



# **MPI** introduction



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# Message passing and shared memory parallelism







shared memory



Multiple *tasks* exchange data via explicit messages

Program splits into *threads* which share data via variables in shared memory





### Message Passing



Unlike the shared memory model, resources are local;

□ Each process operates in its own environment (logical address space) and communication occurs via the exchange of messages;

Messages can be instructions, data or synchronisation signals;

The message passing scheme can also be implemented on shared memory architectures;

Delays are much longer than those due to shared variables in the same memory space;







#### Advantages and Drawbacks

- Advantages
  - Communications hardware and software are important components of HPC system and often very highly optimised;
  - Portable and scalable;
  - Long history (many applications already written for it);
- Drawbacks
  - Explicit nature of message-passing is error-prone and discourages frequent communications;
  - Most serial programs need to be completely re-written;
  - High memory overheads.





# MPI (Message Passing Interface)



**MPI origin**: 1992, "Workshop on Standards for Message Passing in a Distributed Memory Environment"

60 experts from more than 40 organisations (IBM T. J. Watson Research Center, Intel's NX/2, Express, nCUBE's Vertex, p4, PARMACS, Zipcode, Chimp, PVM, Chameleon, PICL, ... ).

Many of them coming from the most important constructors of parallel computers or researchers from University, government and private research centres.







# MPI (Message Passing Interface)

#### **MPI development:**

- MPI-1.0: June 1994;
- MPI-1.1: June 1995;
- MPI-1.2 e MPI-2: June 1997
- MPI-1.3 e MPI-2.1: May, June 2008
- MPI-2.2 : September 2009
- MPI-3.0 : September 2012
- MPI-3.1 : June 2015





#### Goals of the MPI standard



#### MPI's prime goals are:

- To allow efficient implementation
- To provide source-code portability

MPI also offers:

- A great deal of functionality
- Support for heterogeneous parallel architectures

**MPI2** further extends the library power (parallel I/O, Remote Memory Access, Multi Threads, Object Oriented programming)

**MPI3** aims to support exascale by including non-blocking collectives, improved RMA and neighbourhood collectives.





### **MPI** versions



Some of the public domain most used MPI libraries:

- **MPICH** : Argonne National Laboratory
- **Open MPI** : "open source" implementation of MPI-2
- **<u>CHIMP/MPI</u>** : Edinburgh University
- LAM : Ohio Supercomputer Center

To realize a (simple) parallel program *only six MPI functions* are needed.

But if the program is a complex one and the best performances are sought for, the whole MPI library may be used, with more than a hundred functions.





### MPI introduction



What we will learn in this lesson on MPI library:

- Compiling and executing MPI programs
- C and Fortran calling syntax
- Environment
- Point to point communications
- Collective communications
- Synchronization





#### A note about MPI Implementations



- The MPI standard defines the functionalities and the API, i.e. what the C or FORTRAN calls should look like.
- The MPI standard does not define how the calls should be performed at the system level (algorithms, buffers, etc) or how the environment is set up (env variables, mpirun or mpiexec, libraries, etc). This is left to the implementation.
- There are various implementations (IntelMPI, OpenMPI, MPICH, HPMPI, etc) which have different performances, features and standards compliance.
- On some clusters you may choose which MPI to use, on other systems you have only the vendor-supplied version.





## My first program



#### Fortran

```
program first
  character(100) :: &
    & message="Hello"
```

```
write(6,FMT="(A)") message
```

stop
end program first

```
С
#include <stdio.h>
#include <stdlib.h>
int main(int argc, char *argv[])
{
    char message[100]="Hello";
    printf("%s\n",message);
    return 0;
```





# Compiling notes



To compile programs that make use of MPI library:

- mpif90/mpicc/mpiCC -o <executable> <file 1> <file 2> ... <file n>
- Where: <file n> program source files

<executable> - executable file

- To start parallel execution on one node only:
- mpirun -np <processor\_number> <executable> <exe\_params>
- To start parallel execution on many nodes:
- mpirun -np <processor\_number> -machinefile <node\_list\_file> \
   <executable> <exe\_params>





### My first program



Try to compile and run with MPI the example *first*, either in Fortran or in C.





### My first program



Try to compile and run with MPI the example *first*, either in Fortran or in C.

Well, the result is not much useful, but one thing is shown: every MPI process run the entire program code.

How then do we take advantage of parallel execution?







Fortran

```
program first_mpi
  include 'mpif.h'
  integer :: my_rank
  character(100) :: message="Hello from "
  integer :: ierr
 call MPI Init(ierr)
  call MPI_Comm_rank(MPI_COMM_WORLD, my_rank, ierr)
 write(6,FMT="(A,I3)") TRIM(message),my_rank
 call MPI Finalize(ierr)
```

stop
end program first\_mpi







#### С

```
#include "mpi.h"
#include <stdio.h>
#include <stdlib.h>
int main( int argc, char *argv[]) /* first_mpi */
{
    int my rank;
    char message[100]="Hello from ";
    int ierr;
    ierr = MPI_Init(&argc,&argv);
    ierr = MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);
    printf("%s %d\n",message,my_rank);
    MPI Finalize();
    return 0;
```







Try to compile and run the example *first\_mpi*, either in Fortran or in C.

The result is more interesting, and can suggest how the program might be parallelized.

Partitioning the data or program operations on the basis of the process id can lead to parallel execution.







#### Fortran - add the tags -stdin all to run this program

```
program greetings
    include 'mpif.h'
    integer :: my_rank, ierr
    character(100) :: message=", greetings from "
    character(100) :: name
   call MPI Init(ierr)
   call MPI Comm rank(MPI COMM WORLD, my rank, ierr)
  write(6,FMT="(A)") "What's your name?"
   read(5,"(A)") name
  write(6,FMT="(3A,I3)") "Hi ",TRIM(name),TRIM(message),my rank
   call MPI Finalize(ierr)
end program greetings
```





#### C - add the tags -stdin all to run this program

```
#include "mpi.h"
#include <stdio.h>
#include <stdlib.h>
int main( int argc, char *argv[]) { /* greetings */
    int my_rank, ierr;
    char name[100], message[100]=", greetings from ";
    MPI_Init(&argc,&argv);
    MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);
    printf("What's your name?\n");
```

```
scanf("%s",name);
printf("Hi %s %s %d\n",name,message,my_rank);
```

```
MPI_Finalize();
return 0;
```

}







Compile and run with MPI the example *greetings*, either in Fortran or in C.







Compile and run with MPI the example *greetings*, either in Fortran or in C.

Although with the flags '-stdin all' the stdin input is shared among the processes, the query is written many times.

Some things in a program should be carried out by one process only, but so how to share data?







#### Fortran

```
program greetings comm
    include 'mpif.h'
    integer :: my rank, np, sender, recipient, ierr
    integer :: status(MPI_STATUS_SIZE)
    character(100) :: message=", greetings from "
    character(100) :: name="
   call MPI Init(ierr)
   call MPI Comm rank(MPI COMM WORLD, my rank, ierr)
   call MPI Comm size(MPI COMM WORLD, np, ierr)
   sender = my_rank - 1; recipient = my_rank + 1
   if (my rank == 0) then
      write(6,FMT="(A)") "What's your name?"
      read(5,"(A)") name
      ln = len trim(name)
   endif
```







#### Fortran

```
if ( sender >= 0 ) then
      tag = 1
      call MPI Recv(name, 100, MPI CHARACTER, sender, tag, &
    &
                                     MPI COMM WORLD, status, ierr)
   endif
  if ( recipient < np ) then
      tag = 1
      call MPI_Send(name, 100, MPI_CHARACTER, recipient, tag, &
    &
                                              MPI COMM WORLD, ierr)
   endif
   write(6,FMT="(3A,I3)") "Hi ",TRIM(name),TRIM(message),my_rank
   call MPI Finalize(ierr)
end program greetings comm
```





```
С
```

```
#include "mpi.h"
int main( int argc, char *argv[]) /* greetings_comm */
{
    int my_rank, np, sender, recipient, tag, ln, ierr;
    char name[100], message[100]=", greetings from ";
    MPI Status status;
    ierr = MPI Init(&argc,&argv);
    ierr = MPI Comm rank(MPI COMM WORLD,&my rank);
    ierr = MPI Comm size(MPI COMM WORLD,&np);
    sender = my_rank - 1; recipient = my_rank + 1;
    if ( my rank == 0 ) {
      printf("What's your name?\n");
      scanf("%s",name);
      ln = strlen(name);
```





С

#### My first MPI program









```
C
. . .
if ( recipient < np ) {
   tag = 0;</pre>
```

```
MPI_Finalize();
```

```
return 0;
```

}







Compile and run with MPI the example *greetings\_comm*, either in Fortran or in C.

Now input data is carried out by one process only. Process 0 is often used as a 'master process' to perform I/O and to manage data and work distribution.





#### Header files



All Subprogram that contains calls to MPI subroutine must include the MPI header file

**C**:

#include <mpi.h>

Fortran:

include 'mpif.h'

Fortran 90:

USE MPI

Fortran 08 (MPI-3):

USE MPI\_F08

The header file contains definitions of MPI constants, MPI types and functions

FORTRAN note:

The FORTRAN include and module forms are *not equivalent*: the module can also do type checking. Some compilers gave problems with the module but it is now highly recommended to use the module, particularly for FORTRAN 2008 (most rigorous type-checking)





### MPI syntax



Every Fortran subroutine in the MPI library returns, as the last argument, an INTEGER type error code.

Every MPI C function returns an int value representing the error code.

Whenever a MPI function has exited without errors, the error code should have the value MPI\_SUCCESS.

The value of MPI\_SUCCESS is usually 0.







```
include "mpif.h"
integer :: ierror
....
call MPI_send (..., ierror)
if (ierror .ne. MPI_SUCCESS) then
    write (*,*)"SEND operation failed"
    stop 777
end if
```

**Error code values different from MPI\_SUCCESS are implementation dependent.** 





# MPI syntax

#### Generally speaking, MPI functions have the following prototype:



| call | MPI_name | ( parameter,, ier | ror ) fortran |
|------|----------|-------------------|---------------|
| rt = | MPI_Name | (parameter,)      | C/C++         |

To initialize the MPI environment the MPI\_Init function must be called:

| call | MPI_ | INIT | ( | ierror ) | fortran |
|------|------|------|---|----------|---------|
|      |      |      |   |          |         |

| rt | = | MPI | Init | (int | *argc, | char | ***argv) |  |
|----|---|-----|------|------|--------|------|----------|--|
|    |   | -   |      |      |        | -    |          |  |

On ending parallel computations the MPI\_Finalize function should be called, otherwise processes could remain alive on local or remote computing units:

| call MPI_FINALIZE             | ( ierror ) | fortran       |
|-------------------------------|------------|---------------|
| <pre>rt = MPI_Finalize(</pre> | );         | <i>C/C</i> ++ |



C/C++



### Groups of MPI processes



A group is an ordered set of processes.

All MPI processes are organized in groups; each process belongs to one or more groups.

Processes are sequentially ordered in an unambiguous way. In each group each process has its own identifying number or **rank**.





# Groups of MPI processes



Process identifying numbers are integer numbers in the range **0** – *N-1* where *N* is the group size.

On initializing MPI a default group is created containing all the processes: this group is associated to the default communicator **MPI\_COMM\_WORLD**.

If the processes are not many the default group is sufficient. Otherwise it may be convenient to create new groups defined as subsets, either disjoined or not, of the default group or formerly created groups.





#### MPI processes



The following function returns the extension of the group associated to a communicator, i.e. the number of processes belonging to the group:



Where: comm = communicator handle size = number of processes ierr = error code





#### MPI processes



#### The following function returns the rank of the calling process:



#### Where: comm = communicator handle rank = process rank (a number in the range 0 - size-1) ierr = error code



#### Communicator Size and Process Rank / 1

How many processes are contained within a communicator?

SIZE = 8  $P_0$   $P_1$   $P_2$   $P_3$   $P_4$   $P_5$   $P_6$   $P_7$ RANK = 2

size is the number of processes associated to the communicator

rank is the index of the process within a group associated to a communicator (rank = 0,1,...,N-1). The rank is used to identify the source and destination process in a communication


# Communication domains (communicators)



On MPI initialization the default communicator MPI\_COMM\_WORLD is generated. It allows all the activated processes to communicate each other.

Sometimes it is necessary to generate new communicators either by duplicating existing ones, or by associating to newly created groups of processes.





# Communication domains (communicators)



A new communicator should be created every time a new group of processes is generated. A new group is always generated by choosing processes from a wider already existing group.

The creation of a group of processes is a local operation, it is realized at process level. On the contrary, the creation of a new communicator is a global operation and involves (hidden) communications among all the processes of the group.







Point to point communications realize connections between two processes.

From the programmer point of view communications depend on a *communicator* and are identified by a *handle* and a *tag*.

- The communicator defines the processes that can be involved.
- The tag is used to differentiate messages.

The handle may be useful whenever it is necessary to control the completion of the communicating operation.

A communication is said to be locally completed if the process has terminated the operation.

A communication is said to be globally completed when all the involved processes have terminated the operation.



#### **MPI Programming Model**







Communication calls may be **blocking** or **nonblocking**.

The functions relevant to **blocking calls** do not return control unless data in the message can be safely modified without changing the message data.

These functions (MPI\_Send, MPI\_Recv) are **very reliable** but the program execution may be slowed down because the processes are blocked until the message has been received.

The functions relevant to **nonblocking calls** are faster but **care must be taken** that the sent data are actually received and are not corrupted.

Therefore data sent by nonblocking calls can not be modified unless it is safe to do so. The functions MPI\_Wait or MPI\_Test should be called for checking.





### The Message



- Data is exchanged in the buffer, an array of count elements of some particular MPI data type
- One argument that usually must be given to MPI routines is the *type* of the data being passed.
- This allows MPI programs to run automatically in heterogeneous environments
- C types are different from Fortran types.

Messages are identified by their envelopes. A message could be exchanged only if the sender and receiver specify the correct envelope

#### Message Structure

|        | body        |              |     |        |       |          |      |
|--------|-------------|--------------|-----|--------|-------|----------|------|
| source | destination | communicator | tag | buffer | count | datatype | NECA |



### Messages



The receiving process may receive messages in random order if they are sent by different processes.

- Care must be taken to insure the correct receiving order of the messages.
- The following rules are always true:
- Messages with the same tag sent by the same process will be received in the sending sequence.
- Messages sent by nonblocking calls will be received in the sending order. This is important because otherwise large messages could be received after smaller ones sent later.





### Basic data types



MPI messages are sent as arrays of data *homogeneous in type*. In sending and receiving calls only one data type can and shall be specified. The allowed data types may be either *basic* or *derived*. Derived types shall be explicitly defined in the program and explicitly registered in the MPI system.

| Basic types in Fortran | Basic types in C   |
|------------------------|--------------------|
| MPI_INTEGER            | MPI_CHAR           |
| MPI_REAL               | MPI_SHORT          |
| MPI_DOUBLE_PRECISION   | MPI_INT            |
| MPI_COMPLEX            | MPI_LONG           |
| MPI_DOUBLE_COMPLEX     | MPI_UNSIGNED_CHAR  |
| MPI_LOGICAL            | MPI_UNSIGNED_SHORT |
| MPI_CHARACTER          | MPI_UNSIGNED       |
| MPI_BYTE               | MPI_UNSIGNED_LONG  |
| MPI_PACKED             | MPI_FLOAT          |
|                        | MPI_DOUBLE         |
|                        | MPI_LONG_DOUBLE    |
|                        | MPI_BYTE           |
|                        | MPI_PACKED         |





### Sending calls

#### The prototype of a sending function is:



fortran

C/C++

ierror = MPI\_Send( void \*buf, int count, MPI\_Datatype
datatype,int dest, int tag, MPI\_Comm comm);

#### where:

buf = array of data to be sent count = how many elements are sent datatype = type of data to be sent dest = rank of the receiving process tag = identifier of the message comm = communicator connecting sending and receiving processes ierror = error code

The starting position of the array to be sent must be passed to the sending call.



### Receiving calls



The prototype of a receiving call is:

| <pre>integer :: source, status(MPI_STATUS_SIZE)</pre> |         |  |  |
|---|---------|--|--|
| call MPI_recv( buf, count, datatype, source, &        |         |  |  |
| & tag, comm, status, ierror )                         | fortran |  |  |

#### where:

- source = rank of the sending process
- status = message info
- ierror = error code





#### Send and Receive - FORTRAN

PROGRAM send recv

-

USE mpi implicit none

INTEGER ierr, myid, nproc
INTEGER status(MPI\_STATUS\_SIZE)
REAL A(2)

CALL MPI\_INIT(ierr) CALL MPI\_COMM\_SIZE(MPI\_COMM\_WORLD, nproc, ierr) CALL MPI COMM RANK(MPI COMM WORLD, myid, ierr)

```
IF( myid .EQ. 0 ) THEN
A(1) = 3.0
A(2) = 5.0
CALL MPI_SEND(A, 2, MPI_REAL, 1, 10, MPI_COMM_WORLD, ierr)
ELSE IF( myid .EQ. 1 ) THEN
CALL MPI_RECV(A, 2, MPI_REAL, 0, 10, MPI_COMM_WORLD, status, ierr)
WRITE(6,*) myid,': a(1)=',a(1),' a(2)=',a(2)
END IF
```

CALL MPI FINALIZE (ierr)

END





#### Send and Receive - C

```
#include <stdio.h>
#include <mpi.h>
void main (int argc, char * argv[])
{
  int err, nproc, myid;
 MPI Status status;
  float a[2];
  err = MPI Init(&argc, &argv);
  err = MPI Comm size(MPI COMM WORLD, &nproc);
  err = MPI Comm rank (MPI COMM WORLD, &myid);
  if( myid == 0 ) {
    a[0] = 3.0, a[1] = 5.0;
   MPI Send(a, 2, MPI FLOAT, 1, 10, MPI COMM WORLD);
  } else if( myid == 1 ) {
    MPI Recv(a, 2, MPI FLOAT, 0, 10, MPI COMM WORLD, &status);
   printf("%d: a[0]=%f a[1]=%f\n", myid, a[0], a[1]);
  }
  err = MPI Finalize();
}
```









There are 4 modes of sending data in MPI:

- Buffered Data are copied in a memory area explicitly allocated in the program. Either blocking or nonblocking calls are available, but non blocking calls may lead to problems if the buffer is not large enough to keep all the messages waiting to be sent.
- Synchronous Send operation is considered completed only if the receiving operation has been started, i.e. the receiving processes have provided the memory space needed to copy the sent data. Therefore memory allocation is not an issue because memory buffers are always made available by the sender and the receiver. The problem is that if sending and receiving processes are not synchronized the execution may be slowed down.





- Standard The operation is automatically managed by the MPI system. If buffered communications are used, memory space is automatically allocated. Again this may lead to memory problems if data sent are too large.
- Ready This mode should be used with care because when the sender starts operation the receiving process must be ready to receive the message. If this is not the case, errors and undefined results are produced. However, if synchronization is granted, this may be the fastest communication mode.







Receiving calls may be blocking or nonblocking only and do not differentiate sending modes.

#### Summary table

| SEND        | Blocking  | Nonblocking |  |
|-------------|-----------|-------------|--|
| Standard    | MPI_Send  | MPI_Isend   |  |
| Ready       | MPI_Rsend | MPI_Irsend  |  |
| Synchronous | MPI_Ssend | MPI_Issend  |  |
| Buffered    | MPI_Bsend | MPI_lbsend  |  |

| RECEIVE  | Blocking | Nonblocking |
|----------|----------|-------------|
| Standard | MPI_Recv | MPI_Irecv   |





### Non Blocking communications



- Non-blocking send and receive routines will return almost immediately. They do not wait for any communication events to complete
- Non-blocking operations simply "request" the MPI library to perform the operation when it is possible. The user can not predict when that will happen.
- It is unsafe to modify the application buffer until you know for a fact that the requested non-blocking operation was actually performed by the library. There are "wait" routines used to do this.
- Non-blocking communications are primarily used to overlap computation with communication.





#### Non-Blocking Send and Receive

#### **C**:

- int MPI\_Isend(void \*buf, int count, MPI\_Datatype type, int dest, int tag, MPI Comm comm, MPI Request \*req);
- int MPI\_Irecv (void \*buf, int count, MPI\_Datatype type, int source, int tag, MPI\_Comm comm, MPI\_Request \*req);





#### Non-Blocking Send and Receive



#### FORTRAN:

MPI\_ISEND(buf, count, type, dest, tag, comm, req, ierr)
MPI\_IRECV(buf, count, type, source, tag, comm, req, ierr)

| buf   | array of type | type (see table).                               |
|-------|---------------|---|
| count | (INTEGER)     | number of element of <b>buf</b> to be sent      |
| type  | (INTEGER)     | MPI type of <b>buf</b>                          |
| dest  | (INTEGER)     | rank of the destination process                 |
| tag   | (INTEGER)     | number identifying the message                  |
| comm  | (INTEGER)     | communicator of the sender and receiver         |
| req   | (INTEGER)     | output, identifier of the communications handle |
| ierr  | (INTEGER)     | output, error code (if ierr=0 no error occurs   |







The following function stops execution until the data have been safely sent or received:

| SUBROUTINE | MPI_WAIT(REQ,    | STATUS,   | IERR)              |         |
|------------|------------------|-----------|--------------------|---------|
| INTEGER,   | , INTENT (INOUT) | ) :: REQ  |                    | fortran |
| INTEGER,   | , INTENT (OUT)   | :: STATUS | G(MPI_STATUS_SIZE) | jortrun |
| INTEGER,   | , INTENT (OUT)   | :: IERR   |                    |         |
|            |                  |           |                    |         |

int MPI\_Wait(MPI\_Request \*req, MPI\_Status \*status) C/C++

```
Where:
req = iSend or iRecv request
status = communication status
ierr = error code
```

If req=MPI\_REQUEST\_NULL nothing is done.







The following function checks if data have been safely sent or received:

| SUBROUTINE N | MPI_TEST(REQ, | FI   | LAG,  | STATUS   | , IERROR | ())   |         |
|--------------|---------------|------|-------|----------|----------|-------|---------|
| INTEGER,     | INTENT (INOUT | ') : | :: RI | ΞQ       |          |       |         |
| LOGICAL,     | INTENT (OUT)  | ::   | FLA(  | J<br>J   |          |       | fortran |
| INTEGER,     | INTENT (OUT)  | ::   | STA   | TUS(MPI_ | _STATUS_ | SIZE) |         |
| INTEGER,     | INTENT (OUT)  | ::   | IERI  |          |          |       |         |

#### C/C++

#### Where:

req = iSend or iRecv request
flag = true if communication has been completed
status = communication status
ierr = error code





# Notes on communications



- A blocking receiving call returns only when the receiving buffer has been completed.
- The nonblocking call MPI\_Irecv does not return a message status but a message handle MPI\_Request \*request. It can be later used by the function MPI\_Test to check for communication completion or by the function MPI\_Wait to wait for completion.
- Message tags and sending processes may be wildcarded using the constant values MPI\_ANY\_TAG and MPI\_ANY\_SOURCE respectively. These may be used to enhance parallel efficiency.







# Notes on communications

- On exiting the status array will contain useful informations. The array size is MPI\_STATUS\_SIZE and two of the most used infos are:
  - status (MPI\_SOURCE) = rank of the sender. It may be particularly useful when the sender id is MPI ANY SOURCE.
  - status (MPI\_TAG) = message tag. It may be
    particularly useful when message tag is MPI\_ANY\_TAG.





#### An example

```
integer, dimension (2000) :: box
integer :: error_code, msg_tag=5432, sender=2
integer, dimension (MPI_STATUS_SIZE) :: status
call MPI_recv (box(1), 1500, mpi_integer, sender, &
      & msg tag, MPI COMM WORLD, status, error code)
call MPI_recv (box(1501), 500, mpi_integer, &
      & MPI_ANY_SOURCE, MPI_ANY_TAG, MPI_COMM_WORLD, &
      & status, error code)
```

In this example the first 1500 elements of the array box are received from the process with rank 2; the remaining elements are received from whichever the sending process is, without even specifyingCINECA the message tag.



#### DEADLOCK



A Deadlock or a Race condition occurs when 2 (or more) processes are blocked and each is waiting for the other to make progress.







#### Simple DEADLOCK

PROGRAM deadlock USE mpi implicit none INTEGER ierr, myid, nproc INTEGER status (MPI STATUS SIZE) REAL A(2), B(2)CALL MPI INIT(ierr) CALL MPI COMM SIZE (MPI COMM WORLD, nproc, ierr) CALL MPI COMM RANK (MPI COMM WORLD, myid, ierr) IF(myid .EQ. 0) THEN a(1) = 2.0a(2) = 4.0CALL MPI RECV(b, 2, MPI REAL, 1, 11, MPI COMM WORLD, status, ierr) CALL MPI SEND(a, 2, MPI REAL, 1, 10, MPI COMM WORLD, ierr) ELSE IF ( myid .EQ. 1 ) THEN a(1) = 3.0a(2) = 5.0CALL MPI RECV(b, 2, MPI REAL, 0, 10, MPI COMM WORLD, status, ierr) CALL MPI SEND(a, 2, MPI REAL, 0, 11, MPI COMM WORLD, ierr) END IF WRITE(6,\*) myid, ': b(1)=', b(1), ' b(2)=', b(2) CALL MPI FINALIZE(ierr) END







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### Avoiding DEADLOCK

PROGRAM avoid lock USE mpi Implicit none INTEGER ierr, myid, nproc INTEGER status (MPI STATUS SIZE) REAL A(2), B(2)CALL MPI INIT(ierr) CALL MPI COMM SIZE (MPI COMM WORLD, nproc, ierr) CALL MPI COMM RANK (MPI COMM WORLD, myid, ierr) IF( myid .EQ. 0 ) THEN a(1) = 2.0a(2) = 4.0CALL MPI RECV(b, 2, MPI REAL, 1, 11, MPI COMM WORLD, status, ierr) CALL MPI SEND(a, 2, MPI REAL, 1, 10, MPI COMM WORLD, ierr) ELSE IF ( myid .EQ. 1 ) THEN a(1) = 3.0a(2) = 5.0CALL MPI SEND(a, 2, MPI REAL, 0, 11, MPI COMM WORLD, ierr) CALL MPI RECV(b, 2, MPI REAL, 0, 10, MPI COMM WORLD, status, ierr) END IF WRITE(6,\*) myid, ': b(1)=', b(1), ' b(2)=', b(2) CALL MPI FINALIZE(ierr) END









Sending and receiving may be accomplished by one call only:

| type :: SENDBUF, RECVBUF                                  |         |
|---|---------|
| integer :: SENDCOUNT, SENDTYPE, DEST, SENDTAG, RECVCOUNT, | &       |
| & RECVTYPE, SOURCE, RECVTAG, COMM, STATUS, IERROR         |         |
| CALL MOT SENDRECU ( SENDRIF SENDCOINT SENDTYDE S          |         |
| & DEST, SENDTAG, RECVBUF, RECVCOUNT, RECVTYPE, &          |         |
| & SOURCE, RECVTAG, COMM, STATUS, IERROR )                 |         |
|   | fortran |

ierror = MPI\_Sendrecv (void \*sendbuf, int sendcount, MPI\_Datatype sendtype, int dest, int sendtag, void \*recvbuf, int recvcount, MPI\_Datatype recvtype, int source, int recvtag, MPI\_Comm comm, MPI\_Status \*status) C/C++





#### where:

- SENDBUF = data buffer to be sent
- SENDCOUNT = how many sent elements
- SENDTYPE = sent data type
- DEST = rank of the receiving process
- SENDTAG = sent message tag
- RECVBUF = receiving data buffer
- RECVCOUNT = how many receiving elements
- RECVTYPE = receiving data type
- SOURCE = rank of the sending process
- RECVTAG = receiving message tag
- COMM = communicator
- STATUS = message info
- IERROR = error code





}

#### SendRecv example



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

```
int main(int argc, char *argv[])
{
    int myid, numprocs, left, right,i;
    int buffer[1], buffer2[1];
    MPI_Status status;
```

MPI Comm size (MPI COMM WORLD, &numprocs);

MPI Comm rank (MPI COMM WORLD, &myid);

MPI Init(&argc,&argv);



Useful for cyclic communication patterns

```
right = (myid + 1) % numprocs;
left = myid - 1;
if (left < 0)
    left = numprocs - 1;
buffer[0]=myid;
MPI_Sendrecv(buffer, 1, MPI_INT, right, 123, buffer2, 1, MPI_INT, left, 123,
MPI_COMM_WORLD, &status);
printf("I am processor rank %d and I received the rank of processor
%d\n",myid,buffer2[0]);
MPI_Finalize();
```







The following function returns how many elements have been received. The number of bytes received is dependent on the received data type.

call MPI\_get\_count (status, datatype, count, ierr) fortran

| ierror = MPI_ | get_count (MPI | _Status *status, |
|---------------|----------------|------------------|
| MPI_Datatype  | datatype,      | int *count )     |



C/C++





Whenever is necessary to control completion of a lot of communication operations, the following functions may be used instead.

**MPI\_Waitall** does block execution until the operations in LIST\_REQUEST are all completed.

**MPI\_Testall** checks if all the operations in LIST\_REQUEST are completed (FLAG=.TRUE.).

| ierr = MPI Waitall (int count, MPI Request  | C/C++ |
|---|-------|
| list_requests[], MPI_Status list_status[] ) |       |
| ierr = MPI_Testall (int count, MPI_Request  |       |
| list_requests[], int *flag, MPI_Status      |       |
| list_status[])                              |       |



The function MPI\_WAITANY blocks execution until at least one of the operations in LIST REQUEST is locally completed.

The function MPI\_TESTANY checks if at least one of the operations in LIST\_REQUEST is locally completed. On output INDEX is the position in LIST\_REQUESTS of the completed operation and RETURN\_STATUS contains infos about it.

| <pre>call MPI_waitany(count, list_requests, in<br/>return_status, ierr)</pre> | dex, <i>fortran</i> |
|---|---------------------|
| <pre>call MPI_testany(count, list_requests, in<br/>return_status, ierr)</pre> | dex, flag,          |







#### **Exercises**



http://www.hpc.cineca.it/content/training-mpi

Here you will find some exercises of gradual difficulty, with hints about the functions/routines to be used, solutions in C and Fortran and Q/A in some cases

BE SMART! Exercises are for you to learn. Peeking at solutions shouldn't be the easy way to solve the exercises, but rather a way to compare your ideas with the ones provided by the teachers. Your solution may be better than ours!

For Point-to-point communications, you can do exercises from 1 to 6

When programming with MPI, remember to...think in parallel





# Collective communications

Communications is a very important issue in MPI programs, therefore their optimization is a mandatory effort.

In many cases communications involve a lot of processors and realizing them by point-to-point communications become inefficient and an error prone exertion.

For this reason MPI library contains functions optimized to accomplish collective communications. Therefore using collective communications in such cases is much more effective (and easier) than using point-to-point communications.







# Collective communications

- Collective communications do not need tags for messages.
- All collective communications are blocking.
- Collective communication calls carry out both sending and receiving operations.
- The calls to collective communication functions should be issued by all the processes of a given communicator.





# Collective communications



Collective communications may be of two types: **data transfer** and **global computations**.

Data transfer functions can be:

•broadcast - data are shared among all the processes

•gather - data are collected from every process

•scatter - data are distributed to the processes

Global computation functions can be:
•reduction - the result is a computed value
•scanning – partial reduction results




```
subroutine GetData (a, b, n, my rank, num procs)
! Point-to-point version
real :: a, b
integer :: n, p, my rank, num procs, ierr, tag a, tag b, tag n
include 'mpif.h'
tag a=1; tag b=2; tag n=3;
if (my_rank == 0) then
  print *, 'Enter a, b, and n'
  read *, a, b, n
  do p=1, num procs-1
   call MPI_Send(a, 1, MPI_REAL, p, tag_a, MPI_COMM_WORLD, ierr)
    call MPI_Send(b, 1, MPI_REAL, p, tag_b, MPI_COMM_WORLD, ierr)
    call MPI_Send(n, 1, MPI_INTEGER, p, tag_n, MPI_COMM_WORLD, ierr)
```

enddo



```
else
  call MPI_Recv(a, 1, MPI_REAL, 0, tag_a, MPI_COMM_WORLD, &
    status, ierr)
    call MPI_Recv(b, 1, MPI_REAL, 0, tag_b, MPI_COMM_WORLD, &
    status, ierr)
    call MPI_Recv(n, 1, MPI_INTEGER, 0, tag_n, MPI_COMM_WORLD, &
    status, ierr)
endif
return
end subroutine GetData
```

6 x (num\_procs-1) calls issued for sending 3 scalars







The following function may be used to send the same data to all the processes belonging to a communicator. A loop performing point-to-point communications to all the processes gives the same results but is much less efficient.

```
type :: array
integer :: count, datatype, root, comm, ierror
call MPI BCAST( array, count, datatype, root, comm, ierror )
```

```
where: array = data to be sent
    count = how many elements
    datatype = data type of the elements
    root = process owing data to be sent
    comm = communicator
    ierror = error code
```





```
subroutine GetData (a, b, n, my_rank)
! Collective version
real :: a, b
integer :: n, my_rank, ierr
include 'mpif.h'

if (my_rank == 0) then
    print *, 'Enter a, b, and n'
    read *, a, b, n
endif
```

```
call MPI_BCAST (a, 1, MPI_REAL , 0, MPI_COMM_WORLD, ierr )
call MPI_BCAST (b, 1, MPI_REAL , 0, MPI_COMM_WORLD, ierr )
call MPI_BCAST (n, 1, MPI_INTEGER, 0, MPI_COMM_WORLD, ierr )
```

end subroutine GetData







**Gather**: Every process in the communicator send the content of send\_buf to the root process that receives data and orders them in the recv\_buf array according to the rank of the sending processes.





```
subroutine GatherData (my a, vector a, my rank, num procs)
! Point-to-point version
integer :: p, my_rank, num_procs, ierr, tag_a
real :: my_a, vector_a(num_procs)
include 'mpif.h'
integer :: status(MPI STATUS SIZE)
tag a=1
if (my rank == 0) then
 vector_a(1)=my_a
  do p=1, num procs-1
    call MPI Recv(vector a(p+1), 1, MPI REAL, p, tag a, &
&
    MPI_COMM_WORLD, status, ierr)
  enddo
else
  call MPI_Send(my_a, 1, MPI_REAL, 0, tag_a, MPI_COMM_WORLD, iere)
endif; end subroutine GatherData
```





The following function may be used whenever data dispersed among the processes have to be collected in one ROOT process

where:

SEND COUNT - how many elements are sent

RECV COUNT - how many elements have to be received





end subroutine GatherData







The following function may be used to collect data dispersed among the processes if each process owns a different number of elements.

In the function variants with an ending "v" the array RECV\_COUNT (:) specify how many elements are stored in each process.

The array DISP(:) specifies the position in the receiving buffer where data coming from i<sup>th</sup> process must be copied. Positions start from 0 even in Fortran.

call MPI\_Gatherv ( SEND\_BUF, SEND\_COUNT, SEND\_TYPE, RECV\_BUF, & fortran
 & RECV COUNT, DISP, RECV TYPE, ROOT, COMM, IERROR )

ierro = MPI\_Gatherv ( void \*send\_buf, int send\_count, MPI\_Datatype send\_type, void \*recv\_buf, int \*recv\_count, int \*disp, MPI\_Datatype recv\_type, int root, MPI\_Comm comm )







Gathering a dispersed vector when its portions do not have a fixed length is easier (and faster) using MPI\_Gatherv.

Of course the length of each portion of the dispersed vector and the position in the global vector should still be known by the gathering process.

```
subroutine GatherVdata (my_a, l_a, vector_a, l_v, pos, num_proc)
! collective version
integer :: 1 a, 1 v
integer :: p, num_proc, ierr
real :: my_a(l_a), vector_a(l_v)
integer :: pos(num_proc), n_a(num_proc)
include "mpif.h"
```





```
! A vector with the length of each portion is needed
do p = 0, num_proc-2
    n_a(p+1) = pos(p+2)-pos(p+1)
enddo
n_a(num_proc) = 1_v-pos(num_proc)+1
call MPI_Gatherv ( my_a, 1_a, MPI_REAL, vector_a, &
    & n_a, pos, MPI_REAL, 0, MPI_COMM_WORLD, ierr )
```

end subroutine GatherVdata

Remark: the vector pos(:) in this code version must contain the positions of each my\_a in vector\_a(:) beginning from 0







Scatter: the root process disperses the content of send\_buf array to the other processes of the communicator group.

Data are scattered according to the order of the processes.







Dispersing a vector from one process to the others requires at least (num\_proc - 1) \* 2 calls.

```
subroutine ScatterData (vector_a, l_v, a, l_a, my_rank, num_proc)
! Point to point version
    integer :: l_v, l_a, my_rank, num_proc, tag_a, p, ierr
    real :: vector_a(l_v), a(l_a)
    include "mpif.h"
    integer :: status(MPI_STATUS_SIZE)
```





```
tag a=1
  if (my_rank == 0) then
    do p = 1, num_proc-1
      call MPI Send(vector a(l a*p+1), l a, MPI REAL, p, tag a, &
&
                     MPI COMM WORLD, ierr)
    enddo
    a(1:1 a) = vector a(1:1 a)
  else
    call MPI_Recv(a, l_a, MPI_REAL, 0, tag_a, &
&
                    MPI COMM WORLD, status, ierr)
   endif
```

end subroutine ScatterData











```
subroutine ScatterData (vector_a, l_v, a, l_a)
! Collective version
    integer :: l_v, l_a
    real :: vector_a(l_v), a(l_a)
    integer :: ierr
    include "mpif.h"
    call MPI_Scatter ( vector_a, l_a, MPI_REAL, &
```

```
&
```

```
a, l_a, MPI_REAL, 0, MPI_COMM_WORLD, ierr )
```

end subroutine ScatterData







Allgather: Every process in the communicator send the content of send\_buf to all the other processes that receive data and order them in the recv\_buf array according to the rank of the sender.







type :: SEND\_BUF(\*), RECV\_BUF(\*) fortran
integer :: SEND\_COUNT, SEND\_TYPE, RECV\_COUNT, RECV\_TYPE,
COMM, IERROR

call MPI\_Allgather ( SEND\_BUF, SEND\_COUNT, SEND\_TYPE, RECV BUF, RECV COUNT, RECV TYPE, COMM, IERROR )

```
ierror = MPI_Allgather ( void *send_buf, int send_count, C/C++
MPI_Datatype send_type,
void *recv_buf, int recv_count, MPI_Datatype recv_type,
MPI_Comm comm )
```

The above function may be used to collect data from all the processes to all the processes. It is equivalent to a sequence of calls to MPI\_Gather in which each call identifies a different process as root.





Collective communications include global computations, of a reduction type.

The result of the computations may be:

- stored in one process only
- broadcasted to all the processes
- scattered to all the processes

Three functions are available:

- MPI\_Reduce
- MPI\_Allreduce
- MPI\_Reduce\_scatter







In the following example the quadrature of a function is computed between two extremes.

```
program integral
  Point to point version
L
  Domain decomposition and computation
Į.
   x intrvl = (x1-x0)/num procs
  my x0 = my rank*x intrvl; my x1 = my x0+x intrvl
  my_n = 0; x = my_x0; my_s = 0.0
   do while ( x < my_x1 )</pre>
      my s = my s + f(x)
      my n = my n + 1
      x = x + dx
   enddo
```







```
! Gather results and sum them up
  tag s=10; tag n=20
   if ( my_rank == 0 ) then
      s = my s; n = my n
      do p = 1, num_procs-1
         call MPI_Recv(my_s, 1, MPI_DOUBLE_PRECISION, p, tag_s, &
&
                MPI COMM WORLD, status, ierr); s = s + my s
      enddo
  else
      call MPI Send(my s, 1, MPI DOUBLE PRECISION, 0, tag s, &
&
                MPI COMM WORLD, ierr)
   endif
```

if (my\_rank==0) write(6,\*)"After ",n," steps result=",s/dble(n)
end program integral





The following function may be used to compute reduction operations such as sum, product, logical, min/max and others. It must be called by all the processes of the communicator comm. The result is stored in the process identified as root. If count>1 then send\_buf and recv\_buf are arrays and the computation is executed element by element.







send\_buf = data to be used for computation, operands
recv\_buf = result buffer (received by root process only)
count = buffer size

- datatype = type of the elements
- op = reduction operation (es.: MPI\_SUM, MPI\_MAX, ...)
- root = which process stores the results

```
comm = communicator
```

```
ierror = error code
```

As an example, if count=3 and  $op=MPI\_SUM$ , then: Recv\_buf(0) = send\_buf<sub>proc0</sub>(0) + ... + send\_buf<sub>procN-1</sub>(0) Recv\_buf(1) = send\_buf<sub>proc0</sub>(1) + ... + send\_buf<sub>procN-1</sub>(1) Recv\_buf(2) = send\_buf<sub>proc0</sub>(2) + ... + send\_buf<sub>procN-1</sub>(2)







#### The available operations are:

| MPI_MAX    | maximum                    |
|------------|----------------------------|
| MPI_MIN    | minimum                    |
| MPI_SUM    | sum                        |
| MPI_PROD   | product                    |
| MPI_LAND   | logical AND                |
| MPI_BAND   | bit-wise AND               |
| MPI_LOR    | logical OR                 |
| MPI_BOR    | bit-wise OR                |
| MPI_LXOR   | logical XOR                |
| MPI_BXOR   | bit-wise XOR               |
| MPI_MAXLOC | maximum value and location |
| MPI_MINLOC | minimum value and location |







program integral\_c

! Collective version

```
Į.
   Domain decomposition and computation
   x intrvl = (x1-x0)/num procs
   my x0 = my rank*x intrvl; my x1 = my x0+x intrvl
   my_n = 0; x = my_x0; my_s = 0.0
   do while (x < my x1)
      my s = my s + f(x)
      my n = my n + 1
      x = x + dx
   enddo
   call MPI_REDUCE ( my_s, s, 1, MPI_DOUBLE_PRECISION, &
&
                           MPI SUM, 0, MPI COMM WORLD, ierr)
   if (my rank==0) write(6,*)"After ",n," steps result=",s/dble(n)
end program integral c
```







| <pre>type :: OPERAND(*), RESULT(*)</pre>                 | fortran |
|--|---------|
| integer :: COUNT, DATATYPE, OP ,COMM, IERROR             |         |
| call MPI_AllReduce ( OPERAND, RESULT, COUNT, DATATYPE, O | P,      |
| COMM, LERROR )   |         |

This function differs from the previous one because the operation result is stored in all the processes of the communicator comm.

Mpi\_AllReduce = MPI\_Reduce + MPI\_Bcast







```
<type>, IN :: SENDBUF(*)
<type>, OUT :: RECVBUF(*)
INTEGER RECVCOUNTS(*), DATATYPE, OP, COMM, IERROR
call MPI_REDUCE_SCATTER (SENDBUF, RECVBUF, RECVCOUNTS,
```

DATATYPE, OP, COMM, IERROR)

```
fortran
```

Using the function MPI\_Reduce\_scatter, the reduction result is first computed element by element, then the obtained vector is split into disjoined segments and dispersed to all the processes. The array recvcounts(:) is used to specify how many elements each process will store.



## Process synchronization



Whenever it is necessary that all the processes come to a determined point at the same time, then synchronization barriers must be used. To avoid heavy loss of performances barriers should be used with care and only if it is unavoidable, i.e. the implemented algorithm requires it.

The following function can be used to define a synchronising point:

Where: comm- communicator whose processes must be synchronizedierror- error code.

This function returns only after all the processes have called it.





## Performance evaluation



It is often useful to measure computing time of portions of the program. The following functions may be used. Both functions return a double floating point value.



| double t1, dt               |   | C/C++ |
|-----------------------------|---|-------|
| t1 = MPI_Wtime()            | <pre>/* elapsed time in seconds */</pre>    | 0,011 |
| <pre>dt = MPI_Wtick()</pre> | <pre>/* time resolution in seconds */</pre> |       |

Time values are process dependent unless MPI\_WTIME\_IS\_GLOBAL is defined and its value is .TRUE..







http://www.hpc.cineca.it/content/training-mpi

After having learned about collective communications, you have «unlocked» exercises from 7 to 9

If you have not finished the point-to-point yet, you are free to keep working on them. Teacher's suggestion is to try to do some collective exercises in any case, just to fix the concepts.

When programming with MPI, remember to...think in parallel!

