Foundations of High Performance Computing

Lecture 05: Message Passing programming Using MPI

"Foundation of HPC" course

DATA SCIENCE & SCIENTIFIC COMPUTING

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Agenda

- Recap:
  - Message Passing Paradigm
- Basic on Message Passing Interface

- Point-to-Points operation
- Collective operations

2 main parallel paradigms

DIDACTED BY MEMORY ORGANIZATION

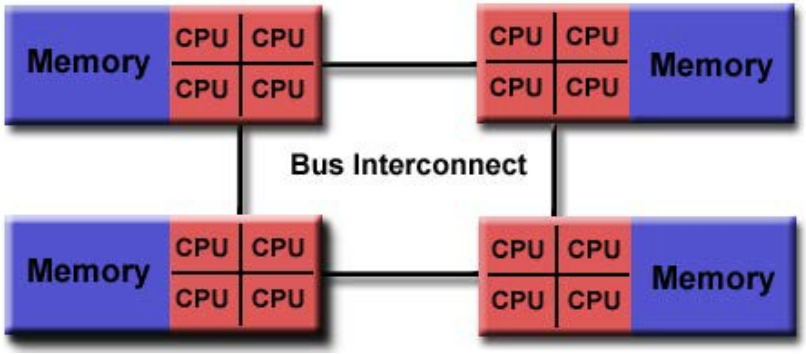
shared memory

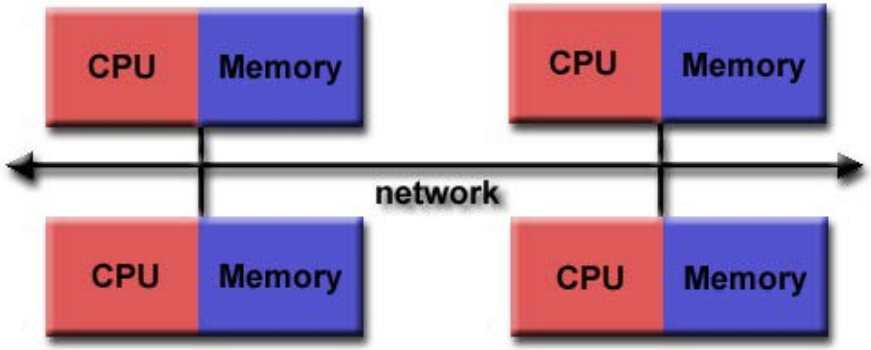
Single memory view, all processes (usually threads) could directly access the whole memory

distributed memory

Message Passing

all processes could directly access only their local memory.

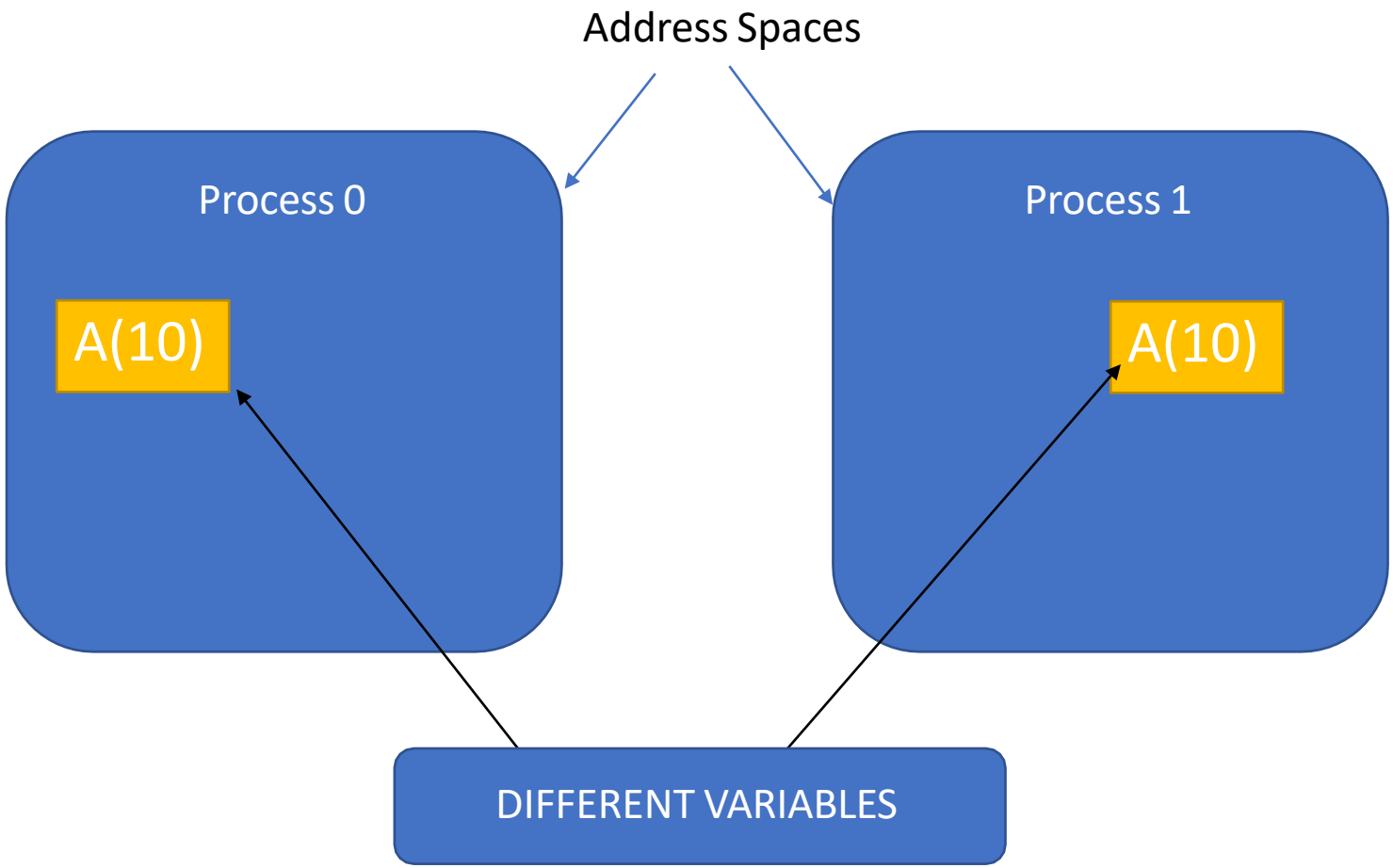




Message Passing paradigm

- Parallel programs consist of separate processes, each with its own address space
- Programmer manages memory by placing data in a particular process
- Data sent explicitly between processes
- Programmer manages
  - memory motion
  - Data distribution

Shared nothing approach



Message Passing Pro&Cons

- Pros
- Memory is scalable with the number of processors. Increase the number of processors and the size of memory increases proportionately.
- Cons
- Data is scattered on separated address spaces
- The programmer is responsible for many of the details associated with data communication between processors.
- Non-uniform memory access times - data residing on a remote node takes longer to access than node local data.

Message Passing approach

- Using the de-facto standard : MPI message passing interface
  - A standard which defines how to send/receive message from a different processes
- Many different implementation
  - OpenMPI
  - Intel-MPI
- They all provide a library which provide all communication routines
- To compile your code you have to link against a library
- Generally a wrapper is provided (mpif90/mpicc)

What is MPI ?

- A message-passing library specification
- An extended message-passing model
- NOT a language or compiler specification
- NOT a specific implementation or product
- For parallel computers, clusters, and heterogeneous networks
- Full-featured
  - Designed to provide access to advanced parallel hardware for end users, library writers, and tool developers
- Latest version of the standard MPI- 3.1

What is MPI ?

A STANDARD...

- The actual implementation of the standard is demanded to the software developers of the different systems
- In all systems MPI has been implemented as a library of subroutines over the network drivers and primitives
- many different implementations
  - MPICH (the original one)
  - OpenMPI
  - IntelMPI

Some reasons to use MPI

- INTERNATIONAL STANDARD
- MPI evolves: MPI 1.0 was first introduced in 1994, most current version is MPI 3.1 (June 2015)
- Available on almost all parallel systems (free MPICH, Open MPI used on many clusters), with interfaces for C/C++ and Fortran
- Supplies many communication variations and optimized functions for a wide range of needs
- Works both on distributed memory (DM) and shared memory (SM) hardware architectures
- Supports large program development and integration of multiple modules

How to program with MPI ?

- MPI is a library:
  - All operations are performed with subroutine calls
- Basic definitions are in
  - mpi.h for C/C++
  - mpif.h for Fortran 77 and 90
  - MPI module for Fortran 90 (optional)

How to compile MPI Programs

- NO STANDARD: left to the implementations:
- Generally:
  - You should specify the appropriate include directory (i.e. -I/mpidir/include)
  - You should specify the mpi library (i.e. -L/mpidir/lib -lmpi)
- Usually MPI compiler wrappers do this job for you. (i.e. mpicc)

How to run MPI programs ?

- The MPI Standard does not specify how to run an MPI program, just as the Fortran standard does not specify how to run a Fortran program.
- In general, starting an MPI program is dependent on the implementation of MPI you are using, and might require various scripts, program arguments, and/or environment variables.
- Many implementations provided `mpirun -np 4 a.out` to run an MPI program
- The specific commands to run a program on a parallel system are defined by the environment installed on the parallel computer

How to write an MPI program ?

- Modify your serial program to insert MPI routines which distribute data and loads to different processors.

WHICH MPI ROUTINES DO I NEED ?

Basic Features of MPI routines

- Calls may be roughly divided into four classes:
  - Calls used to initialize, manage, and terminate communications
  - Calls used to communicate between pairs of processors. (Pair communication)
  - Calls used to communicate among groups of processors. (Collective communication)
  - Calls to create data types.

Minimal set of MPI routines

- MPI_INIT: initialize MPI
- MPI_COMM_SIZE: how many Processors?
- MPI_COMM_RANK: identify the Processor
- MPI_SEND : send data
- MPI_RECV: receive data
- MPI_FINALIZE: close MPI

(Almost) All you need is to know this 6 calls

Our first program

Fortran

```
PROGRAM hello
 INCLUDE ‘mpif.h‘
 INTEGER err
 CALL MPI_INIT(err)
 call  MPI_COMM_RANK(MPI_COMM_WORLD,rank,ierr)
 call  MPI_COMM_SIZE(MPI_COMM_WORLD,size,ierr)
 print *, 'I am ', rank, ' of ', size
 CALL MPI_FINALIZE(err)
END
```

C

```
#include <stdio.h>
#include <mpi.h>
int main (int argc, char * argv[])
{
  int rank, size;
  MPI_Init( &argc, &argv );
  MPI_Comm_rank( MPI_COMM_WORLD,&rank);
  MPI_Comm_size( MPI_COMM_WORLD,&size );
  printf( "I am %d of %d\n", rank, size );
  MPI_Finalize();
```

Some notes/observations

- All MPI programs begin with MPI_Init and end with MPI_Finalize
- MPI_COMM_WORLD is defined by mpi.h (in C) or mpif.h (in Fortran) and designates all processes in the MPI "job"
- Each statement executes independently in each process including the printf/print statements
- I/O not part of MPI-1 (MPI-IO part of MPI-2)
- print and write to standard output or error not part of MPI-1 or MPI-2 or MPI-3
- output order is undefined (may be interleaved by character, line, or blocks of characters),
- A consequence of the requirement that non-MPI statements execute independently

Inizialing/Finalizing MPI program

- Initializing the MPI environment
  - C:

```
int MPI_Init(int *argc, char ***argv);
```

  - Fortran:

```
INTEGER IERR
CALL MPI_INIT(IERR)
```

- Finalizing MPI environment
  - C:

```
int MPI_Finalize()
```

  - Fortran:

```
INTEGER IERR
CALL MPI_FINALIZE(IERR)
```

This two subprograms should be called by all processes, and no other MPI calls are allowed before **mpi_init** and after **mpi_finalize**

MPI Communicator

- The Communicator is a variable identifying a group of processes that are allowed to communicate with each other.
- It identifies the group of all processes.
- All MPI communication subroutines have a communicator argument. The Programmer could define many communicators at the same time

There is a default communicator (automatically defined):

MPI_COMM_WORLD

Communicator size and processor rank

How many processors are associated with a communicator?

C:

```
MPI_Comm_size(MPI_Comm comm, int *size)
```

Fortran:

```
INTEGER COMM, SIZE, IERR
CALL MPI_COMM_SIZE(COMM, SIZE, IERR)
```

OUTPUT: SIZE

What is the ID of a processor in a group?

C:

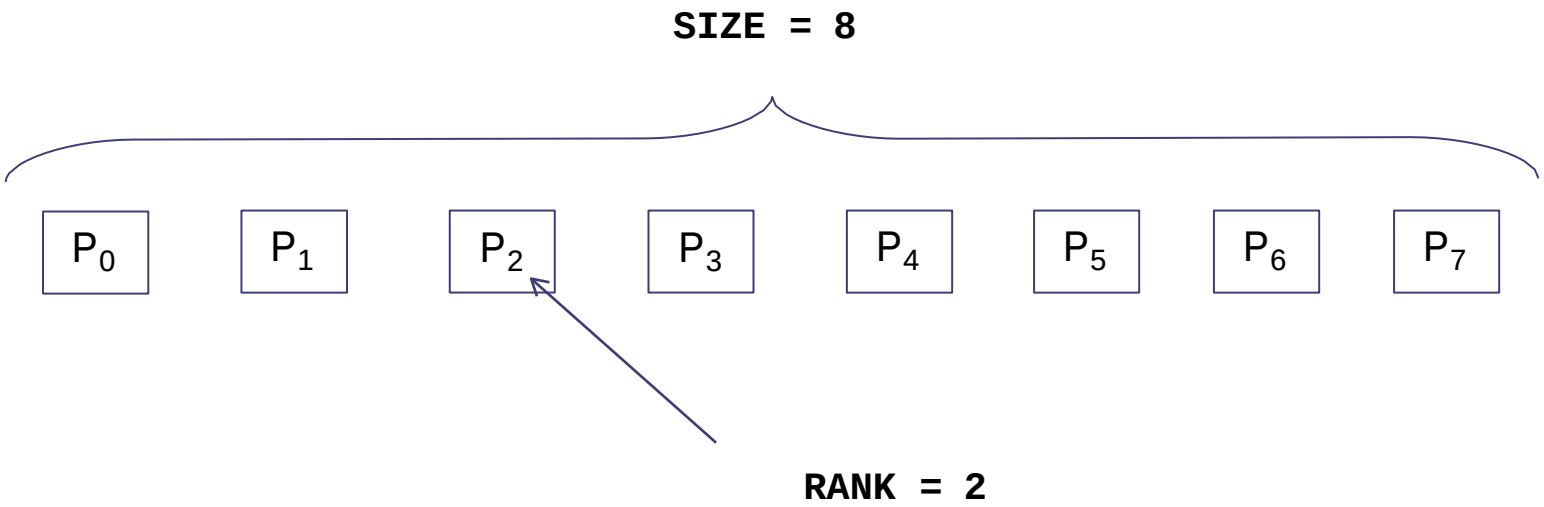
```
MPI_Comm_rank(MPI_Comm comm, int *rank)
```

Fortran:

```
INTEGER COMM, RANK, IERR
CALL MPI_COMM_RANK(COMM, RANK, IERR)
```

OUTPUT: RANK

Communicator size and processor rank



Size is the number of processors associated to the communicator

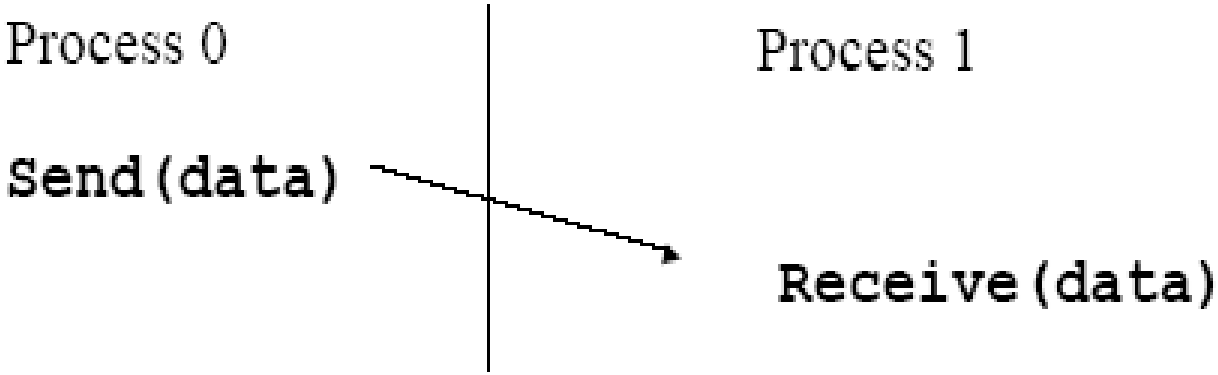
rank is the index of the process within a group associated to a communicator (**rank** = 0,1,...,N-1). The rank is used to identify the source and destination process in a communication

Basic elements of a message

- To send a message via mail we typically have:
  - An envelope (with possibly some hints on the content itself… i.e., advertisement, bills, greetings....)
  - A message
  - A destination address
  - A sender address
  - A tools to send the message (phone/mailer/ messenger)

For MPI it is exactly the same thing...

Basic Send/Receive



- How will “data” be described? datatypes
- How will processes be identified? rank/comm
- How will the receiver recognize messages? tag
- What will it mean for these operations to complete? blocking/non-blocking ()

Describing data

- The data in a message to send or receive is described by a triple (address, count, datatype), where an MPI datatype is recursively defined as:
  - predefined, corresponding to a data type from the language (e.g., MPI_INT, MPI_DOUBLE)
  - a contiguous array of MPI datatypes
  - a strided block of datatypes
  - an indexed array of blocks of datatypes
  - an arbitrary structure of datatypes
- There are MPI functions to construct custom datatypes, in particular ones for subarrays

MPI data type: Fortran language

MPI Data type	Fortran Data type
MPI_INTEGER	INTEGER
MPI_REAL	REAL
MPI_DOUBLE_PRECISION	DOUBLE PRECISION
MPI_COMPLEX	COMPLEX
MPI_DOUBLE_COMPLEX	DOUBLE COMPLEX
MPI_LOGICAL	LOGICAL
MPI_CHARACTER	CHARACTER(1)
MPI_PACKED	
MPI_BYTE	

MPI data type: C language

MPI Data type	C Data type
MPI_CHAR	signed char
MPI_SHORT	signed short int
MPI_INT	signed int
MPI_LONG	Signed log int
MPI_UNSIGNED_CHAR	unsigned char
MPI_UNSIGNED_SHORT	unsigned short int
MPI_UNSIGNED	unsigned int
MPI_UNSIGNED_LONG	unsigned long int
MPI_FLOAT	float
MPI_DOUBLE	double
MPI_LONG_DOUBLE	long double
MPI_BYTE	
MPI_PACKED	

MPI data tag

- Messages are sent with an accompanying user-defined integer tag, to assist the receiving process in identifying the message
- Messages can be screened at the receiving end by specifying a specific tag, or not screened by specifying MPI_ANY_TAG as the tag in a receive

Our first send message…

The simplest call:

```
MPI_send(buffer, count, data_type,
destination,tag,communicator)
```

where:

BUFFER: data to send

COUNT: number of elements in buffer .

DATA_TYPE : which kind of data types in buffer ?

DESTINATION the receiver

TAG: the label of the message

COMMUNICATOR set of processors involved

And our first receiver..

The simplest call:

```
MPI_recv( buffer, count, data_type, source,
tag, communicator, status)
```

Similar to send with the following differences:

- SOURCE is the sender ; can be set as MPI_any_source (receive a message from any processor within the communicator)
- TAG the label of message: can be set as MPI_any_tag: receive any kind of message
- STATUS integer array with information on message in case of error

The status array

Status is a data structure allocated in the user's program.

In C:

```
int recvd_tag, recvd_from, recvd_count;
MPI_Status status;
MPI_Recv(..., MPI_ANY_SOURCE, MPI_ANY_TAG, ..., &status )
recvd_tag = status.MPI_TAG;
recvd_from = status.MPI_SOURCE;
MPI_Get_count( &status, datatype, &recvd_count );
```

In Fortran:

```
integer recvd_tag, recvd_from, recvd_count
integer status(MPI_STATUS_SIZE)
call MPI_RECV(..., MPI_ANY_SOURCE, MPI_ANY_TAG, .. status, ierr)
tag_recvd = status(MPI_TAG)
recvd_from = status(MPI_SOURCE)
call MPI_GET_COUNT(status, datatype, recvd_count, ierr)
```

A fortran example

```
Program MPI
   Implicit None
!
   Include 'mpif.h'
!
   Integer                                   :: rank
   Integer                                   :: buffer
   Integer, Dimension( 1:MPI_status_size ) :: status
   Integer                                   :: error
!
   Call MPI_init( error )
   Call MPI_comm_rank( MPI_comm_world, rank, error )
!
   If( rank == 0 ) Then
      buffer = 33
      Call MPI_send( buffer, 1, MPI_integer, 1, 10, &
                     MPI_comm_world, error )
   End If
!
   If( rank == 1 ) Then
      Call MPI_recv( buffer, 1, MPI_integer, 0, 10, &
                     MPI_comm_world, status, error )
      Print*, 'Rank ', rank, ' buffer=', buffer
      If( buffer /= 33 ) Print*, 'fail'
   End If
   Call MPI_finalize( error )
End Program MPI
```

Questions for you:

- How many processors should I run this program on ?
- Can I run this program on 1000 processors ?

Blocking vs Non blocking calls

Q: When is a SEND instruction complete?
A: When it is safe to change the data that we sent.

Q: When is a RECEIVE instruction complete?
A: When it is safe to access the data we received.

Blocking vs Non blocking calls

With both communications (send and receive) we have two choices:

1. Start a communication and wait for it to complete: BLOCKING approach

2. Start a communication and return control to the main program:
   NON-BLOCKING approach

The Non-Blocking approach REQUIRES us to check for completion
before we can modify/access the sent/received data!!!

MPI_send/MPI_recv

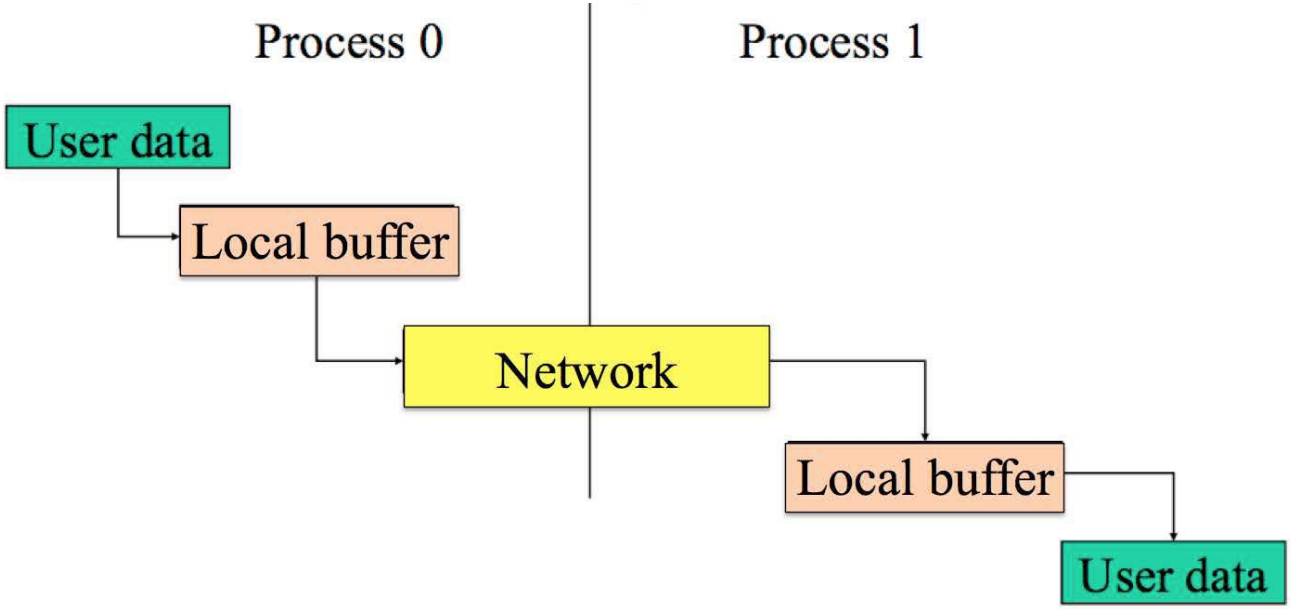
MPI_SEND() and MPI_RECV()
are blocking operations.

Are they really blocking ?

MPI_SEND() and MPI_RECV() are blocking operations.

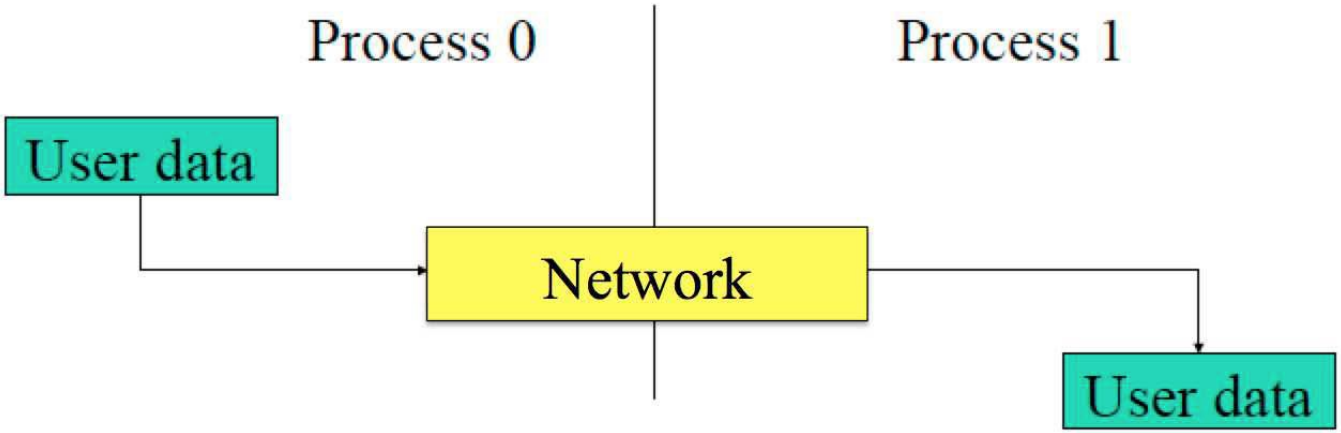
- However: often a system buffer is used that allows small messages to be non-blocking send-recv handshakes, but large messages will be blocking.
- MPI implementation (not the MPI standard) decides this.
- Blocking communication can be unsafe and may lead to deadlocks.

To make it clear:



Small messages make use of system-supplied buffer

To make it clear:



Large message are really blocking

Pros and Cons of Non-Blocking Send/ Receive

- Non-Blocking communications allows the separation between the initiation of the communication and the completion.
- Advantages:
  - between the initiation and completion the program could do other useful computation (latency hiding).
- Disadvantages:
  - the programmer has to insert code to check for completion.

Communication mode

- 4 different send types:
  - Standard: let MPI decide the best strategy...
  - Synchronous: it is complete when the receiver acknowledged the reception of the message
  - Buffered: it is complete when the data has been copied to a local buffer
  - Ready: requires a receiver to be already waiting for the message
- 1 single receive type

Communication mode and MPI routines

Mode	**Completion Condition**	Blocking subroutine	Non-blocking subroutine
Standard send	**Message sent (receive state unknown)**	**`MPI_SEND`**	**`MPI_ISEND`**
receive	**Completes when a message has arrived**	**`MPI_RECV`**	**`MPI_IRECV`**
Synchronous send	**Only completes when the receive has completed**	`MPI_SSEND`	`MPI_ISSEND`
Buffered send	**Always completes, irrespective of receiver**	`MPI_BSEND`	`MPI_IBSEND`
Ready send	**Always completes, irrespective of whether the receive has completed**	`MPI_RSEND`	`MPI_IRSEND`

Non blocking send/receive (Fortran)

```
MPI_ISEND(buf, count, type, dest, tag, comm, req, ierr)
MPI_IRECV(buf, count, type, dest, tag, comm, req, ierr)
```

buf	array of type **type** see table.	
count	(INTEGER)	number of element of **buf** to be sent
type	(INTEGER)	MPI type of **buf**
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)

Non blocking send/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 dest, int tag, MPI_Comm comm, MPI_Request *req);
```

Waiting for completion…

- Fortran:

```
MPI_WAIT(req, status, ierr)
```

- A call to this subroutine cause the code to wait until the communication pointed by req is complete.
- **Req (**INTEGER) input/output, communication handler (initiated by **MPI_ISEND** or **MPI_IRECV**).
- **Status** (INTEGER) array of size **MPI_STATUS_SIZE**,
- if **Req** was associated to a call to **MPI_IRECV**, **status** contains informations on the received message, otherwise **status** could contain an error code.
- **ierr** (INTEGER) output, error code (if **ierr=0** no error occours).
- C:

```
int MPI_Wait(MPI_Request *req, MPI_Status *status);
```

Testing for completition

- Fortran:

```
MPI_TEST(req, flag, status, ierr)
```

- A call to this subroutine sets flag to .true. if the communication pointed by req is complete, sets flag to .false. otherwise.
- **Flag**(LOGICAL) output, .true. if communication req has completed .false. Otherwise
- **Req (**INTEGER) input/output, communication handler (initiated by **MPI_ISEND** or **MPI_IRECV**).
- **Status** (INTEGER) array of size **MPI_STATUS_SIZE**,
- if **Req** was associated to a call to **MPI_IRECV**, **status** contains informations on the received message, otherwise **status** could contain an error code.
- **ierr** (INTEGER) output, error code (if **ierr=0** no error occours).
- C:

```
int MPI_Wait(MPI_Request *req, int *flag, MPI_Status *status);
```

MPI: a case study

Problem: exchanging data between two processes

```
If( rank == 0 ) then
     Call MPI_send( buffer1, 1, MPI_integer, 1, 10, &
                    MPI_comm_world, error )
     Call MPI_recv( buffer2, 1, MPI_integer, 1, 20, &
                    MPI_comm_world, status, error )
  Else If( rank == 1 )then
     Call MPI_send( buffer2, 1, MPI_integer, 0, 20, &
                    MPI_comm_world, error )
     Call MPI_recv( buffer1, 1, MPI_integer, 0, 10, &
                    MPI_comm_world, status, error )
End If
```

DEADLOCK

Solution A

USE BUFFERED SEND: bsend
send and go back so the deadlock is avoided

```
If( rank == 0 ) then
     Call MPI_Bsend( buffer1, 1, MPI_integer, 1, 10, &
                     MPI_comm_world, error )
     Call MPI_recv( buffer2, 1, MPI_integer, 1, 20, &
                     MPI_comm_world, status, error )
  Else If( rank == 1 )then
     Call MPI_Bsend( buffer2, 1, MPI_integer, 0, 20, &
                     MPI_comm_world, error )
     Call MPI_recv( buffer1, 1, MPI_integer, 0, 10, &
                     MPI_comm_world, status, error )
End If
```

Requires a copy therefore is not efficient
for large data set memory problems

Solution B

Use non blocking SEND : isend
send go back but now is not safe to change the buffer

```
 If( rank == 0 ) then
      Call MPI_Isend( buffer1, 1, MPI_integer, 1, 10, &
                      MPI_comm_world, error )
      Call MPI_recv( buffer2, 1, MPI_integer, 1, 20, &
                      MPI_comm_world, status, error )
   Else If( rank == 1 )then
      Call MPI_Isend( buffer2, 1, MPI_integer, 0, 20, &
                      MPI_comm_world, error )
      Call MPI_recv( buffer1, 1, MPI_integer, 0, 10, &
                      MPI_comm_world, status, error )
 End If
Call MPI_wait( REQUEST, status ) ! Wait until send is complete
```

1 A handle is introduced to test the status of message.
2. More efficient of the previous solutions

Solution C

Use non blocking SEND : isend
send go back but now is not safe to change the buffer

```
If( rank == 0 ) then
      Call MPI_send( buffer1, 1, MPI_integer, 1, 10, &
                     MPI_comm_world, error )
      Call MPI_recv( buffer2, 1, MPI_integer, 1, 20, &
                     MPI_comm_world, status, error )
   Else If( rank == 1 )then
      Call MPI_recv( buffer1, 1, MPI_integer, 0, 10, &
                     MPI_comm_world, status, error )
      Call MPI_send( buffer2, 1, MPI_integer, 0, 20, &
                     MPI_comm_world, error )
End If
```

the most efficient one and the recommended one

Home Works..

- Compile/Run and understand usage of MPI programs
  - mpi_pi.c
  - hello_world.c/f90
  - send_message.f90
- First MPI exercise: fix deadlock problems on a ring
- Second MPI exercise: play with different MPI_send call on mpi_pi.c
- Third MPI exercise: implement the sum of N number using MPI paradigm