

Introduction to the Message Passing Interface (MPI)

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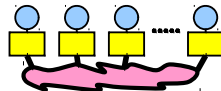
November 05, 2019



Outline

1 MPI Overview

- one program on several processors work and data distribution



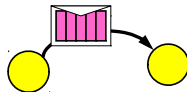
2 Process model and language bindings

- starting several MPI processes

```
MPI_Init()  
MPI_Comm_rank()
```

3 Messages and point-to-point communication

- the MPI processes can communicate



4 Non-blocking communication

- to avoid idle time and deadlocks



5 Collective communication

- e.g., broadcast



Deploying in-class exercises on ICSMaster

1 C program compilation (pi0_example.zip):

```
$ module load openmpi
$ mpicc -O3 pi0.c -o pi0
```

2 Create a job configuration file to execute the program using 4 processes on 2 nodes for 30 min max:

```
$ cat prun
#!/bin/bash -l
#SBATCH --job-name=hpc-class          # job name
#SBATCH --time 00:30:00               # wall-clock time (hrs:mins::secs)
#SBATCH --nodes=2                    # number of compute nodes
#SBATCH --ntasks=4                   # number of total MPI tasks
#SBATCH --error=job.%J.err           # error file name
#SBATCH --output=job.%J.out          # output file name
# load modules
module load gcc
module load openmpi
# your commands
mpirun $@
```

Deploying in-class exercises on ICSMaster

- 1 Submit the job for execution, passing the program name and arguments:

```
sbatch prun ./pi0 100000000000
```

- 2 Program output shall appear in file job.XXXXXX.out (live updating)
- 3 Error output shall appear in file job.XXXXXX.err (live updating)

Deploying in-class exercises on **your Mac**

1 Install MPI from ports:

```
$ sudo port install openmpi
```

2 Install MPI from Homebrew:

```
$ brew install open-mpi
```

3 C program compilation - same as on ICSMaster:

```
$ mpicc -std=c99 -O3 pi0.c -o pi0
```

4 There is no MPI job queue on your machine \Rightarrow MPI programs are executed right away:

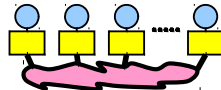
```
$ mpirun -np 8 ./pi0 10000000000
```

5 Program output shall appear in the owning terminal

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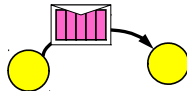
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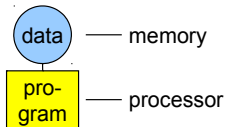
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- e.g., broadcast

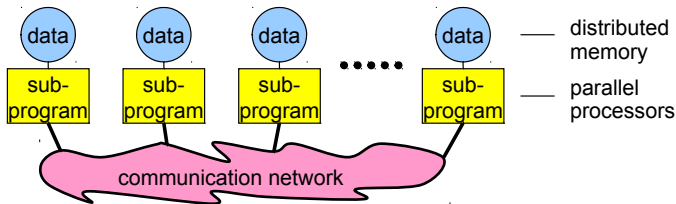


The Message-Passing Programming Paradigm

■ Sequential Programming Paradigm



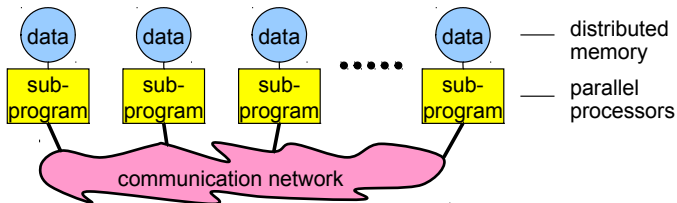
■ Message-Passing Programming Paradigm



The Message-Passing Programming Paradigm

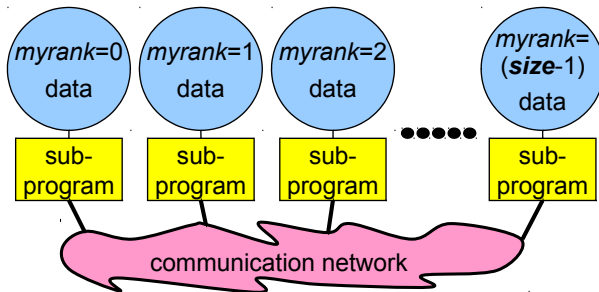
■ Each processor in a message passing program runs a sub-program:

- written in a conventional sequential language, e.g., C or C++,
- typically the same on each processor (SPMD),
- the variables of each sub-program have
 - the same name
 - but different locations (distributed memory) and different data!
 - i.e., all variables are private
- communicate via special send & receive routines (message passing)



Data and Work Distribution

- the value of **myrank** is returned by special library routine
- the system of size processes is started by special MPI initialization program (mpirun or mpiexec)
- all distribution decisions are based on **myrank**
- i.e., which process works on which data

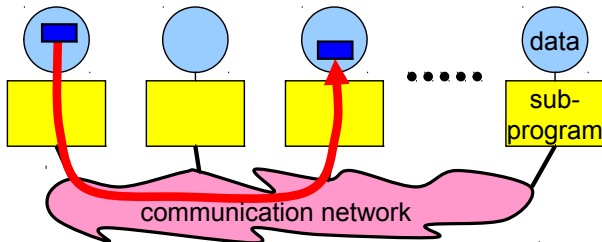


What is SPMD?

- Single Program, Multiple Data
- Same (sub-)program runs on each processor
- MPI allows also MPMD, i.e., Multiple Program, ...
- but some vendors may be restricted to SPMD
- MPMD can be emulated with SPMD
- Emulation of Multiple Program (MPMD), Example:

```
int main(int argc, char **argv)
{
    ...
    if (myrank < .... /* process should run the ocean model */)
    {
        ocean( /* arguments */ );
    } else {
        weather( /* arguments */ );
    }
    ...
}
```

Messages



- Messages are packets of data moving between sub-programs
- Necessary information for the message passing system:
 - sending process rank
 - source location
 - source data type
 - source data size
 - receiving process rank
 - destination location
 - destination data type
 - destination buffer size

- A sub-program needs to be connected to a message passing system
- A message passing system is similar to:
 - mail box
 - phone line
 - fax machine
 - etc.
- MPI:
 - sub-program must be linked with an MPI library
 - sub-program must use include file of this MPI library
 - the total program (i.e., all sub-programs of the program) must be started with the MPI startup tool

Addressing

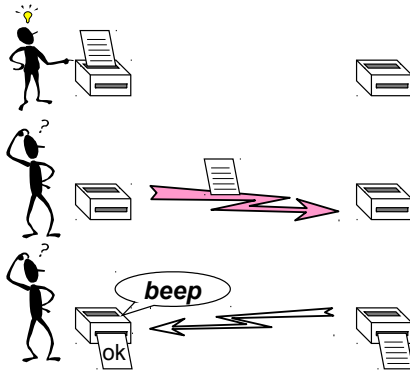
- Messages need to have addresses to be sent to
- Addresses are similar to:
 - mail addresses
 - phone number
 - fax number
 - etc.
- MPI: addresses are ranks of the MPI processes (sub-programs)

Point-to-Point Communication

- Simplest form of message passing
- One process sends a message to another
- Different types of point-to-point communication:
 - synchronous send
 - buffered = asynchronous send

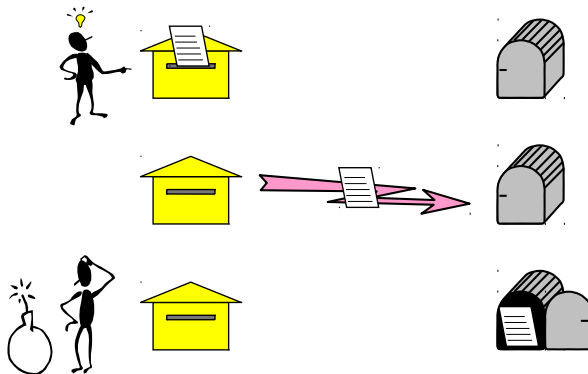
Synchronous Sends

- The sender gets an information that the message is received.
- Analogue to the beep or okay-sheet of a fax.



Buffered = Asynchronous Sends

- Only know when the message has left

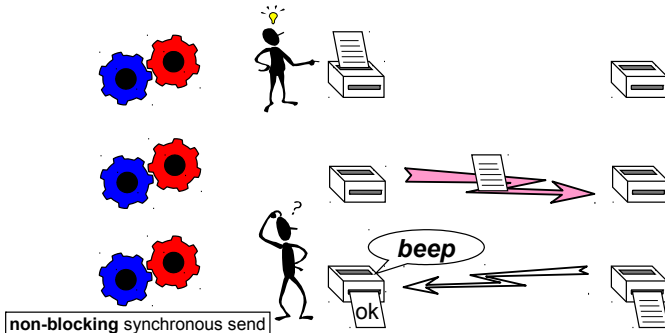


Blocking Operations

- Operations are local activities, e.g.,
 - sending (a message)
 - receiving (a message)
- Some operations may block until another process acts:
 - synchronous send operation blocks until receive is posted;
 - receive operation blocks until message was sent.
- Relates to the completion of an operation.
- Blocking subroutine returns only when the operation has completed.

Non-Blocking Operations

- Non-blocking operation: returns immediately and allow the sub-program to perform other work.
- At some later time the sub-program must **test** or **wait** for the completion of the non-blocking operation.



Non-Blocking Operations (cont'd)

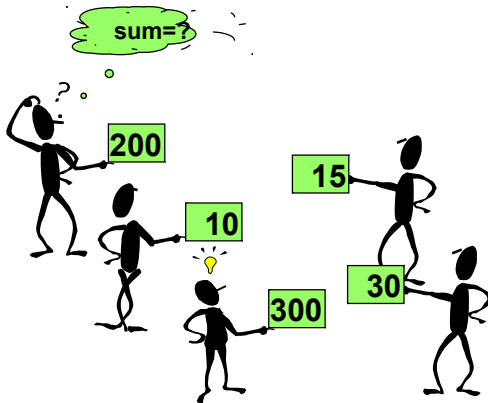
- All non-blocking operations must have matching wait (or test) operations.
(Some system or application resources can be freed only when the non-blocking operation is completed.)
- A non-blocking operation immediately followed by a matching wait is equivalent to a blocking operation.
- Non-blocking operations are not the same as sequential subroutine calls:
the operation may continue while the application executes the next statements!

Collective Communications

- Collective communication routines are higher level routines.
- Several processes are involved at a time.
- May allow optimized internal implementations, e.g., tree based algorithms
- Can be built out of point-to-point communications.

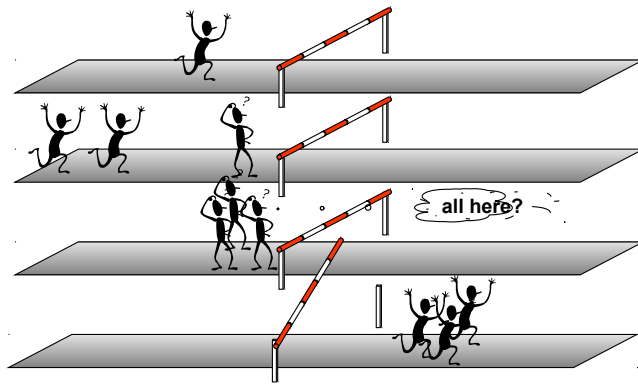
Reduction Operations

- Combine data from several processes to produce a single result.



Barriers

- Synchronize processes.



■ MPI-1 Forum

- First message-passing interface standard.
- Sixty people from forty different organizations.
- Users and vendors represented, from US and Europe.
- Two-year process of proposals, meetings and review.
- Message-Passing Interface document produced.
- MPI-1.0 — June, 1994.
- MPI-1.1 — June 12, 1995.

MPI-2 and MPI-3 Forum

■ MPI-2 Forum

- Same procedure (e-mails, and meetings in Chicago, every 6 weeks).
- MPI-2: Extensions to the Message-Passing Interface (July 18, 1997).

containing:

- MPI-1.2 — mainly clarifications.
- MPI-2.0 — extensions to MPI-1.2.

■ MPI-3 Forum

- Started Jan. 14-16, 2008 (1st meeting in Chicago)
- Using e-mails, wiki, meetings every 8 weeks (Chicago and San Francisco), and telephone conferences
- MPI-2.1 — June 23, 2008, mainly combining MPI-1 and MPI-2 books to one book
- MPI-2.2 — September 4, 2009: Clarifications and a few new func.
- MPI-3.0 — September 21, 2012: Important new functionality



Goals and Scope of MPI

■ MPI's primary goals

- To provide a message-passing interface.
- To provide source-code portability.
- To allow efficient implementations.

■ It also offers:

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

■ With MPI-2:

- Important additional functionality.
- No changes to MPI-1.

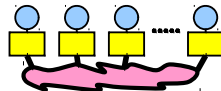
■ With MPI-2.1, 2.2, 3.0:

- Important additional functionality to fit on new hardware principles.
- Deprecated MPI routines moved to chapter "Deprecated Functions"
- With MPI-3.0, some deprecated features were removed

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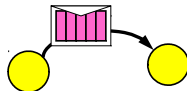
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- e.g., broadcast



MPI Header files and MPI Function Format

```
#include <mpi.h>
error = MPI_Xxxxxx( parameter, ... );
MPI_Xxxxxx( parameter, ... );
```

definition in the standard:

```
MPI_Comm_rank(..., int *rank);
MPI_Recv(..., MPI_Status *status);
```

usage in your code:

```
main...
{
    int myrank;
    MPI_Status rcv_status;
    MPI_Comm_rank(..., &myrank);
    MPI_Recv(..., &rcv_status);
}
```

- MPI_..... namespace is reserved for MPI constants and routines, i.e. application routines and variable names must not begin with MPI_.

Initializing MPI

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

```
#include <mpi.h>
int main(int argc, char **argv)
{
    MPI_Init(&argc, &argv);
    ...
}
```

- In MPI-2.0 and higher could also be: `MPI_Init(NULL, NULL);`
- Must be first MPI routine that is called
(only a few exceptions, e.g., `MPI_Initialized`)

Starting the MPI Program

- Start mechanism is implementation-dependent:

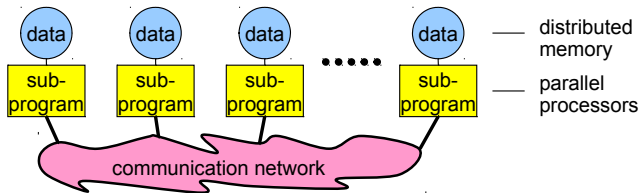
- Most implementations:

```
$ mpirun -np number_of_processes ./executable
```

- With MPI-2 and later:

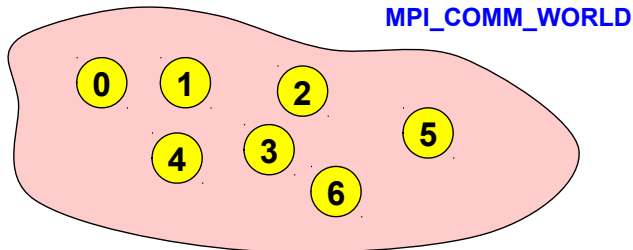
```
$ mpiexec -n number_of_processes ./executable
```

- The parallel MPI processes exist at least after `MPI_Init` was called.



Communicator `MPI_COMM_WORLD`

- All processes (= sub-programs) of one MPI program are combined in the **communicator** `MPI_COMM_WORLD`.
- `MPI_COMM_WORLD` is a predefined **handle** in `mpi.h`.
- Each process has its own **rank** in a communicator:
 - starting with 0
 - ending with (size-1)



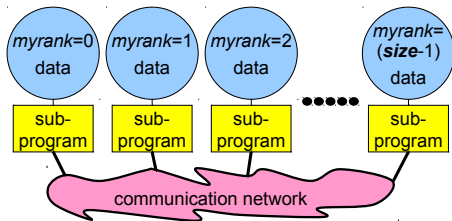
Handles

- Handles identify **MPI** objects.
- For the programmer, handles are
 - predefined constants in `mpi.h`
 - Example: `MPI_COMM_WORLD`
 - Can be used in initialization expressions or assignments.
 - The object accessed by the predefined constant handle exists and does not change only between `MPI_Init` and `MPI_Finalize`.
 - values returned by some MPI routines, to be stored in variables, that are defined as
 - in C: special MPI typedefs, e.g., `MPI_Comm`
- Handles refer to internal MPI data structures

Rank

- The rank identifies different processes.
- The rank is the basis for any work and data distribution.
- C:

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



```
MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
```


Size / Exiting MPI

■ How many processes are contained within a communicator?

■ C:

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

■ Exiting MPI

■ C:

```
int MPI_Finalize();
```

- Must be called last by all processes.
- After `MPI_Finalize`:
 - Further MPI-calls are forbidden
 - Especially re-initialization with `MPI_Init` is forbidden

In Class Exercise: Hello World

- Write a minimal MPI program which prints “hello world” by each MPI process.
- Compile and run it on a single processor.
- Run it on several processors in parallel.
- Modify your program so that:
 - every process writes its rank and the size of `MPI_COMM_WORLD`,
 - only process ranked 0 in `MPI_COMM_WORLD` prints “hello world”.
- Why is the sequence of the output non-deterministic?

```
I am 2 of 4
Hello world
I am 0 of 4
I am 3 of 4
I am 1 of 4
```

In Class Exercise: Hello World (Solution)

Advanced exercise: Hello World with deterministic output

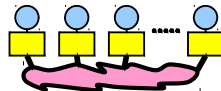
- 1 Discuss with your neighbor, what must be done, that the output of all MPI processes on the terminal window is in the sequence of the ranks.
- 2 Or is there no chance to guarantee this?

In Class Exercise: Hello World (Solution)

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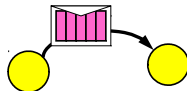
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- e.g., broadcast



Messages

- A message contains a number of elements of some particular datatype.
- MPI datatypes:
 - Basic datatype (see next slide).
 - Derived datatypes. 
- Derived datatypes can be built up from basic or derived datatypes.
- Datatype handles are used to describe the type of the data in the memory.

Example: message with 5 integers

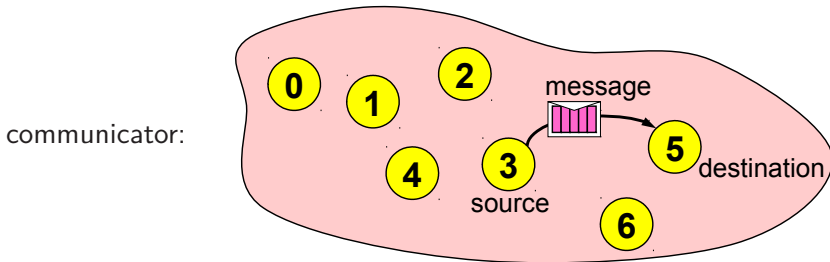
2345	654	96574	-12	7676
-------------	------------	--------------	------------	-------------

MPI Basic Datatypes – C

MPI Datatype	C datatype	Remarks
MPI_CHAR	char	Treated as printable character
MPI_SHORT	signed short int	
MPI_INT	signed int	
MPI_LONG	signed long int	
MPI_LONG_LONG	signed long long	
MPI_SIGNED_CHAR	signed char	Treated as integral value
MPI_UNSIGNED_CHAR	unsigned char	Treated as integral value
MPI_UNSIGNED_SHORT	unsigned short int	
MPI_UNSIGNED	unsigned int	
MPI_UNSIGNED_LONG	unsigned long int	
MPI_UNSIGNED_LONG_LONG	unsigned long long	
MPI_FLOAT	float	
MPI_DOUBLE	double	
MPI_LONG_DOUBLE	long double	
MPI_BYTE		
MPI_PACKED		

Point-to-Point Communication

- Communication between two processes.
- Source process sends message to destination process.
- Communication takes place within a communicator, e.g., `MPI_COMM_WORLD`.
- Processes are identified by their ranks in the communicator.



Sending a Message: `MPI_Send`

■ C:

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

- buf is the starting point of the message with count elements, each described with datatype.
- dest is the rank of the destination process within the communicator comm.
- tag is an additional non-negative integer piggyback information, additionally transferred with the message.
- The tag can be used by the program to distinguish different types of messages.

Sending a Message: `MPI_Ssend`

■ C:

```
int MPI_Ssend(void *buf, int count, MPI_Datatype datatype, int dest,
              int tag, MPI_Comm comm);
```

- buf is the starting point of the message with count elements, each described with datatype.
- dest is the rank of the destination process within the communicator comm.
- tag is an additional non-negative integer piggyback information, additionally transferred with the message.
- The tag can be used by the program to distinguish different types of messages.

Receiving a Message: `MPI_Recv`

■ C:

```
int MPI_Recv(void *buf, int count, MPI_Datatype datatype, int source, int tag,  
             MPI_Comm comm, MPI_Status *status);
```

- `buf/count/datatype` describe the receive buffer.
- Receiving the message sent by process with rank `source` in `comm`.
- Envelope information is returned in `status`.
- `status` is output argument (highlighted).
- Only messages with matching `tag` are received.

Requirements for Point-to-Point Communications

For a communication to succeed:

- Sender must specify a valid destination rank.
- Receiver must specify a valid source rank.
- The communicator must be the same.
- Tags must match.
- Message datatypes must match.
- Receiver's buffer must be large enough.

Wildcarding

- Receiver can wildcard.
- To receive from any source – source = `MPI_ANY_SOURCE`
- To receive from any tag – tag = `MPI_ANY_TAG`
- Actual source and tag are returned in the receiver's status parameter.

Communication Modes

- Send communication modes:

- synchronous: [MPI_SSEND](#)

- Only completes when the receive has started

- standard: [MPI_SEND](#)

- Tries to complete when the send buffer is available for reuse (copies into an internal buffer). May fall back to [MPI_SSEND](#), if internal buffer is not large enough for the message.

- Receiving all modes: [MPI_RECV](#)

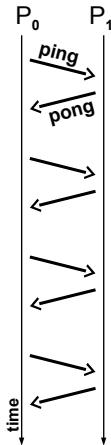
- Completes when a message has arrived (no SRECV mode)

In Class Exercise: Ping-pong

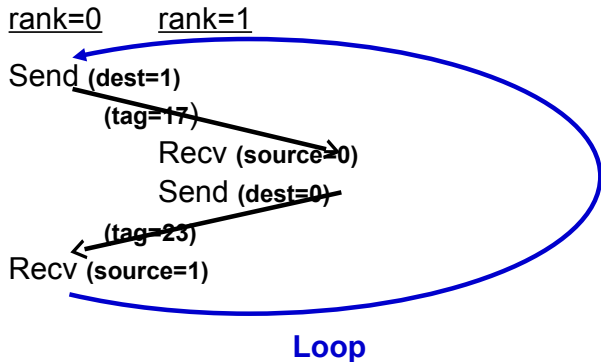
- Write a program according to the time-line diagram:
 - process 0 sends a message to process 1 (ping)
 - after receiving this message, process 1 sends a message back to process 0 (pong)
- Repeat this ping-pong with a loop of length 50
- Add timing calls before and after the loop:

```
double MPI_Wtime(void);
```

- Only at process 0: print out the transfer time of **one** message in μs ,
i.e. $\Delta_{time}/(2 \times 50) \times 10^6$



In Class Exercise: Ping-pong



```
if (my_rank == 0)
{
    MPI_Send( ... dest=1 ...);
    MPI_Recv( ... source=1 ...);
}
else
{
    MPI_Recv( ... source=0 ...);
    MPI_Send( ... dest=0 ...);
}
```

In Class Exercise: Ping-Pong (Solution)

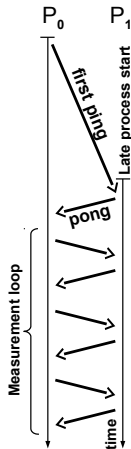
- show template pingpong_template/pingpong.c
- show solution pingpong/pingpong.c

Advanced Exercises – Ping pong latency and bandwidth

- Exclude startup time problems from measurements:
 - Execute a first ping-pong outside of the measurement loop
- latency = transfer time for short messages
- bandwidth = message size (in bytes) / transfer time
- Print out message transfer time and bandwidth
 - for following send modes:
 - for standard send (`MPI_Send`)
 - for synchronous send (`MPI_Ssend`)
 - for following message sizes:

```

    8  B (e.g., one double or double precision value)
  512  B (= 8*64 bytes)
   32 KB (= 8*64**2 bytes)
    2 MB (= 8*64**3 bytes)
    
```



In Class Exercise: Ping-Pong (Solution)

- show solution pingpong/pingpong_advanced_send.cpp ([MPI_Send](#))
- show solution pingpong/pingpong_advanced_ssend.cpp ([MPI_Ssend](#))

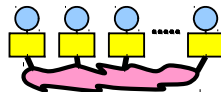
Results for ping-pong on ICSMaster (2 processes, 2 nodes)

2 bytes	0.000022 sec	1.485531 MB/s
2048 bytes	0.000018 sec	111.906391 MB/s
131072 bytes	0.000093 sec	1413.472037 MB/s
8388608 bytes	0.002661 sec	3152.936229 MB/s

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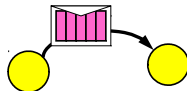
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Deadlock in a process ring

- The following code in each MPI process:

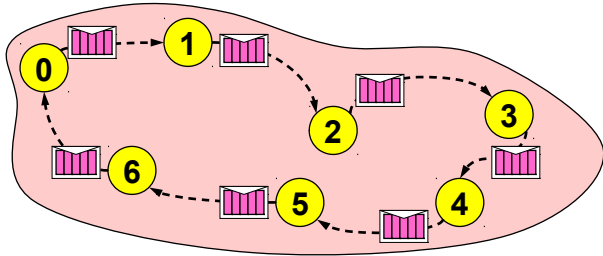
```
MPI_Ssend(..., right_rank, ...);
MPI_Recv(..., left_rank, ...);
```

will block and never return, because
`MPI_Recv` cannot be called in the
right-hand MPI process

- Same problem with standard send mode (`MPI_Send`), if MPI implementation chooses synchronous protocol

- Solution:

- `MPI_Sendrecv`, or
- nonblocking Send and Receive



MPI_Sendrecv

- `MPI_Sendrecv` is just like an `MPI_Send` followed by an `MPI_Recv`, except that it's much better than that.
- With `MPI_Send` and `MPI_Recv`, these are your choices:
 - Everyone calls `MPI_Recv`, and then everyone calls `MPI_Send`.
 - Everyone calls `MPI_Send`, and then everyone calls `MPI_Recv`.

Why `MPI_Sendrecv`?

- Suppose that everyone calls `MPI_Recv`, and then everyone calls `MPI_Send`.
 - Well, these routines are synchronous (also called blocking), meaning that the communication has to complete before the process can continue with the program.
 - That means that, when everyone calls `MPI_Recv`, they're waiting for someone else to call `MPI_Send`. We call this deadlock.
- Suppose that everyone calls `MPI_Send`, and then everyone calls `MPI_Recv`.
 - Well, this will only work if there's enough buffer space available to hold everyone's messages until after everyone is done sending.
 - Sometimes, there isn't enough buffer space.

Why MPI_Sendrecv?

- **MPI_Sendrecv** allows each processor to **simultaneously** send to one processor and **receive** from another. For example, P_1 could send to P_0 while simultaneously receiving from P_2 .

```
#include <mpi.h>

int 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);
```

MPI_Sendrecv_replace

- `MPI_Sendrecv_replace` sends and receives using a single buffer:

```
#include <mpi.h>

int MPI_Sendrecv_replace(void *buf,
                          int count,
                          MPI_Datatype datatype,
                          int dest,
                          int sendtag,
                          int source,
                          int recvtag,
                          MPI_Comm comm,
                          MPI_Status *status);
```

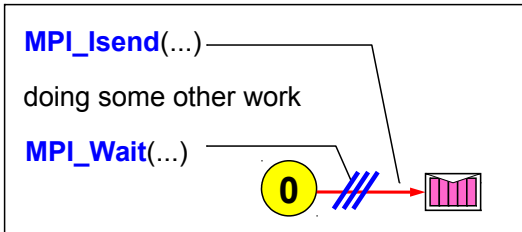
Non-Blocking Communications

Separate communication into three phases:

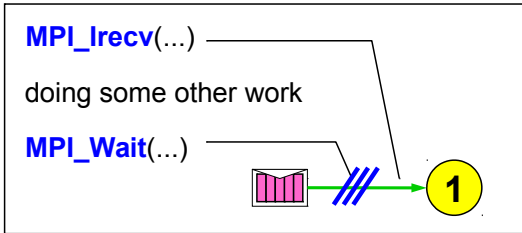
- 1 Initiate non-blocking communication
 - returns immediately
 - routine name starting with `MPI_I...`
- 2 Do some work (perhaps involving other communications?)
- 3 Wait for non-blocking communication to complete

Non-Blocking Examples

■ Non-blocking **send**:



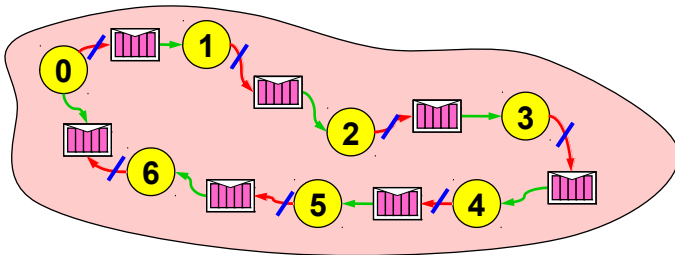
■ Non-blocking **receive**:



/// – waiting until operation locally completed

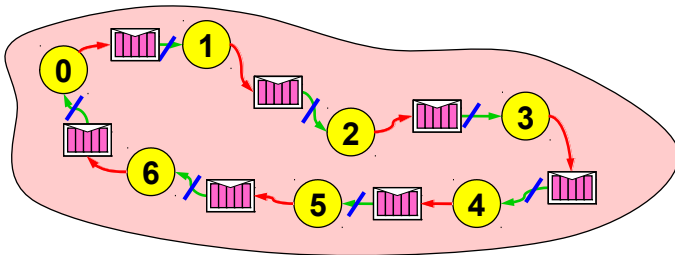
Non-Blocking Send

- Initiate non-blocking send
 - in the ring example: Initiate non-blocking send to the right neighbor
- Do some work:
 - in the ring example: Receiving the message from left neighbor
- Now, the message transfer can be completed
- Wait for non-blocking send to complete: —



Non-Blocking Receive

- Initiate non-blocking receive
 - in the ring example: Initiate non-blocking receive from left neighbor
- Do some work:
 - in the ring example: Sending the message to the right neighbor
- Now, the message transfer can be completed
- Wait for non-blocking receive to complete: —



Handles and MPI_Request

Predefined handles

- defined in `mpi.h`
- communicator, e.g., `MPI_COMM_WORLD`
- datatype, e.g., `MPI_INT`, `MPI_INTEGER`, ...

Handles **can** also be stored in local variables:

- memory for datatype handle: `MPI_Datatype name_of_var`
- memory for communicator handles: `MPI_Comm name_of_var`

Request handles

- are used for **non-blocking communication**
- **must** be stored in local variables: `MPI_Request name_of_var`
- the value
 - **is generated** by a non-blocking communication routine
 - **is used** (and freed) in the `MPI_WAIT` routine

Non-blocking Synchronous Send / Non-blocking Receive

■ C:

```
MPI_Issend(buf, count, datatype, dest, tag, comm, OUT &request_handle);  
..  
MPI_Wait(INOUT &request_handle, &status);
```

- buf must not be modified between `MPI_Issend` and `MPI_Wait`

■ C:

```
MPI_Irecv(buf, count, datatype, source, tag, comm, OUT &request_handle);  
..  
MPI_Wait(INOUT &request_handle, &status);
```

- buf must not be used between `MPI_Irecv` and `MPI_Wait`

Completion

■ C:

```
MPI_Wait(&request_handle, &status);
MPI_Test(&request_handle, &flag, &status);
```

■ one must

- WAIT or
- loop with TEST until request is completed, i.e., `flag == 1` (C) or `.TRUE.` (Fortran)

You have several request handles:

- Wait or test for completion of **one** message: `MPI_Waitany` / `MPI_Testany`
- Wait or test for completion of **all** messages: `MPI_Waitall` / `MPI_Testall`

Exercise – MPI Ring

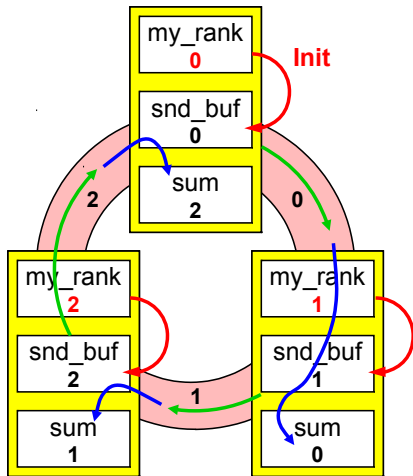
- A set of MPI processes are arranged in a ring.
- The program shall rotate information around a ring, each process calculates sum of all ranks

Algorithm:

- 1 Each process stores its rank in `MPI_COMM_WORLD` into an integer variable `snd_buf`. ↪
- 2 Each process passes this on to its neighbor on the right. ↻
- 3 Each processor calculates the sum of all values. ↪
- 4 Repeat 2-4 with “size” iterations (size = number of processes), i.e. **each process calculates sum of all ranks.**

Use non-blocking `MPI_Issend`:

- to avoid deadlocks
- to verify the correctness, because blocking synchronous send will cause a deadlock



Exercise – Rotating information around a ring

Initialization: ①

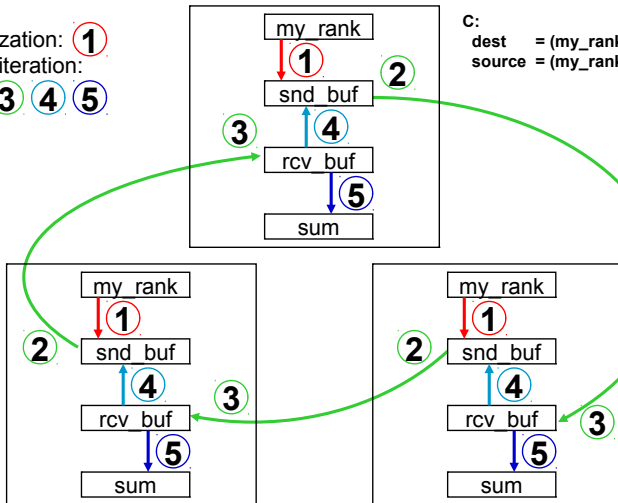
Each iteration:

② ③ ④ ⑤

C:

```
dest  = (my_rank+1) % size;  
source = (my_rank-1+size) % size;
```

Single
Program !!!



In Class Exercise: Ring (Solution)

- show solution pingpong/ring.c

Advanced Exercises – Irecv instead of Issend

- Substitute the `Issend-Recv-Wait` method by the `Irecv-Ssend-Wait` method in your ring program.

Or

- Substitute the `Issend-Recv-Wait` method by the `Irecv-Issend-Waitall` method in your ring program.

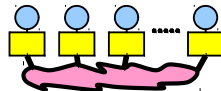
In Class Exercise: Ring (Solution)

- show solution `pingpong/ring_advanced_irecv_issend.c`
- show solution `pingpong/ring_advanced_irecv_ssend.c`

Outline

1 MPI Overview

- one program on several processors work and data distribution



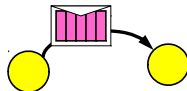
2 Process model and language bindings

- starting several MPI processes

```
MPI_Init()  
MPI_Comm_rank()
```

3 Messages and point-to-point communication

- the MPI processes can communicate



4 Non-blocking communication

- to avoid idle time and deadlocks

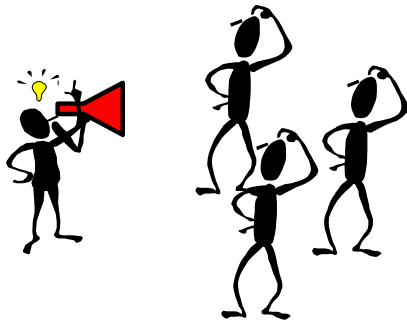


5 Collective communication

- e.g., broadcast



Broadcast and Collective Communication



- A one-to-many communication
- Communications involving a group of processes.
- Called by all processes in a communicator.
- Examples:
 - Broadcast, scatter, gather.
 - Global sum, global maximum, etc.

Broadcast and Collective Communication

- Use slides on collective communications (second PDF on icorsi)