball value is :
12
 Process           0 iter           5 ball value is :
15
 Process           0 iter           6 ball value is :
18
 Process           1 iter           1 ball value is :
 Process           1 iter           2 ball value is :
 Process           1 iter           3 ball value is :
 Process           1 iter           4 ball value is :
10
 Process           1 iter           5 ball value is :
13
 Process           1 iter           6 ball value is :
16
```

Point to point communications

Synchronous Send or Receive data

Synchronous Send/Receive data :

Theses communications are synchronous.

The process will wait here until data is sent or received.

In order to make it work, you have to choose an order : a process send it's data while the receiver waits it. When its done, reverse : the first one waits for the data and the second one send it.

This is laborious, we will see some bypass after.

Use Sendrecv to do both at the same time !

Point to point communications

Synchronous Send/Receive data

Fortran :

```
call MPI_SENDRECV ( val , 1 , MPI_INTEGER , 1 , tag ,        data to send
                    val0 , 1 , MPI_INTEGER , 1 , tag ,       data to receive
                    MPI_COMM_WORLD , status , ierror )
```

C :

```
MPI_Sendrecv ( &val , 1 , MPI_INTEGER , 1 , tag , &val0 , 1 ,
MPI_INTEGER , 1 , tag , MPI_COMM_WORLD , MPI_STATUS_IGNORE  );
```

```
 if(rank==0) then
    call MPI_SENDRECV ( val , 1 , MPI_INTEGER , 1 , tag , val0 , 1 , MPI_INTEGER , 1 , tag ,
MPI_COMM_WORLD , statu , ierror )
    val = val0
 end if
 if(rank==1) then
    call MPI_SENDRECV ( val , 1 , MPI_INTEGER , 0 , tag , val0 , 1 , MPI_INTEGER , 0 , tag ,
MPI_COMM_WORLD , statu , ierror )
    val = val0
 end if
```

Fortran :

call MPI_SENDRECV (val , 1 , MPI_INTEGER , 1 , tag , — data to send

val0 , 1 , MPI_INTEGER , 1 , tag , — data to receive

MPI_COMM_WORLD , status , ierror) — (context)

C :

MPI_Sendrecv (&val , 1 , MPI_INTEGER , 1 , tag , &val0 , 1 ,
MPI_INTEGER , 1 , tag , MPI_COMM_WORLD , MPI_STATUS_IGNORE);

Point to point communications

Exercises 1.3, 1.4

MPI – Message Passing Interface

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4. **Collective communications**
5. **Communicators**

Collective communications

MPI collective communications

Apply to all processes of the specified communicator

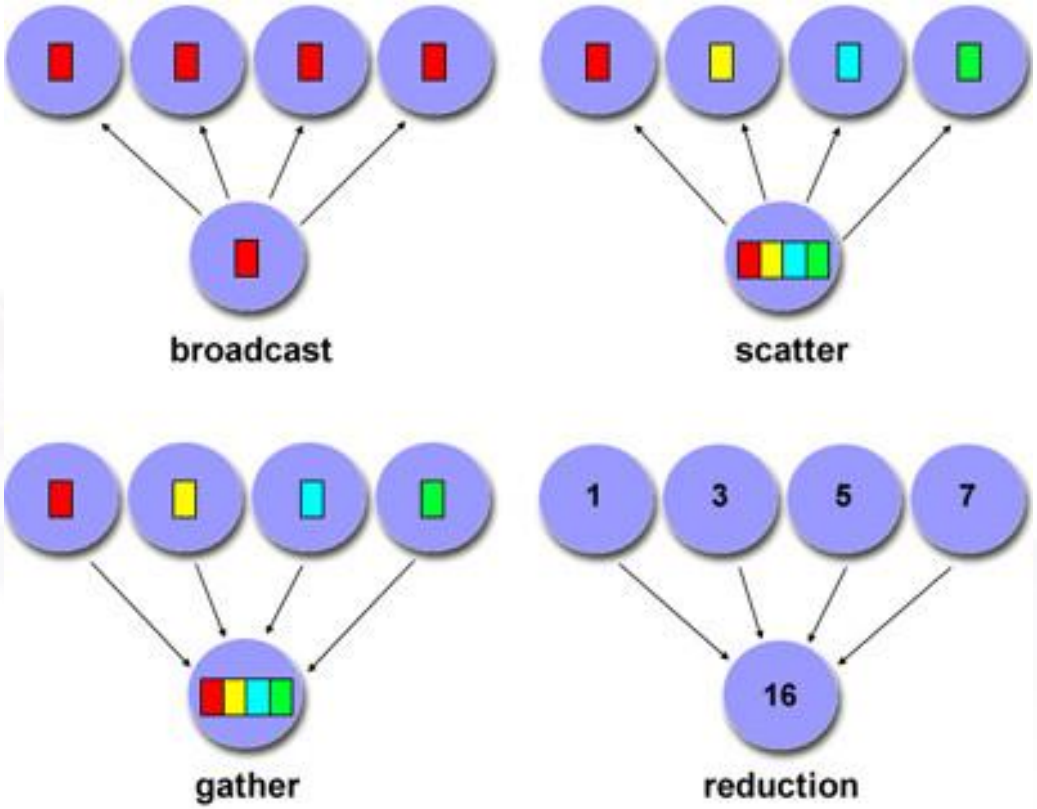
Available :

- Synchronization
- Reductions (Max, Min, SUM, PROD, etc)
- Global broadcast or gather, and derivatives

Collective communications

MPI collective communications

MPI_BARRIER
MPI_REDUCE
MPI_ALLREDUCE
MPI_BCAST
MPI_SCATTER
MPI_GATHER
MPI_ALLGATHER
MPI_GATHERV
MPI_ALLTOALL



Collective communications

Synchronization

As for OpenMP, you can use barriers to ensure all processes stay synchronize before or after a specific action.

MPI_BARRIER

Fortran : call MPI_BARRIER(MPI_COMM_WORLD,ierror)

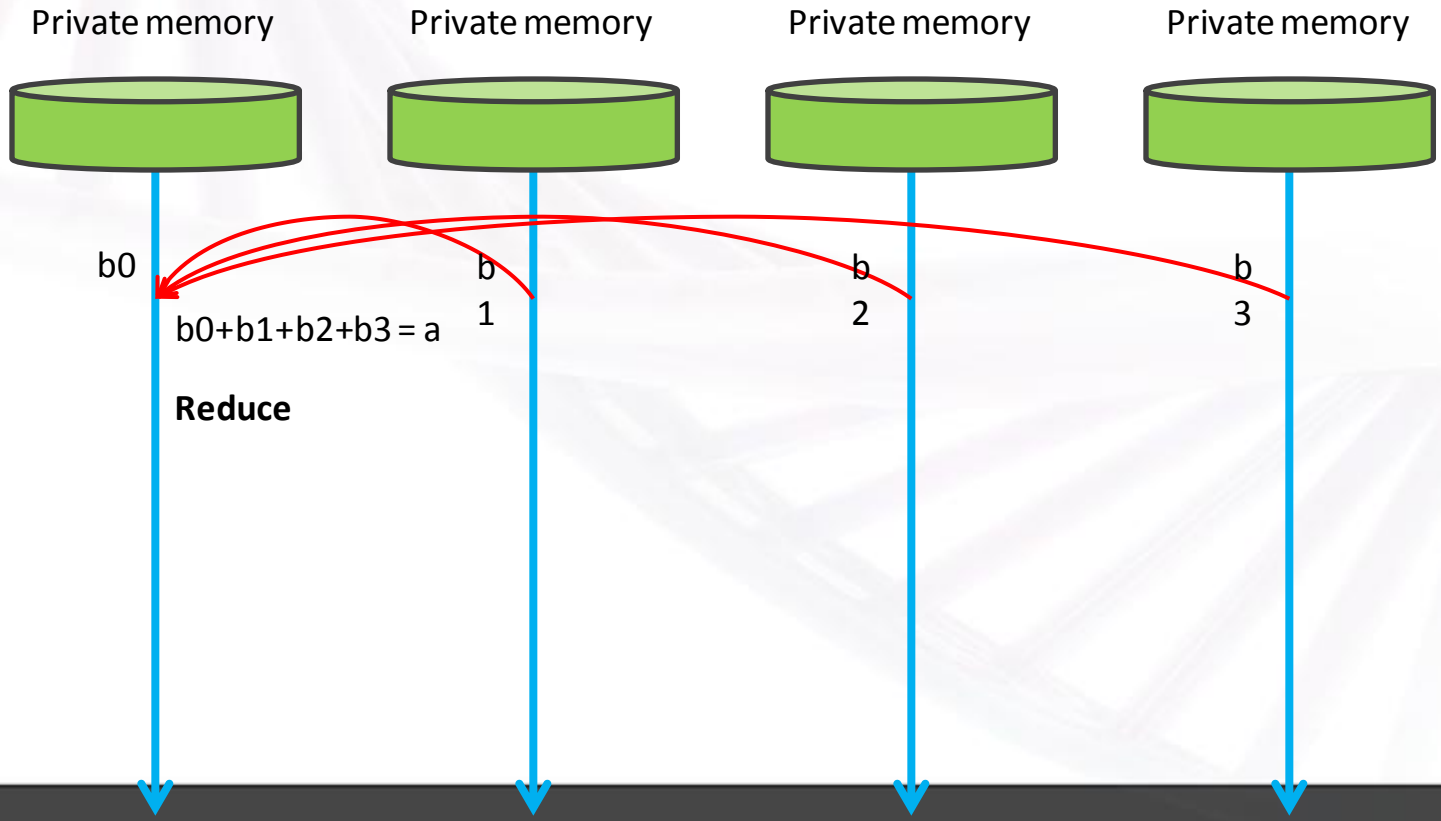
C : MPI_Barrier(MPI_COMM_WORLD);

Collective communications

Reductions : REDUCE

get result on only one process : REDUCE

get result on all processes : ALLREDUCE

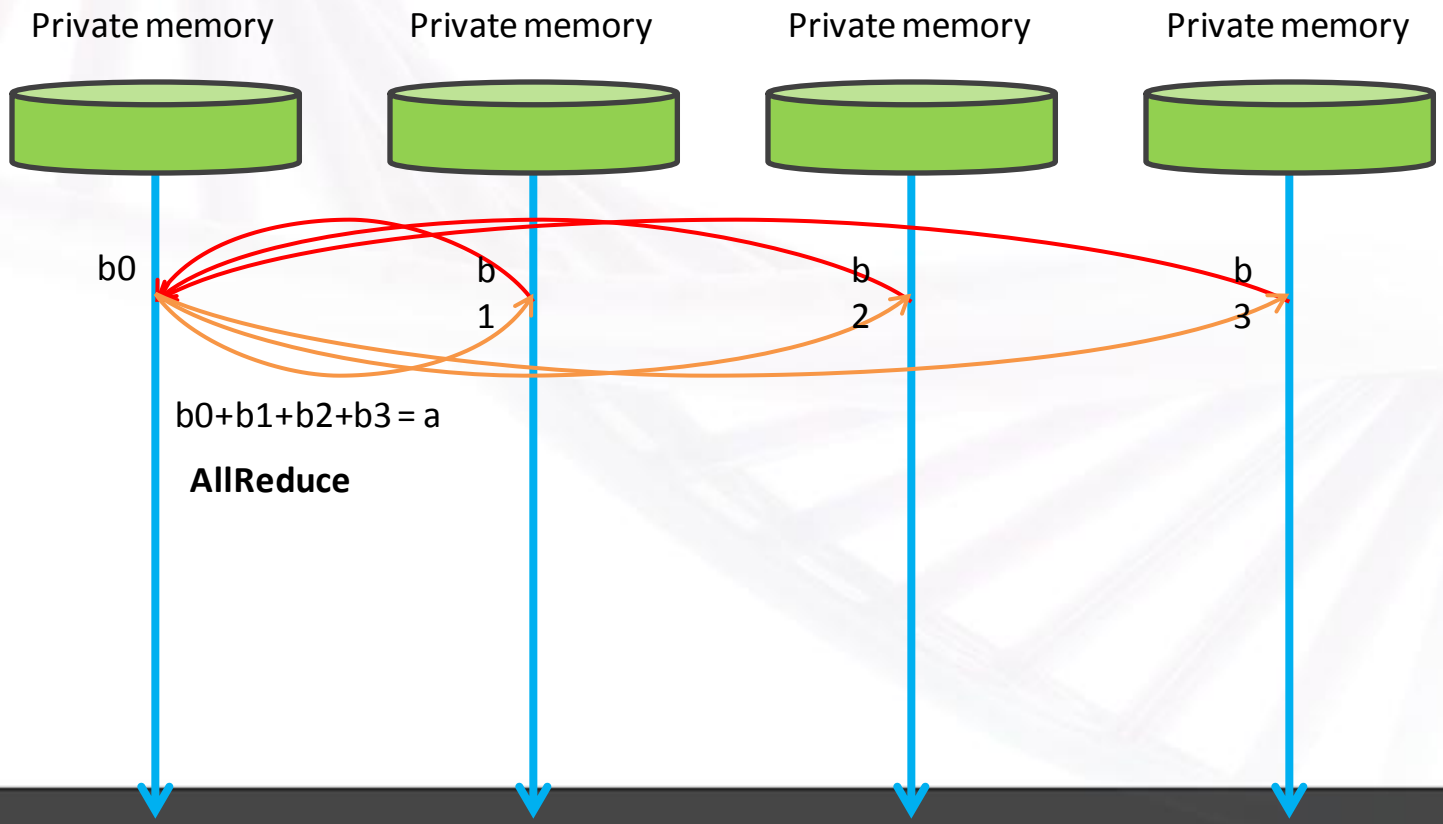


Collective communications

Reductions : ALLREDUCE

get result on only one process : REDUCE

get result on all processes : ALLREDUCE



Collective communications

MPI_ALLREDUCE

Fortran :

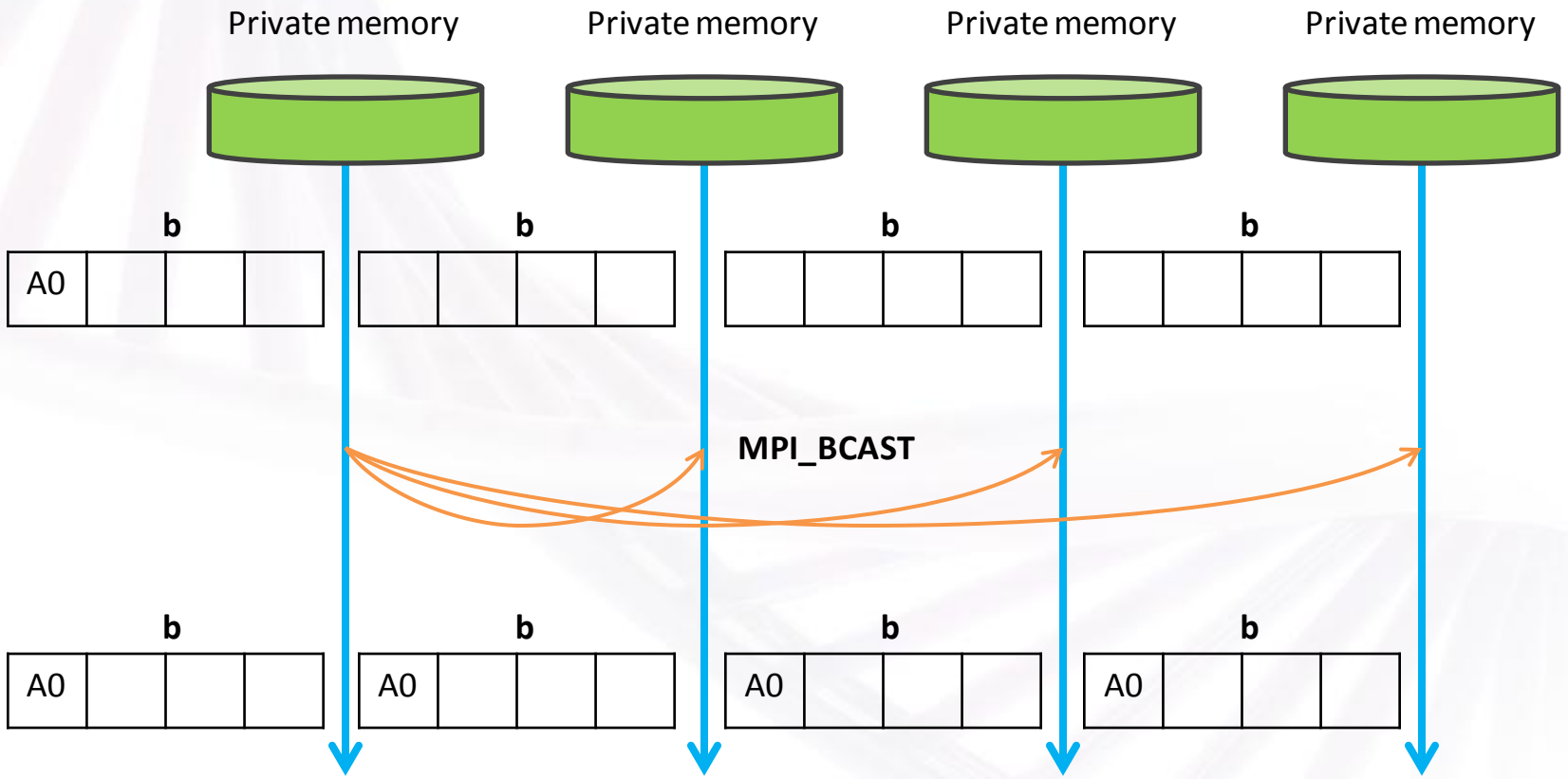
```
CALL MPI_ALLREDUCE ( val , sum_val , 1 , MPI_DOUBLE_PRECISION ,
MPI_SUM , MPI_COMM_WORLD , ierror)
```

C :

```
MPI_Allreduce(&val , &val , 1, MPI_DOUBLE, MPI_SUM,
MPI_COMM_WORLD);
```

Collective communications

Broadcast : MPI_BCAST



Collective communications

MPI_BCAST

Fortran :

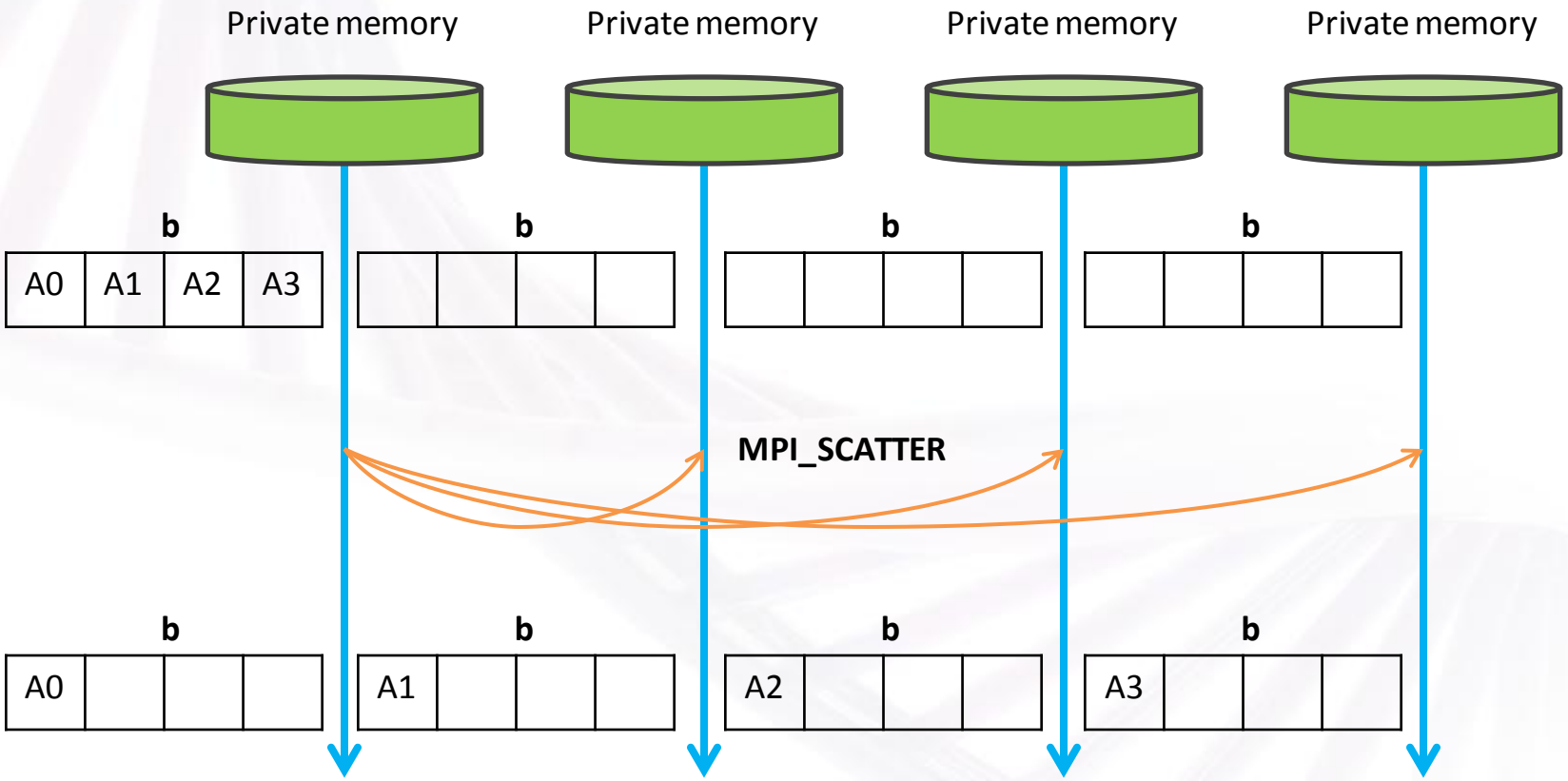
```
CALL MPI_BCAST ( val , 1 , MPI_DOUBLE_PRECISION  , 0 ,
MPI_COMM_WORLD , ierror)
```

C :

```
MPI_Bcast(&val , &val , 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
```

Collective communications

Broadcast : MPI_SCATTER



Collective communications

MPI_SCATTER

Fortran :

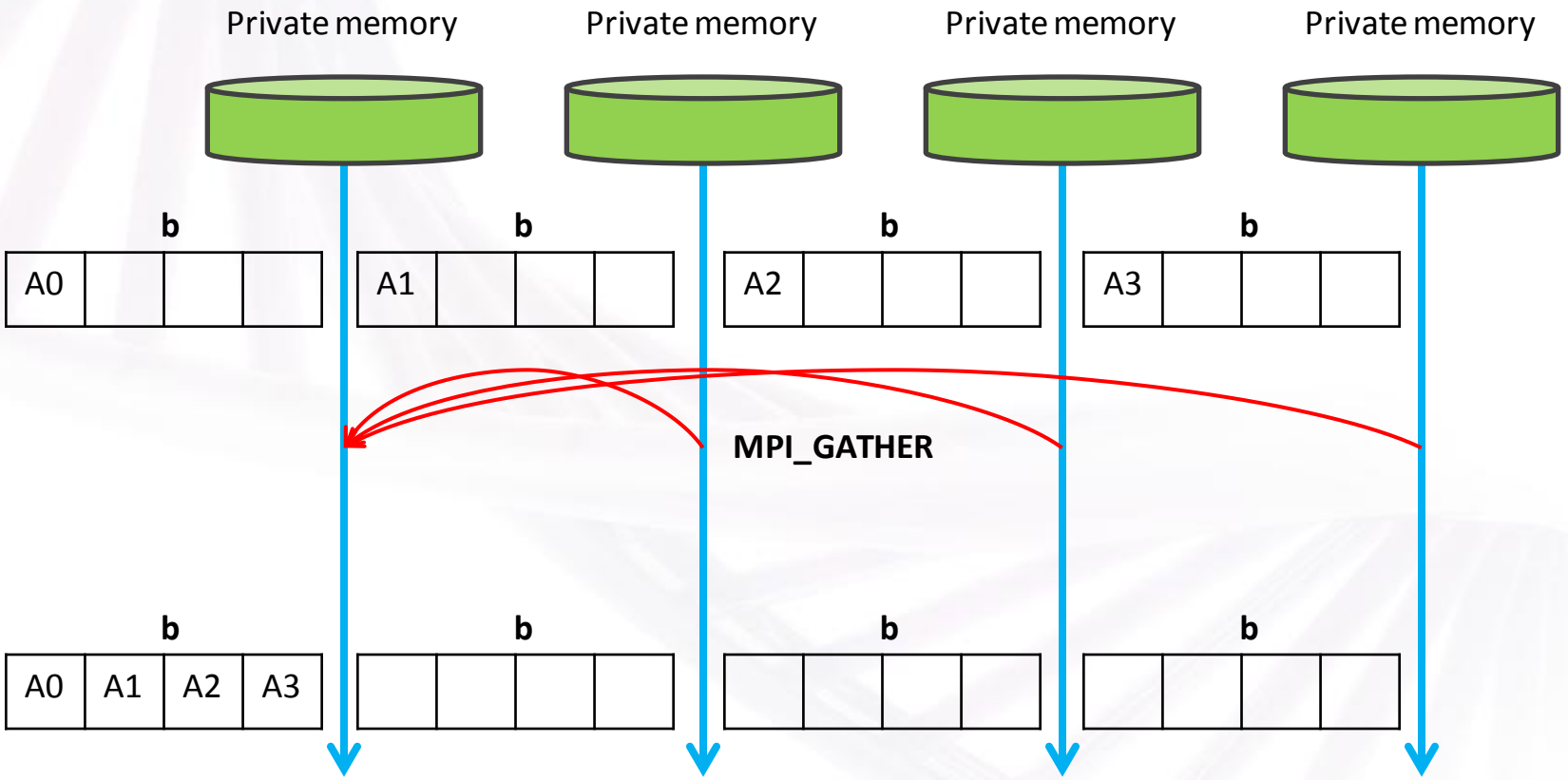
```
CALL MPI_SCATTER (aval(1:8), 2, MPI_DOUBLE_PRECISION,
bval(1:2), 2 , MPI_DOUBLE_PRECISION,  3,
MPI_COMM_WORLD, ierror)
```

C :

```
MPI_Scatter (&aval, 2, MPI_REAL, &bval, 2 , MPI_REAL, 3,
MPI_COMM_WORLD);
```

Collective communications

Broadcast : MPI_GATHER



Collective communications

MPI_GATHER

Fortran :

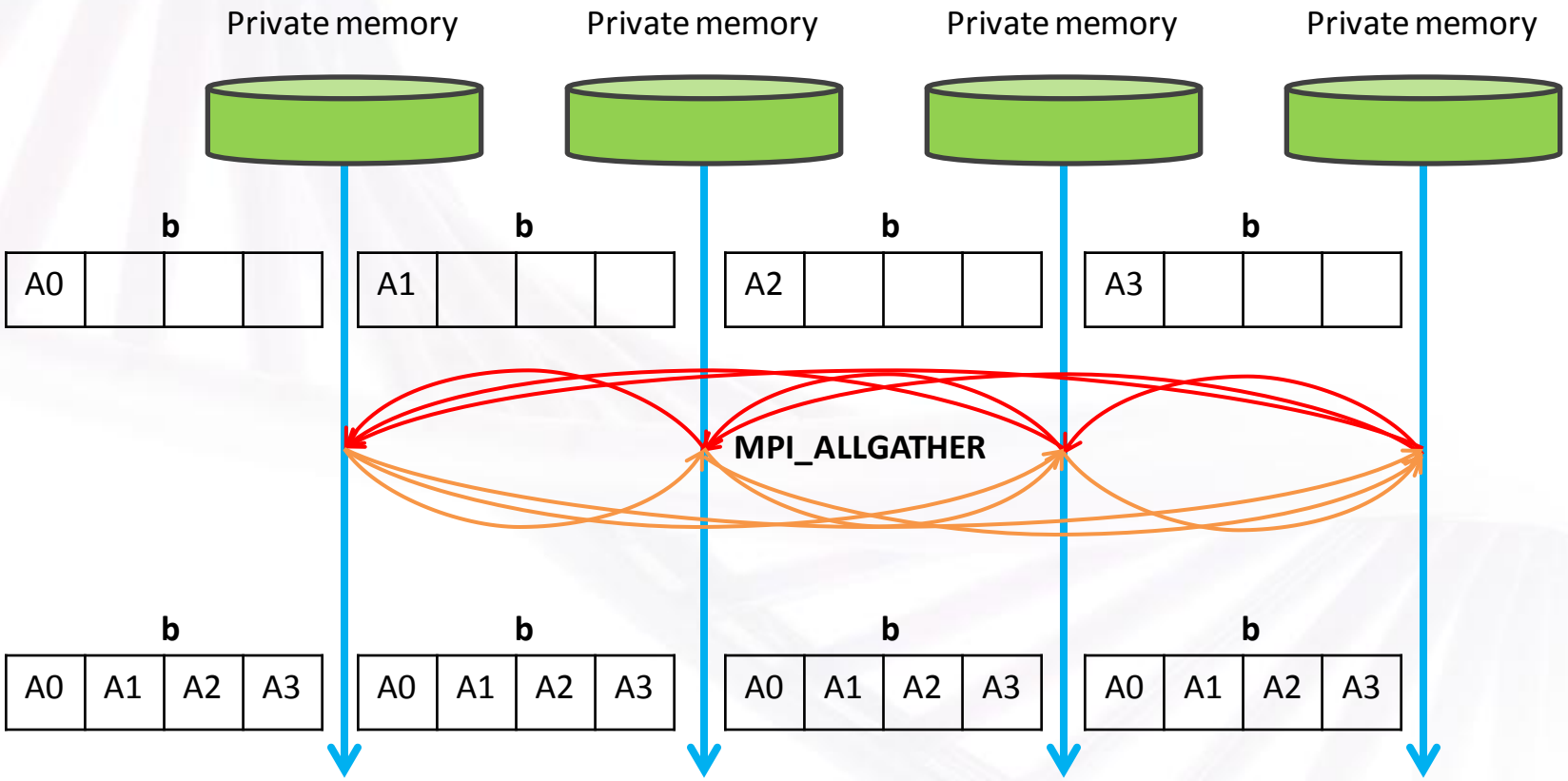
```
CALL MPI_GATHER( val, 1, MPI_DOUBLE_PRECISION, cval(1:4), 1 ,
MPI_DOUBLE_PRECISION, 3, MPI_COMM_WORLD, ierror)
```

C :

```
MPI_Gather (val, 1, MPI_DOUBLE_PRECISION, &cval, 1 ,
MPI_DOUBLE_PRECISION, 3, MPI_COMM_WORLD);
```

Collective communications

Broadcast : MPI_ALLGATHER



Collective communications

MPI_ALLGATHER

Fortran :

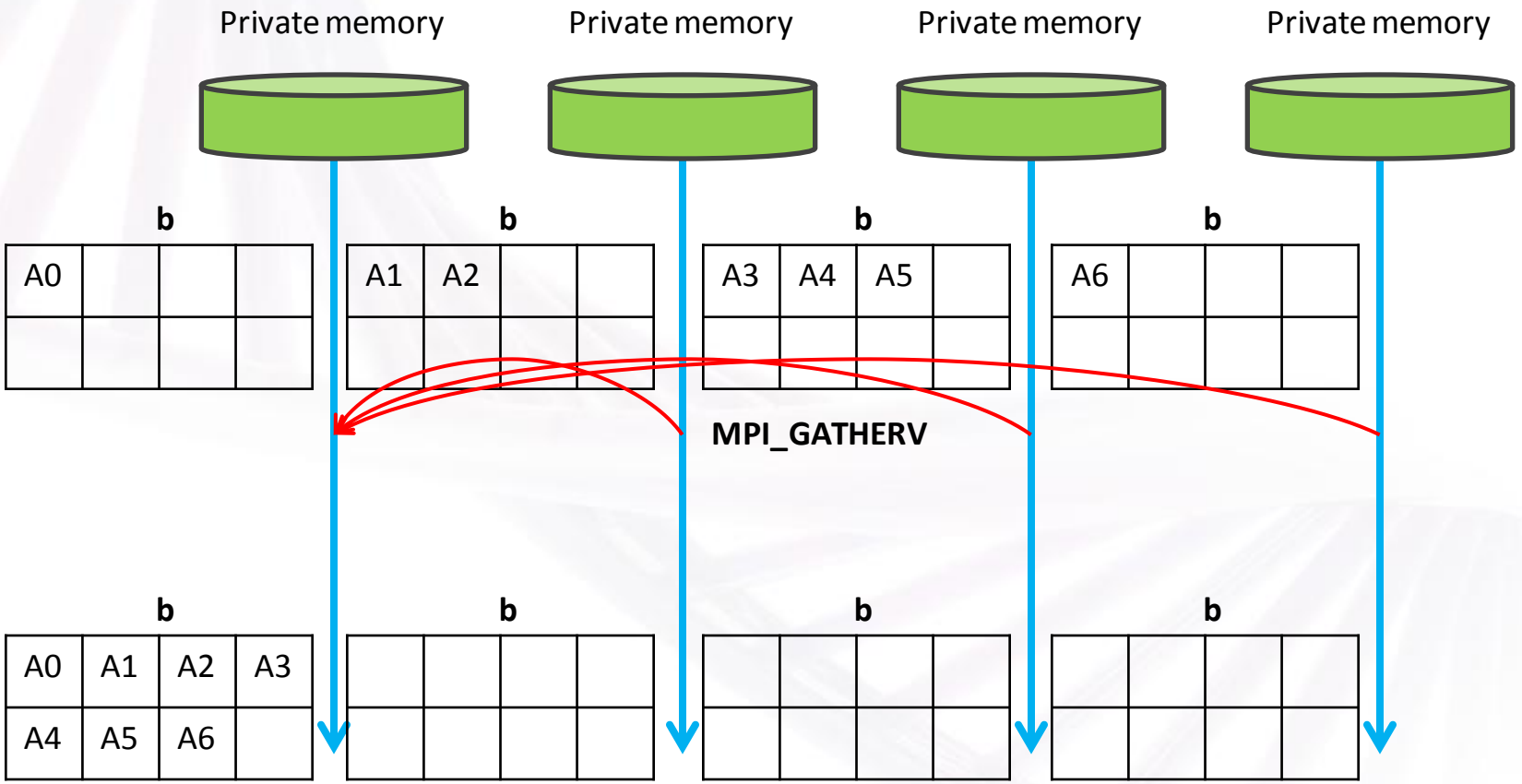
```
CALL MPI_ALLGATHER( val, 1, MPI_DOUBLE_PRECISION,
cval(1:4), 1 , MPI_DOUBLE_PRECISION, MPI_COMM_WORLD,
ierror)
```

C :

```
MPI_Allgather(val, 1, MPI_DOUBLE_PRECISION, &cval, 1 ,
MPI_DOUBLE_PRECISION, MPI_COMM_WORLD);
```

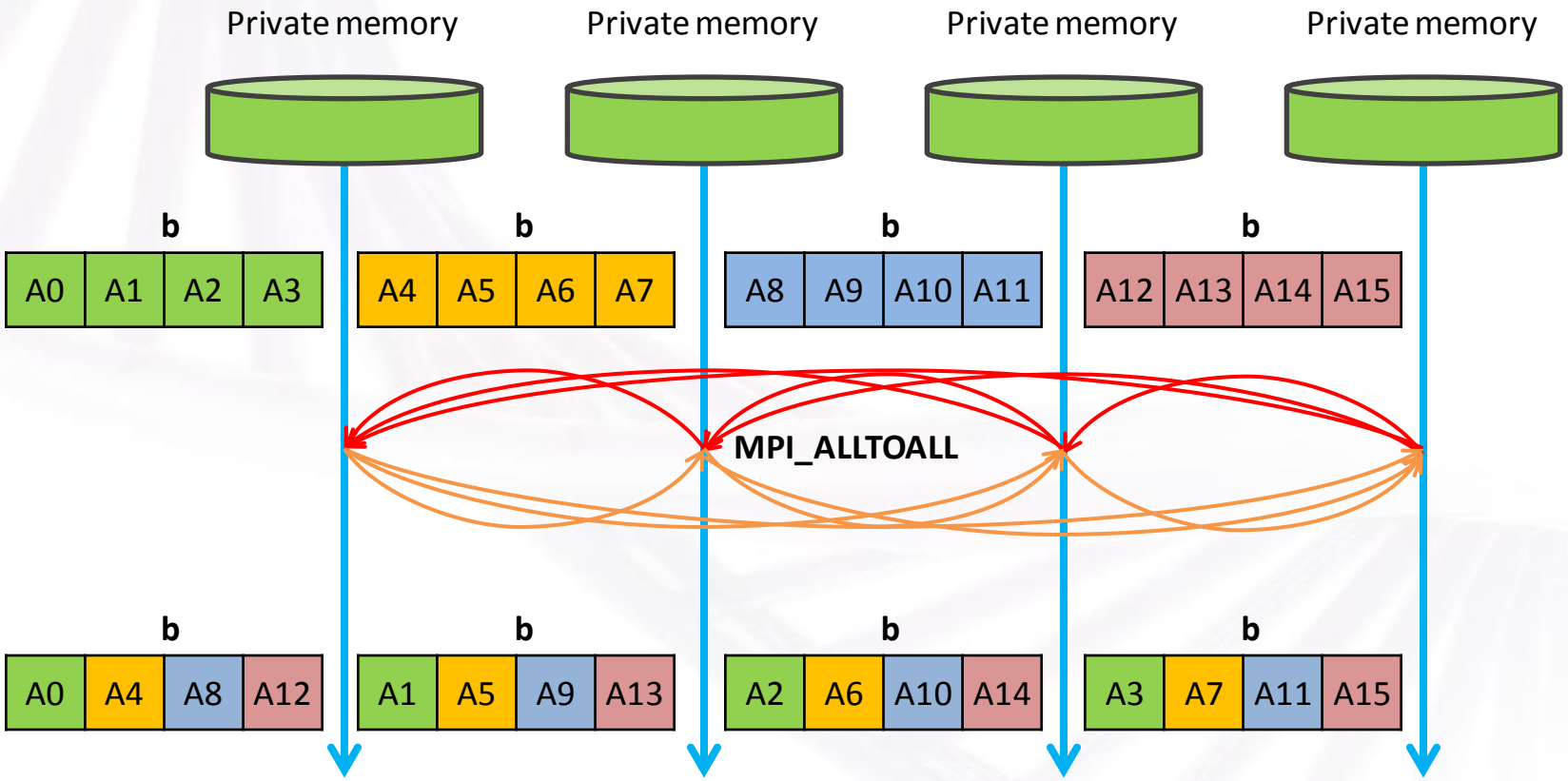
Collective communications

Broadcast : MPI_GATHERV



Collective communications

Broadcast : MPI_ALLTOALL



Collective communications

Others available, not covered in this training :

- MPI_SCATTERV()
- MPI_GATHERV()
- MPI_ALLGATHERV()
- Etc.

All information can be found here :

http://www.mpich.org/static/docs/v3.0.x/www3/

Collective communications

Exercises 1.5

MPI – Message Passing Interface

1. *Introduction*
2. **Acquire information**
3. **Point to point communications**
4. **Collective communications**
5. **Communicators**

Communicators

Communicators

Cartesian communicator

Specific communicator dedicated to Cartesian organization

User tuned communicator

Users can defined their own communicators for specific purposes

Communicators

Cartesian communicator

6	7	8
3	4	5
0	1	2

Communicators

Cartesian communicator

0,2	1,2	2,2
0,1	1,1	2,1
0,0	1,0	2,0

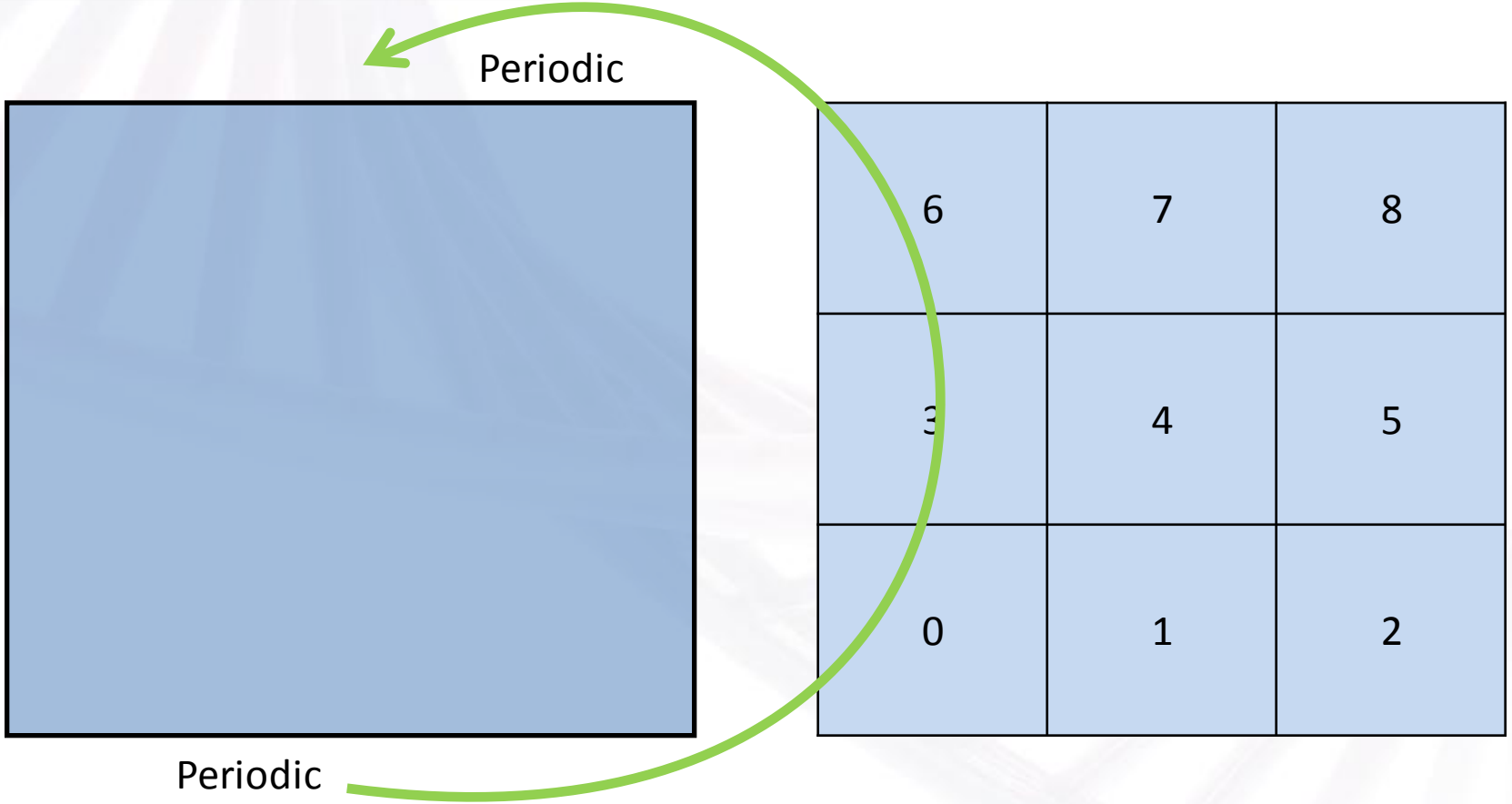
Communicators

Cartesian communicator

MPI_PROC_NULL	MPI_PROC_NULL	MPI_PROC_NULL	MPI_PROC_NULL	MPI_PROC_NULL
MPI_PROC_NULL	6	7	8	MPI_PROC_NULL
MPI_PROC_NULL	3	4	5	MPI_PROC_NULL
MPI_PROC_NULL	0	1	2	MPI_PROC_NULL
MPI_PROC_NULL	MPI_PROC_NULL	MPI_PROC_NULL	MPI_PROC_NULL	MPI_PROC_NULL

Communicators

Cartesian communicator



Communicators

Cartesian communicator

MPI_PROC_NULL	0	1	2	MPI_PROC_NULL
MPI_PROC_NULL	6	7	8	MPI_PROC_NULL
MPI_PROC_NULL	3	4	5	MPI_PROC_NULL
MPI_PROC_NULL	0	1	2	MPI_PROC_NULL
MPI_PROC_NULL	6	7	8	MPI_PROC_NULL

Communicators

Cartesian communicator

When you communicate with MPI_PROC_NULL, communication does not occur, but does not stop computation.

- **Useful to simplify source code.**

Why using Cartesian communicator when you can do it manually ? Reorganize !

- **This function tune your ranks numbers depending on their proximity in the super computer to maximize performances.**

Communicators

Cartesian communicator

```
nb_process_axe(1) = 4
cart_boundaries(1) = .false. ! Means not periodic, .true. Means periodic

call MPI_CART_CREATE( MPI_COMM_WORLD , ndim , nb_process_axe(1:ndim) , &
& cart_boundaries(1:ndim) , .true. , MPI_COMM_CART , ierror )

call MPI_CART_COORDS( MPI_COMM_CART , rank , ndim , cart_position(1:ndim) , ierror )

call MPI_CART_SHIFT (MPI_COMM_CART, 0, 1, cart_neigh(-1), cart_neigh(+1), ierror)
```

Communicators

User tuned communicator

int, reference communicator

int, new communicator

Fortran :

```
CALL MPI_COMM_SPLIT(MPI_COMM_WORLD, color, key, MY_COM, ierror)
```

C :

```
MPI_Comm_split(MPI_COMM_WORLD, color, key, &MY_COM);
```

```
 integer ::  key, color, MY_COMMUNICATOR
 […]
 color=MPI_UNDEFINED
 if (rank == 0 .OR. rank == 1) color = 1
 if (rank == 2 .OR. rank == 3) color = 2
 key=rank
 CALL MPI_COMM_SPLIT(MPI_COMM_WORLD,color,key,MY_COMMUNICATOR,ierror)

 CALL MPI_ALLREDUCE ( rank , ranksum , 1 , MPI_INTEGER , MPI_SUM ,
MY_COMMUNICATOR , ierror)

 print *,"I am proc",rank,ranksum
```

```
 I am proc           2
5
 I am proc           0
1
 I am proc           1
```

Collective communications

Exercises 1.6, 1.7

MPI – The Complete Reference : Volume 1, The MPI Core, by Marc Snir, Steve Otto, Steven Huss-Lederman, David Walker and Jack Dongarra, 1998

https://computing.llnl.gov/tutorials/mpi/

http://www.idris.fr/data/cours/parallel/mpi/choix_doc.html

http://www.mpich.org/static/docs/v3.0.x/www3/ (API)

http://www.open-mpi.org/doc/v1.6/ (API)

http://semelin.developpez.com/cours/parallelisme/ (FR)