Introduction to the Message Passing Interface (MPI)

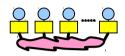
Juraj Kardos, Pratyuksh Bansal, Prof. Olaf Schenk

(TA: Tim Holt, Malik Lechekhab)

November 2, 2021



- 1 MPI Overview
 - one program on several processors, work and data distribution



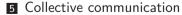
- 2 Process model and language bindings
 - starting several MPI processes

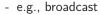
MPI Init() MPI Comm rank()

- Messages and point-to-point communication
 - the MPI processes can communicate



- 4 Non-blocking communication
 - to avoid idle time and deadlocks









Deploying in-class exercises on ICSMaster

1 C program compilation (pi0_example):

```
$ module load openmpi
$ mpicc -03 pi0.c -o pi0
```

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

```
$ cat prun
#!/bin/bash -1
#SBATCH --job-name=hpc-class
                                          # iob 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

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

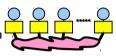
```
sbatch prun ./pi0 1000000000
```

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

- Install MPI from Homebrew:
 - \$ brew install open-mpi
- **2** C program compilation same as on ICSMaster:
 - \$ mpicc -std=c99 -03 pi0.c -o pi0
- **3** There is no job queue on your machine \Rightarrow MPI programs are executed right away:
 - \$ mpirun -np 8 --oversubscribe ./pi0 1000000000
- 4 Program output shall appear in the owning terminal

MPI Overview

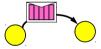
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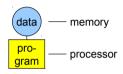


- e.g., broadcast

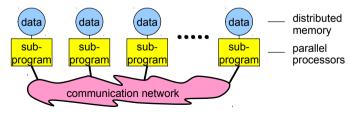




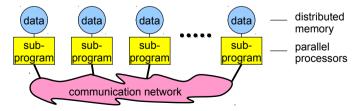
■ Sequential Programming Paradigm



■ Message-Passing Programming Paradigm

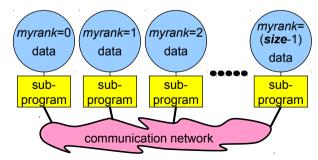


- Each processor in a message passing program runs a sub-program:
 - written in a conventional sequential language, e.g., C or C++,
 - typically the same on each processor (SPMD),
 - the variables of each sub-program have
 - the same name
 - but different locations (distributed memory) and different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



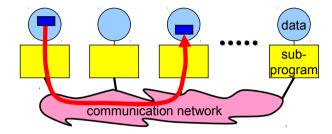
Data and Work Distribution

- 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



- 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 */ );
}
...
}</pre>
```



- 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

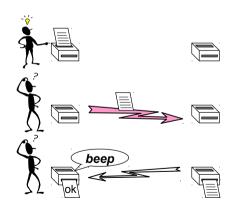
- Messages need to have addresses to be sent to
- Addresses are similar to:
 - mail addresses
 - phone number
 - fax number
 - etc.
- MPI: addresses are ranks of the MPI processes (sub-programs)

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Point-to-Point Communication

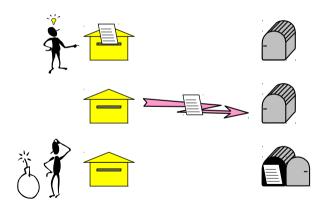
- Simplest form of message passing
- One process sends a message to another
- Different types of point-to-point communication:
 - synchronous send
 - buffered = asynchronous send

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



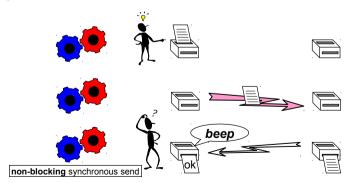
Buffered = Asynchronous Sends

■ Only know when the message has left



- 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 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!

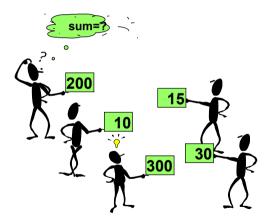
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Collective Communications

- 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.

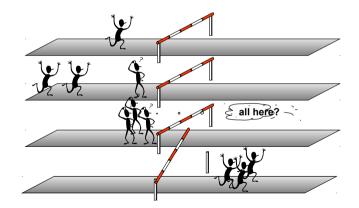
Reduction Operations

■ 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
- MPI-3.1 June 4, 2015: Adds clarifications and minor extensions to MPI-3.0



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.

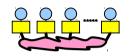
■ With MPI-2:

- 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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- 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 the first MPI routine that is called (only a few exceptions, e.g., MPI_Initialized)

 "The MPI Standard does not say what a program can do before an MPI_Init or after an MPI_Finalize.

 In the Open MPI implementation, it should do as little as possible. In particular, avoid anything that changes the external state of the program, such as opening files, reading standard input, or writing to standard output."

Starting the MPI Program

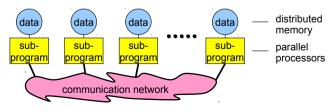
- Start mechanism is implementation-dependent:
 - Most implementations:

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

- With MPI-2 and later:

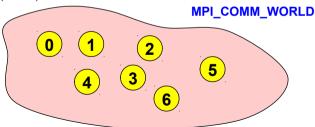
```
$ mpiexec -n number_of_processes ./executable
```

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



Communicator MPI COMM WORLD

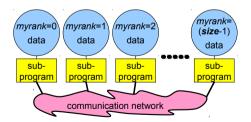
- All processes (= sub-programs) of one MPI program are combined in the **communicator** MPI COMM WORLD.
- MPI_COMM_WORLD is a predefined handle in mpi.h.
- Each process has its own **rank** in a communicator:
 - starting with 0
 - ending with (size-1)



- Handles 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

- 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);
```

■ 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?

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

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In Class Exercise: Hello World (Solution)

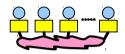
Advanced exercise: Hello World with deterministic output

- What must be done such 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?

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In Class Exercise: Hello World (Solution)

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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

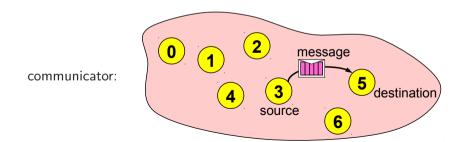
2345	654	96574	-12	7676

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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					

- 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:

- <u>buf</u> 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.
- <u>tag</u> 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:

- <u>buf</u> 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:

- buf/count/datatype describe the receive buffer.
- Receiving the message sent by process with rank source in comm.
- Envelope information is returned in <u>status</u>.
- <u>status</u> 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.

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

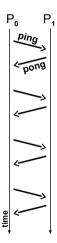
Communication Modes

- 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)

- 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

```
rank=0
           rank=1
Send (dest=1)
       (tag=1
           Recv (source=0)
           Send (dest=0)
Recv (source=1)
                     Loop
```

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

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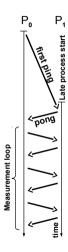
In Class Exercise: Ping-Pong (Solution)

- 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)
```





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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 (MPI_Send)

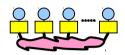
salloc -n2 -N2 -exclusive

	message size	transfer time	bandwidth
	32 bytes	0.000019 sec	1.670995 MB/s
9	2048 bytes	0.000021 sec	97.300019 MB/s
	131072 bytes	0.000281 sec	465.999629 MB/s
	8388608 bytes	0.007252 sec	1156.749400 MB/s

salloc -n2 -N1 -exclusive

	message size	transfer time	bandwidth
	32 bytes	0.000001 sec	49.587033 MB/s
9	2048 bytes	0.000003 sec	782.533605 MB/s
	131072 bytes	0.000017 sec	7498.930130 MB/s
	8388608 bytes	0.001189 sec	7057.169276 MB/s

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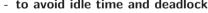
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- 5 Collective communication
 - e.g., broadcast



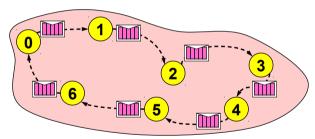
Deadlock in a process ring

■ 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.
 - These routines are synchronous (also called blocking), meaning that the communication has to complete before the process can continue with the program.
 - It 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.
 - This will only work if there's enough <u>buffer space</u> 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 recytag.
                 MPI Comm comm.
                 MPI Status *status):
```

MPI_Sendrecv_replace

■ MPI_Sendrecv_replace sends and receives using a single buffer:

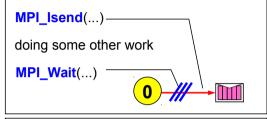
Non-Blocking Communications

Separate communication into three phases:

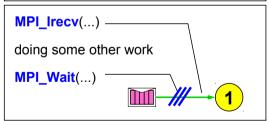
- Initiate non-blocking communication
 - returns Immediately
 - routine name starting with MPI_I...
- 2 Do some work (perhaps involving other communications?)
- 3 Wait for non-blocking communication to complete

Non-Blocking Examples

■ Non-blocking **send**:

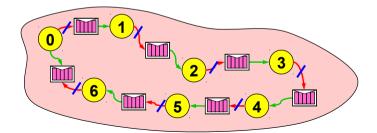


■ Non-blocking **receive**:

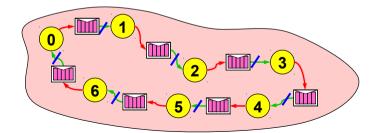


/// waiting until operation locally completed

- 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: —



- 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: —



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

■ 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

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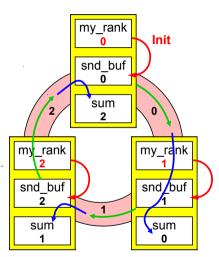
- A set of MPI processes are arranged in a ring.
- The program shall rotate information around a ring, each process calculates sum of all ranks

Algorithm:

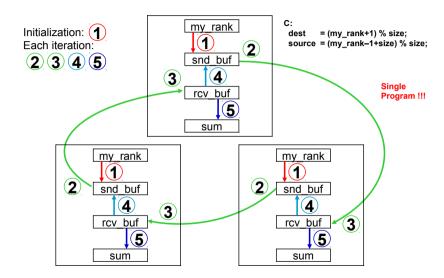
- Each process stores its rank in MPI_COMM_WORLD into an integer variable snd_buf.)
- 2 Each process passes this on to its neighbor on the right. •
- 3 Each processor calculates the sum of all values.
- 4 Repeat 2-4 with "size" iterations (size = number of processes), i.e. each process calculates sum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



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In Class Exercise: Ring (Solution)

■ show solution ring/ring.c



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Advanced Exercises – Irecv instead of Issend

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

Or

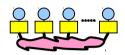
■ Substitute the Issend-Recv-Wait method by the Irecv-Issend-Waitall method in your ring program.

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In Class Exercise: Ring (Solution)

- show solution ring/ring_advanced_irecv_issend.c
- show solution ring/ring_advanced_irecv_ssend.c

- 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



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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.

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Broadcast and Collective Communication

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