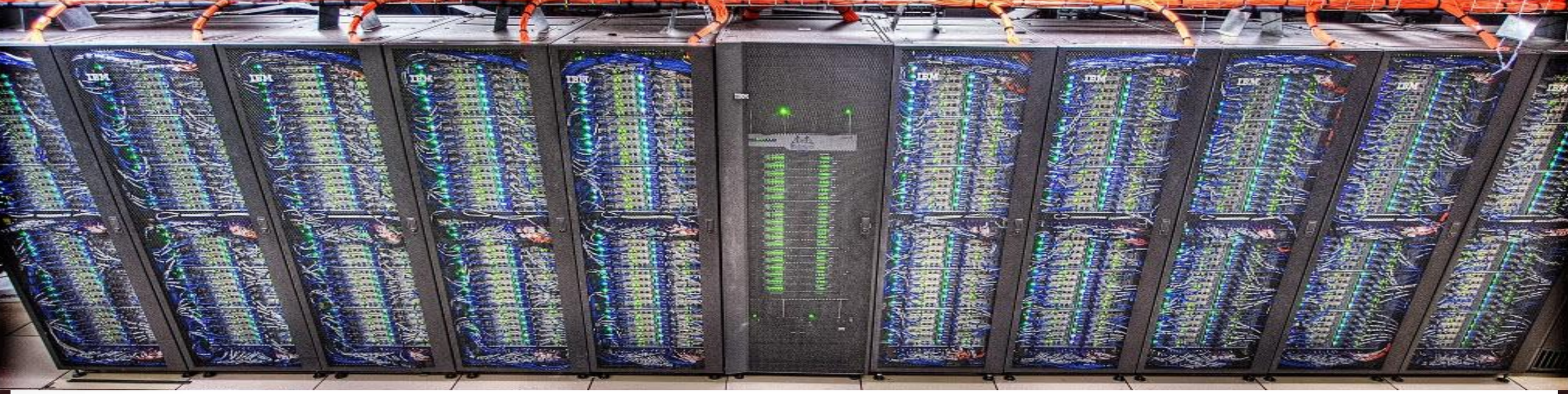

Introduction to Code Parallelization Using MPI

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November 20, 2020

Original slides created by **Ping Luo**

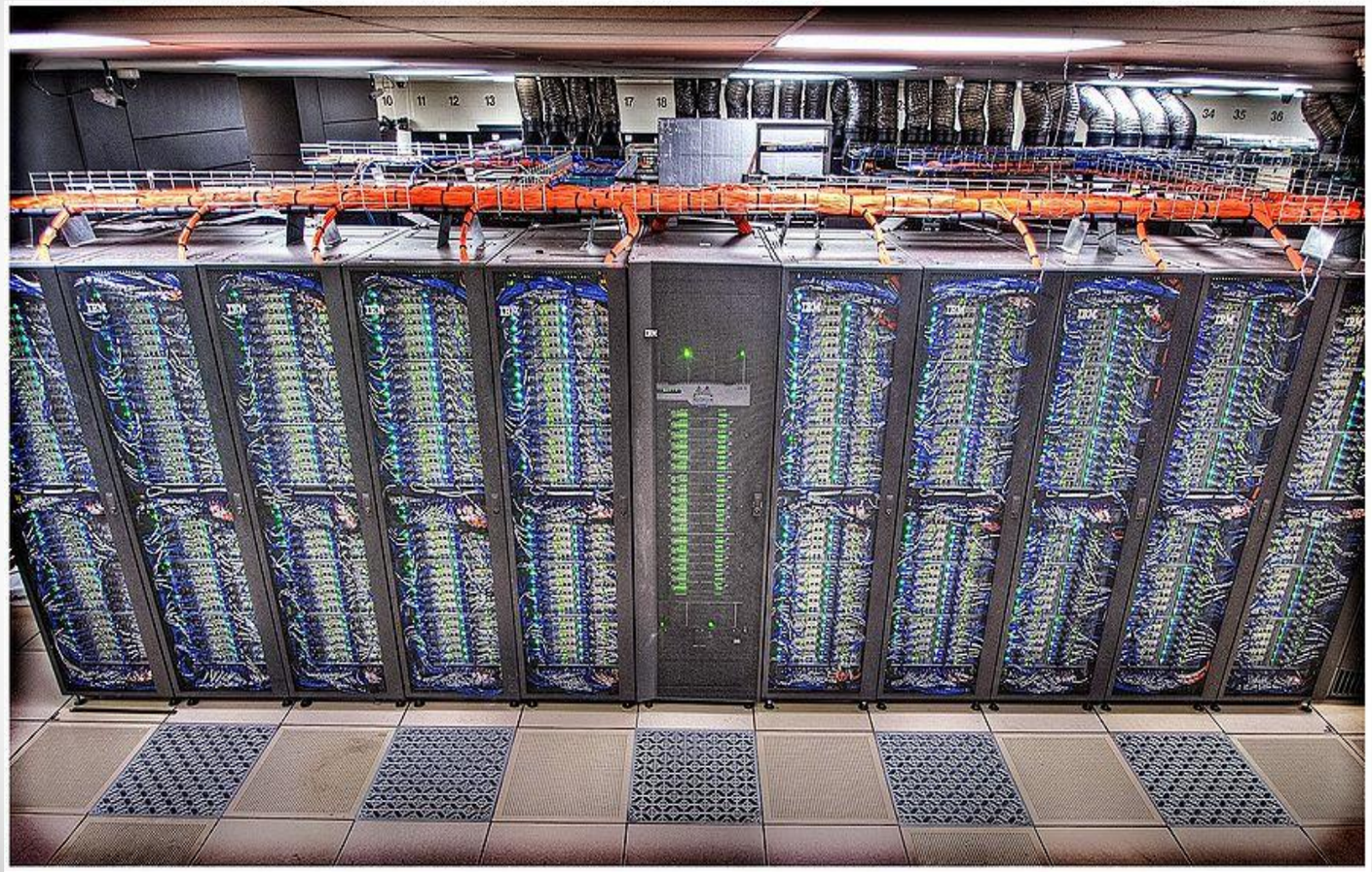
Outline

- Parallel programming models
- Layout of an MPI program
- Compiling and running an MPI program
- Basic MPI concepts
- Point-to-point communication
- Collective communication

To setup examples, type: /scratch/training/mpi/setup.sh (terra and ada)

tamu github repo: git@github.tamu.edu:pennings/hprc_shortcourse_mpi.git

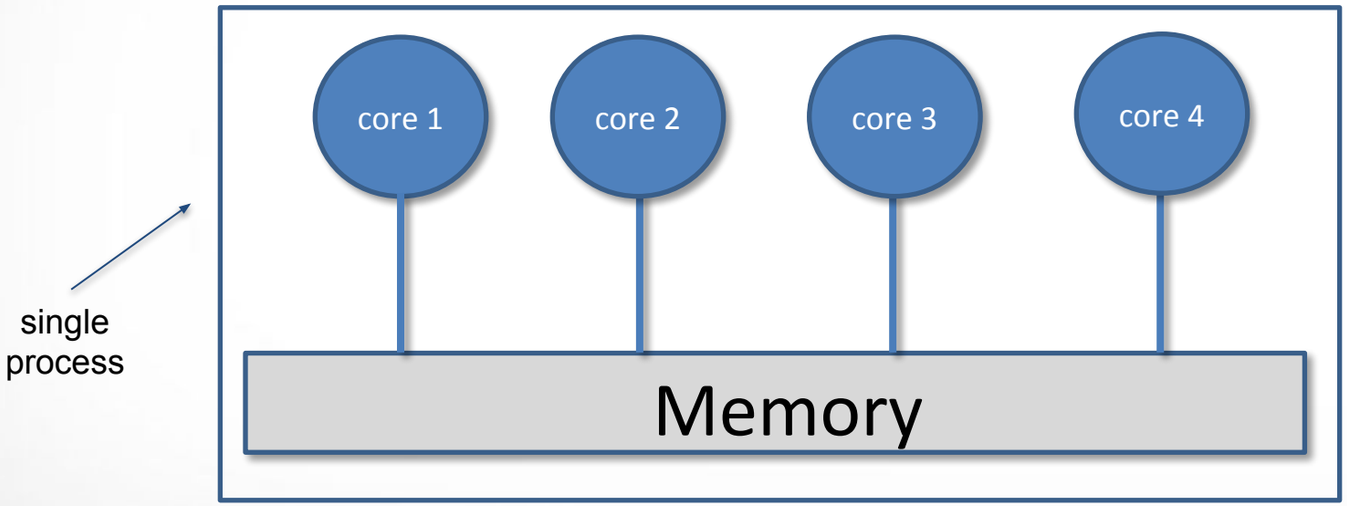
HPRC Systems Summary



- terra: 304 compute nodes, 28 cores per node, 64GB per node
- ada: 852 compute nodes, 20 cores per node. 64GB per node
- *grace: 917 compute nodes, 48 cores per node, 384GB per node*

Parallel Programming Models

- Shared Memory System – an abstraction of a parallel system where all processors share the same memory subsystem



Examples:

- single terra/ada node
- your desktop/laptop

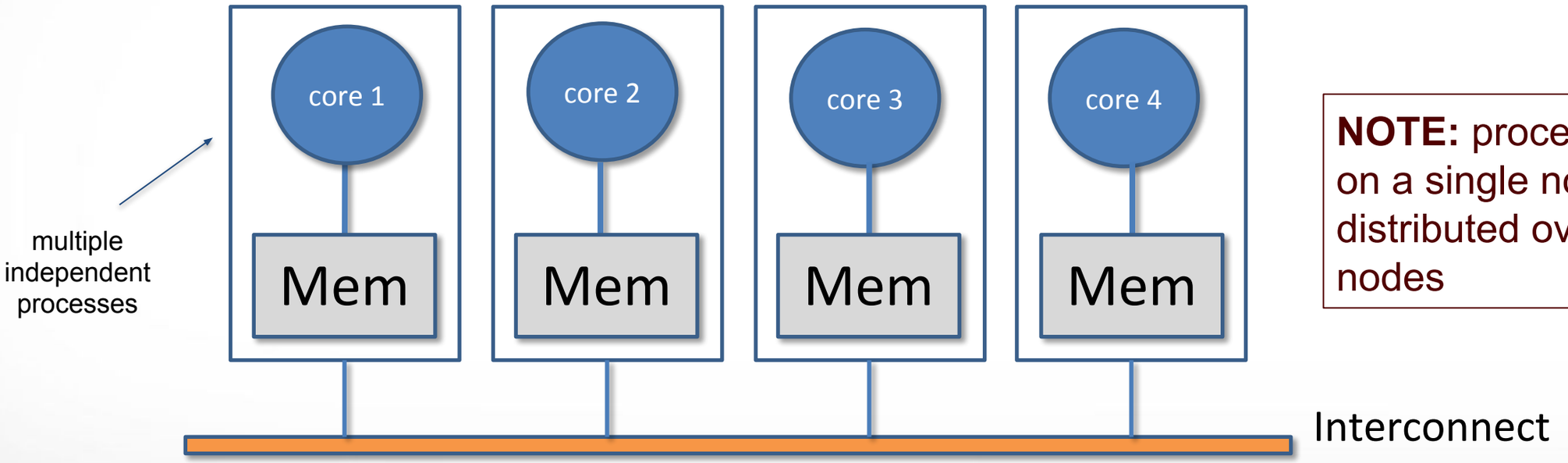
NOTE: every node on terra has 28 cores (48 on grace and 20 on ada). Average desktop/laptop has 4 - 8 cores

Programming model for shared memory Systems: OpenMP

(OpenMP is most popular programming model for shared memory parallelism)

Parallel Programming Models

- Distributed Memory System – an abstraction of a parallel system where each processor has its own local memory

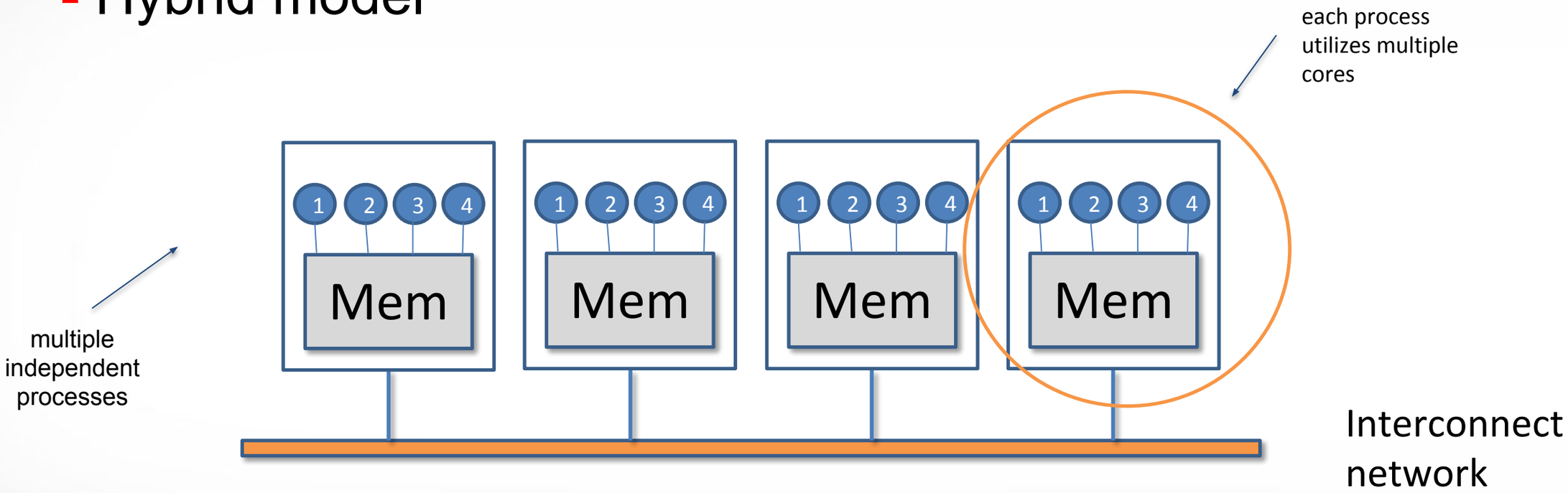


NOTE: processes can be on a single node or distributed over multiple nodes

Programming model for distributed memory Systems: MPI

Parallel Programming models

- Hybrid model



Hybrid Programming model: MPI + OpenMP

(for example: one MPI task per node with 4 OpenMP threads per MPI task)

What is MPI?

- **M**essage **P**assing **I**nterface: a specification for the library interface that implements message passing in parallel programing.
- Is standardized by the MPI forum for implementing portable, flexible, and reliable codes for **distributed memory systems**, regardless of underneath architecture.
  - First edition: MPI-1(1994)
  - Evolving over time: MPI-2(1998), MPI-3(2012), MPI-3.1(2015)
  - MPI-4.0 is under discussion (last draft specification November 2020)
- Has C/C++/Fortran bindings.
  - C++ binding deprecated since MPI-2.2
- Different implementations (libraries) available: **Intel MPI**, MPICH, OpenMPI, etc.
- It is the most widely used parallel programing paradigm for large scale scientific computing.

Example 1: Hello World (C/C++)

Serial C Code

```
#include <stdlib.h>

int main(int argc, char **argv){

    printf("Hello, world\n");

}
```

Parallel C Code Using MPI

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

int main(int argc, char **argv){
    MPI_Init(&argc, &argv);
    printf("Hello, world\n");
    MPI_Finalize();
}
```

Example 1: Hello World (Fortran)

Serial Fortran Code

```
program hello
implicit none


print *, “Hello, world”

end program hello
```

Parallel Fortran Code using MPI

```
program hello
use mpi
implicit none

call MPI_INIT(ierr)
print *, “Hello, world”
call MPI_Finalize(ierr)
end program hello
```

demo example1-hello_world. How to compile?

Compiling and Linking MPI Programs

We will use Intel MPI implementation in the examples

(Using Intel compiler underneath)

```
mpiicc    prog.c   [flags] -o prog.exe   (C)
mpiicpc    prog.cpp [flags] -o prog.exe   (C++)
mpiifort prog.f   [flags] -o prog.exe   (Fortran)
```

(Using GNU compilers underneath)

```
mpicc     prog.c   [flags] -o prog.exe   (C)
mpicxx    prog.cpp [flags] -o prog.exe   (C++)
mpif90    prog.f   [flags] -o prog.exe   (Fortran)
```

don’t forget to load an mpi toolchain. We will use intel/2019b here

demo how to compile? Try to run

Running an MPI Program

- Load the module

```
module load intel/2019b
```

- Use mpirun to run your program

```
mpirun -np n [options] prog.exe [prog_args]
(n is number of "tasks" that will be started
```

- Useful MPI options

```
-ppn/-perhost, -hosts, -hostfile
example:mpirun -np 4 -hosts login1,login2 -ppn 1 mympi.exe
(NOTE: some flags are specific per MPI implementation)
```

how are tasks distributed?

NOTE: When testing always try on single node before running on multiple nodes

https://hprc.tamu.edu/wiki/Ada:Compile:All#MPI_Programs

run example, single/multiple node, also use hostname

Running MPI Program in Batch

ada

```
#BSUB -J MPIBatchExample
#BSUB -L /bin/bash
#BSUB -W 24:00
#BSUB -n 40
#BSUB -R "span[ptile=20]"
#BSUB -R "rusage[mem=2560]"
#BSUB -M 2560
#BSUB -o MPIBatchExample.%J

module load intel/2019b
mpirun prog.exe
```

terra/grace

```
#!/bin/bash
#SBATCH --export=NONE
#SBATCH --get-user-env=L
#SBATCH --job-name=MPIBatchExample
#SBATCH --time=24:00:00
#SBATCH --ntasks=56
#SBATCH --ntasks-per-node=28
#SBATCH --mem=56000M
#SBATCH --output=MPIBatchExample.%j

module load intel/2019b
mpirun prog.exe
```

No need to specify number of tasks when running MPI jobs using the batch system?

Layout of an MPI Program

C

```
#include <mpi.h>
int main(
   int argc, char **argv)
{
   …        no mpi calls
   MPI_Init(&argc, &argv);

   MPI_Finalize();
   …        no mpi calls
}
```

mpi calls happen here

multiple concurrent **processes** execute at their own pace unless synchronization is applied.

Fortran

```
PROGRAM SAMPLE1
USE MPI !F90
!f77: include "mpif.h"
integer ierr
…    no mpi calls
CALL MPI_INIT(ierr)

CALL MPI_FINALIZE(ierr)
…    no mpi calls
END PROGRAM SAMPLE1
```

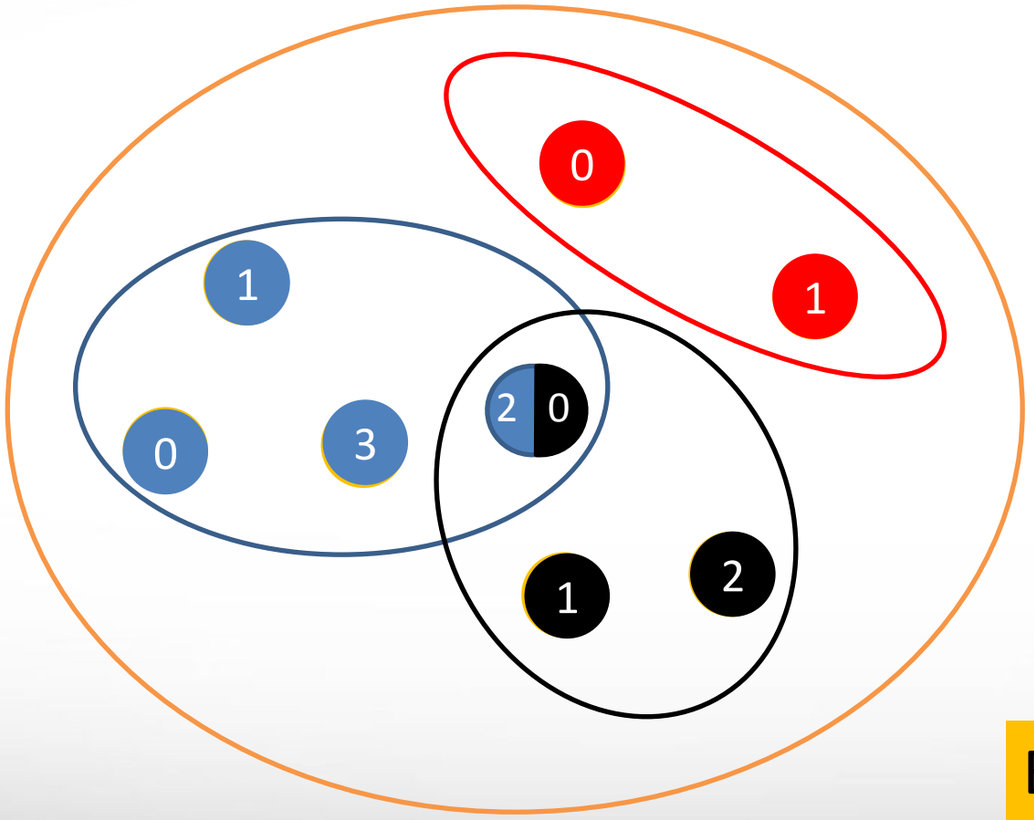
mpi calls happen here

MPI Communicator

- A communicator is a software structure that specifies and maintains a group of processes.
- Each process (also named task) inside a communicator is assigned a unique rank (an integer) ranging from 0 to (group_size -1). group_size is the size of the communicator.
- The constant **MPI_COMM_WORLD** (obtained from MPI include file) is the main communicator that includes all the MPI tasks spawned by mpirun
- Communicators are especially useful for characterizing the tasks that different groups of processes carry out.

MPI Communicator

communicator, size, rank



Communicator: MPI_COMM_WORLD
Size: 8
Rank: 0, 1, …, 7
Communicator: comm1
Size: 2
Rank: 0, 1
Communicator: comm2
Size: 4
Rank: 0, 1, 2, 3
Communicator: comm3
Size: 3
Rank: 0, 1, 2

Every MPI communication must specify a communicator.

Size and Rank

- How many processes in a communicator?

C	`int MPI_Comm_size(MPI_Comm comm, int *size)`
Fortran	`SUBROUTINE MPI_COMM_SIZE(comm, size, ierr)` `integer comm, size, ierr`

- What's the rank (id) of each process in a communicator?

C	`int MPI_Comm_rank(MPI_Comm comm, int *rank)`
Fortran	`SUBROUTINE MPI_COMM_RANK(comm, rank, ierr)` `integer comm, rank, ierr`

exercise ex1_hello_tasks

Example: Hello world (part 2)

C

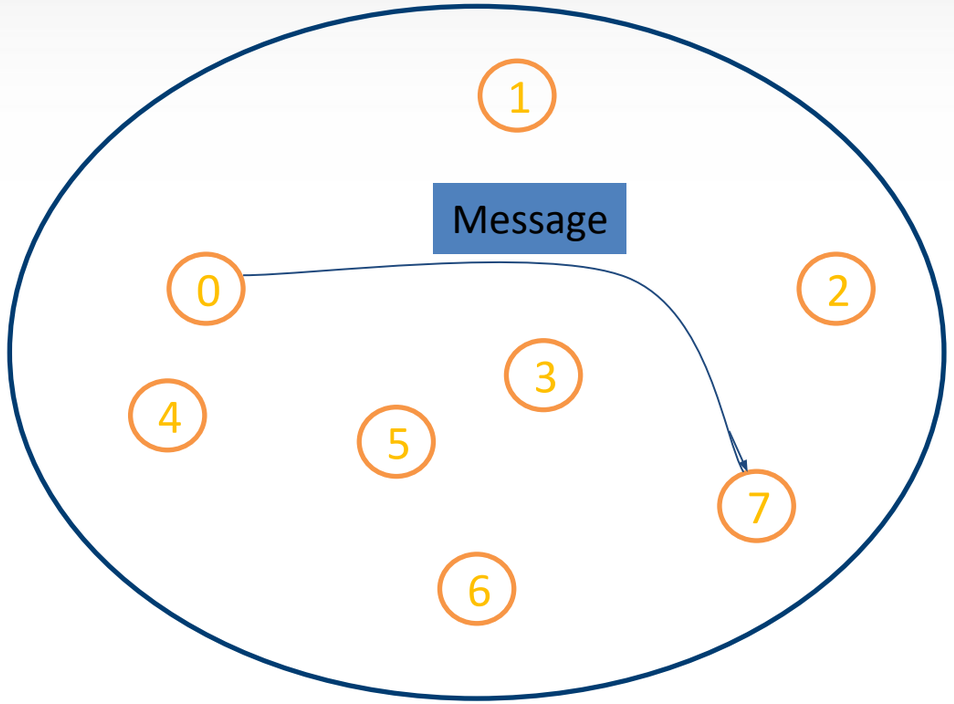
```
#include <stdlib.h>
#include <mpi.h>

int main(int argc, char **argv){
   int np, rank, number;
   MPI_Status status;

   MPI_Init(&argc, &argv);

   MPI_Comm_size(MPI_COMM_WORLD, &np);
   MPI_Comm_rank(MPI_COMM_WORLD, &rank);

    fprinf("Hello from task %d out of %d tasks",rank,np);
    MPI_Finalize();
}
```

Fortran

```
program simple
use mpi
implicit none
integer ierr, np, rank, number, status ;

call MPI_INIT(ierr)

call MPI_COMM_SIZE(MPI_COMM_WORLD, np, ierr)
call MPI_COMM_RANK(MPI_COMM_WORLD, rank, ierr)

print *, "hello  from task ", rank, "out of ", np, " tasks"

call MPI_Finalize(ierr)
end program simple
```

exercise ex1

Point-to-Point Communication



- Blocking `MPI_Send, MPI_Recv`
- Non-blocking `MPI_Isend, MPI_Irecv`
- Send-Receive `MPI_Sendrecv`

Blocking Send

C

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

Fortran

```
MPI_SEND(buf, count, datatype, dest, tag, comm, ierr)
<type> buf(*)
integer count, datatype, dest, tag, comm, ierr
```

buf	starting address of send buffer
count	number of elements in send buffer
datatype	datatype of each send buffer element
dest	rank of destination
tag	message tag
comm	communicator

Blocking Receive

C

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

Fortran

```
MPI_RECV(buf, count, datatype, source, tag, comm, status, ierr)
<type> buf(*)
integer count, datatype, source, tag, comm, ierr, status[MPI_STATUS_SIZE]
```

buf	initial address of receive buffer
count	number of elements in receive buffer
datatype	datatype of each receive buffer element
source	rank of source or MPI_ANY_SOURCE
tag	message tag or MPI_ANY_TAG
comm	communicator
status	status object

MPI_ANY_SOURCE and MPI_ANY_TAG are MPI defined wildcards.

example2-send_receive

Example 2 – One Sender and One Receiver

C

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

int main(int argc, char **argv){
   int np, rank, number;
   MPI_Status status;
   MPI_Init(&argc, &argv);
   MPI_Comm_size(MPI_COMM_WORLD, &np);
   MPI_Comm_rank(MPI_COMM_WORLD, &rank);
   if (rank == 0){
      number = 1234;
      MPI_Send(&number, 1, MPI_INT, 1, 0,
                  MPI_COMM_WORLD);
     printf("Process %d sends %d to process 1\n", rank,
number);
   }else if(rank == 1){
      MPI_Recv(&number, 1, MPI_INT, 0, 0,
                  MPI_COMM_WORLD, &status);
     printf("Process %d receives %d from process 0\n",
rank,number);
   }
   MPI_Finalize();
}
```

Fortran

```
program simple
use mpi
implicit none
integer ierr, np, rank, number, status ;
call MPI_INIT(ierr)
call MPI_COMM_SIZE(MPI_COMM_WORLD, np, ierr)
call MPI_COMM_RANK(MPI_COMM_WORLD, rank, ierr)
if (rank == 0) then
   number = 1234
   call MPI_SEND(number, 1, MPI_INTEGER 1, 0,
                  MPI_COMM_WORLD, ierr)
   print *, "process ", rank, " sends ", number

else if (rank == 1) then
   call MPI_RECV(number, 1, MPI_INTEGER, 0, 0, MPI_COMM_WORLD,
status, ierr)
   print *, "process ",rank," receives ", number
endif
call MPI_Finalize(ierr)
end program simple
```

example2-send_receive

Send and Receive a Message

```
program simple
use mpi
implicit none
integer ierr, np, rank, number, status ;

if (rank == 0) then
   number = 1234
   call MPI_SEND(number, 1, MPI_INTEGER 1, 0, MPI_COMM_WORLD, ierr)
   print *, "process ", rank, " sends ", number

else if (rank ==
   call MPI_REC                , 1, MI                , 0, 0, MPI_COMM_WORLD, status, ierr)
   print *, "process ",rank," receives ", number
endif

call MPI_Finalize(ierr)
end program simpleC
```

Destination

Data | Envelope

MPI_SEND(number, 1, MPI_INTEGER, 1, 0, MPI_COMM_WORLD, ierr)

MPI_RECV(number, 1, MPI_INTEGER, 0, 0, MPI_COMM_WORLD, status, ierr)

Buffer starting address

Data count

MPI datatype

source

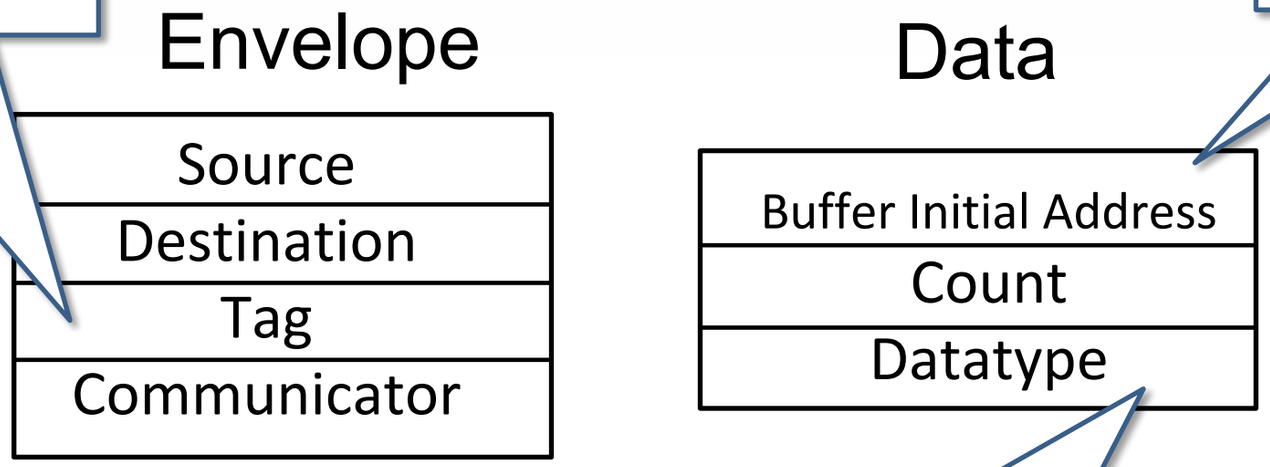
tag

communicator

Message

Tag is an integer used in a message to differentiate one message from other messages.

Where to fetch/store the data



Type of the data to be sent or received. Datatype can be predefined or user defined.
Commonly used predefined datatypes, also called MPI basic datatypes in Fortran:
MPI_INTEGER, MPI_REAL, MPI_REAL8, MPI_CHARACTER, MPI_LOGICAL

Comments on Blocking Send

MPI_SEND(buf, count, datatype, dest, tag, comm)

- The calling process sends a contiguous block of data (count elements, type datatype), starting at buf.
- The message sent by MPI_SEND can be received by either MPI_RECV or MPI_IRECV.
- MPI_SEND doesn't return (i.e., blocked) until it is safe to write to the send buffer.
  - Safe means the message has been copied either into a system buffer, or into the receiver's buffer, depending on which mode the send call is currently working under (see https://www.codingame.com/playgrounds/349/introduction-to-mpi/communication-modes for the various modes)

Comments on Blocking Receive

```
MPI_RECV(buf,count,datatype,source,tag,comm,status)
```

- The calling process attempts to receive a message with specified envelope (source, tag, communicator).
  - **MPI_ANY_SOURCE** and **MPI_ANY_TAG** are valid values.
- When the matching message arrives, elements of the specified datatype are placed in the buffer, starting at the address buf.
- The buffer starting at buf is assumed pre-allocated and has capacity for at least count many datatype elements.
  - An error returns if buf is smaller than amount of data received.

Comments on Blocking Receive

```
MPI_RECV(buf,count,datatype,source,tag,comm,status)
```

- MPI_RECV can receive a message send by MPI_SEND or MPI_ISEND.
- Agreement in datatype between the send and receive is required.
- MPI_RECV is blocked until the message has been copied into buf.
- The actual size of the message received can be extracted with MPI_GET_COUNT.

Return Status

- The argument status in MPI_Recv provides a way of retrieving message source, message tag, and message error from the message.
- status is useful when MPI wildcards (MPI_ANY_SOURCE, MPI_ANY_TAG) are used in MPI_Recv.
- status can be ignored with MPI_STATUS_IGNORE

C

```
MPI_Status status
…
MPI_Recv(…,&status)
Source_id = status.MPI_SOURCE
tag       = status.MPI_TAG
```

Fortran

```
integer status(MPI_STATUS_SIZE)
…
CALL MPI_RECV(…,status,ierr)
source_id = status(MPI_SOURCE)
tag       = status(MPI_TAG)
```

Timing

MPI_WTIME()

- returns a floating-point number in seconds, representing elapsed wall clock time since some time in the past.

C/C++

```
double t1, t2, elapsed;
t1 = MPI_Wtime();
…
// code segment to be timed
…
t2 = MPI_Wtime();
elapsed = t2 – t1;
```

Fortran

```
real*8 t1, t2
real*8 elapsed
t1 = MPI_WTIME()
…
! Code segment to be timed
…
t2 = MPI_WTIME()
elapsed = t2 – t1
```

Case Study: Computing Pi (1)

Monte Carlo method to compute Pi:

- **assume a circle with radius 1, the enclosing box will be 2 by 2**
- **surface of circle = pi*r^2 = pi*1^2 = pi , surface enclosing box = 2*2=4**
- **if you pick a very large number of random points (x and y between 0 and 1) the fraction of the number of points inside the circle will be pi/4. To compute pi:**
  - **Generate a large number of random points (x,y)**
  - **Count #points inside the circle (inside if sqrt(x^2+y^2) <= 1)**
  - **#inside / #total == pi/4 → pi = (4*#inside)/#total**

First (very naive) Attempt

1. Root distributes the large array of random points among all the tasks
2. every task locally computes #points inside the circle
3. every task sends local #points back to root
4. root adds up all the local #points and computes pi using the formula

Non-blocking Send

MPI_ISEND(buf, count, datatype, dest, tag, comm, request)

IN	buf	initial address of send buffer
IN	count	number of elements in send buffer (non-negative integer)
IN	datatype	datatype of each send buffer element
IN	dest	rank of destination
IN	tag	message tag
IN	comm	communicator
OUT	request	communication request (a handle that can be used later to refer the outstanding receive)

Non-blocking Receive

MPI_IRECV(buf, count, datatype, source, tag, comm, request)

IN	buf	initial address of send buffer
IN	count	number of elements in receive buffer (non-negative integer)
IN	datatype	datatype of each receive buffer element
IN	source	rank of source or MPI_ANY_SOURCE
IN	tag	message tag or MPI_ANY_TAG
IN	comm	communicator
OUT	request	communication request (a handle that can be used later to refer the outstanding receive)

Auxiliary Routines for Non-blocking Send/Receive

- Auxiliary routines are used to complete a non-blocking communication or communications.
- Commonly used auxiliary routines:

MPI_Wait(request, status)	The calling process waits for the completion of a non-blocking send/receive identified by *request*.
MPI_Waitall(count, requests, statuses)	The calling process waits for all pending operations in a list of *requests*.
MPI_Test(request, flag, status)	The calling process tests a non-blocking send/receive specified by *request* has completed delivery/receipt of a message.

Non-blocking Send/Receive

- A non-blocking send/receive call initiates the send/receive operation, and returns immediately with a request handle, before the message is copied out/into the send/receive buffer.
- A separate send/receive complete call is needed to complete the communication before the buffer can be accessed again.
- A non-blocking send can be matched by a blocking receive; a non-blocking receive can be matched by a blocking send.
- Used correctly, non-blocking send/receive can improve program performance.
- They also make the point-to-point transfers “safer” by not depending on the size of the system buffers.
  - No deadlock caused by unavailable buffer
  - No buffer overflow

MPI_WAIT

MPI_WAIT(request, status)

request	request (handle)
status	status object (Status)

C

```
MPI_Request request;
MPI_Status  status;
…
MPI_Irecv(recv_buf,count,…,
                  comm,&request);

//do some computations …

MPI_Wait(&request, &status);
```

Fortran

```
integer request
integer status(MPI_STATUS_SIZE)
…
call MPI_IRECV(recv_buf,count,…&
                     comm,request,ierr)

!do some computations …

call MPI_WAIT(request,status,ierr)
```

status can be ignored with MPI_STATUS_IGNORE

MPI_WAITALL

MPI_WAITALL(count, requests, statuses)

count	lists length (non-negative integer)
requests	array of requests (array of handles)
statuses	array of status objects (array of Status)

C

```
MPI_Request reqs[4];
MPI_Status  status[4];
…
MPI_Isend(…,&reqs[0]);
MPI_Irecv(…,&reqs[1]);
MPI_Isend(…,&reqs[2]);
MPI_Irecv(…,&reqs[3]);
…
… do some com computations …
…
MPI_Waitall(4,reqs,statuses);
```

Fortran

```
integer reqs(4)
integer statuses(MPI_STATUS_SIZE,4)
…
call MPI_ISEND(…,reqs(1),ierr)
call MPI_IRECV(…,reqs(2),ierr)
call MPI_ISEND(…,reqs(3),ierr)
call MPI_IRECV(…,reqs(4),ierr)
…
… do some computations …
…
call
MPI_WAITALL(4,reqs,statuses,ierr)
```

status can be ignored with MPI_STATUSES_IGNORE

example4-non_blocking_send_receive

Example 4 (non blocking send)

C

```
MPI_Request *requests;
   ….
if (rank == 0){
   printf("Type any number from the input: ");
   scanf("%d", &number);
   requests = (MPI_Request*)(malloc(npof(MPI_Request)*(np-1)));

   for (i=1; i<np; i++)
      MPI_Isend(&number, 1, MPI_INT, i, 0, MPI_COMM_WORLD,
                                                &requests[i-1]);
   MPI_Waitall(np-1, requests, MPI_STATUSES_IGNORE);
   free(requests);
}else{
   MPI_Recv(&number, 1, MPI_INT, 0, 0, MPI_COMM_WORLD,
                                          MPI_STATUS_IGNORE);
   printf("My id is %d. I received %d\n", rank, number);
}
```

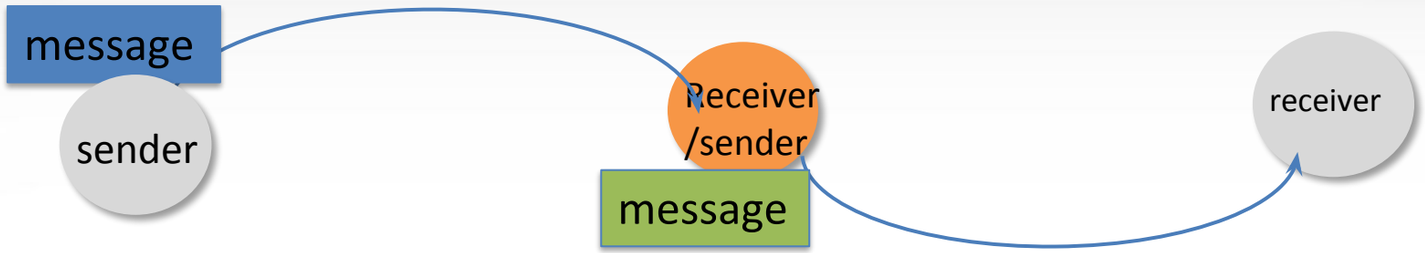
Fortran

```
integer, allocatable::requests(:)
  ….
if (rank == 0) then
   print *, "Type an integer from the input"
   read *, number
   allocate(requests(np-1))
   do i=1, np-1
      call MPI_ISEND(number, 1, MPI_INTEGER, i, 0,   &
                              MPI_COMM_WORLD, ierr)
   enddo
   call MPI_WAITALL(np-1, requests, MPI_STATUSES_IGNORE, ierr)
   deallocate(requests)
else
   call MPI_RECV(number, 1, MPI_INTEGER, 0, 0,    &
                          MPI_COMM_WORLD, MPI_STATUS_IGNORE, ierr)
   print "(2(A,I6))","Process ",rank, " received ", number
endif
```

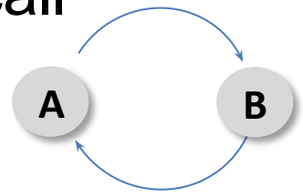
example4-non_blocking_send_receive

Send-Receive

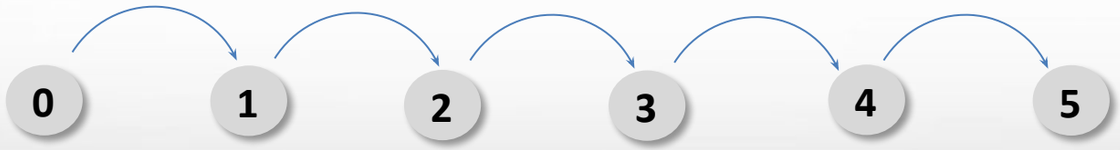
MPI_SENDRECV(sendbuf, sendcount, sendtype, dest, sendtag, recvbuf, recvcount, recvtype, source, recvtag, comm, status)



- Combines send and receive operations in one call
- The source and destination can be the same.



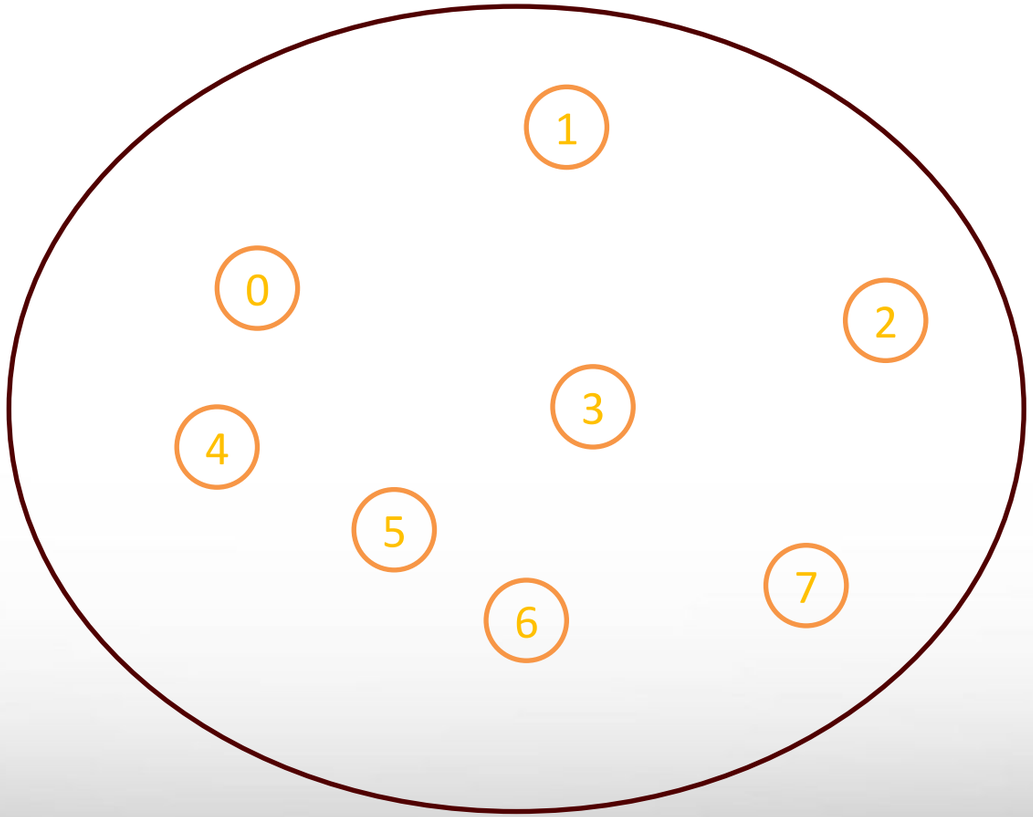
- The message sent out by send-receive can be received by blocking/non-blocking receive or another send-receive
- It can receive a message sent by blocking/non-blocking send or another send-receive.
- Useful for executing a shift operation across a chain of processes.



- Dependencies will be taken care of by the communication subsystem to eliminate the possibility of deadlock.

Collective Communication

- A collective communication refers to a communication that involves all processes in a communicator.



Routines for Collective Communication

MPI_BARRIER	All processes within a communicator will be blocked until all processes within the communicator have entered the call.
MPI_BCAST	Broadcasts a message from one process to members in a communicator.
MPI_REDUCE	Performs a reduction operation to the vector of elements in the sendbuf of the group members and places the result in recvbuf on root.
MPI_GATHER MPI_GATHERV	Collects data from the sendbuf of all processes in comm and place them consecutively to the recvbuf on root based on their process rank.
MPI_SCATTER MPI_SCATTERV	Distribute data in sendbuf on root to recvbuf on all processes in comm.
MPI_ALLREDUCE	Same as MPI_REDUCE, except the result is placed in recvbuf on all members in a communicator.
MPI_ALLGATHER MPI_ALLGATHERV	Same as GATHER/GATHERV, except now data are placed in recvbuf on all processes in comm.

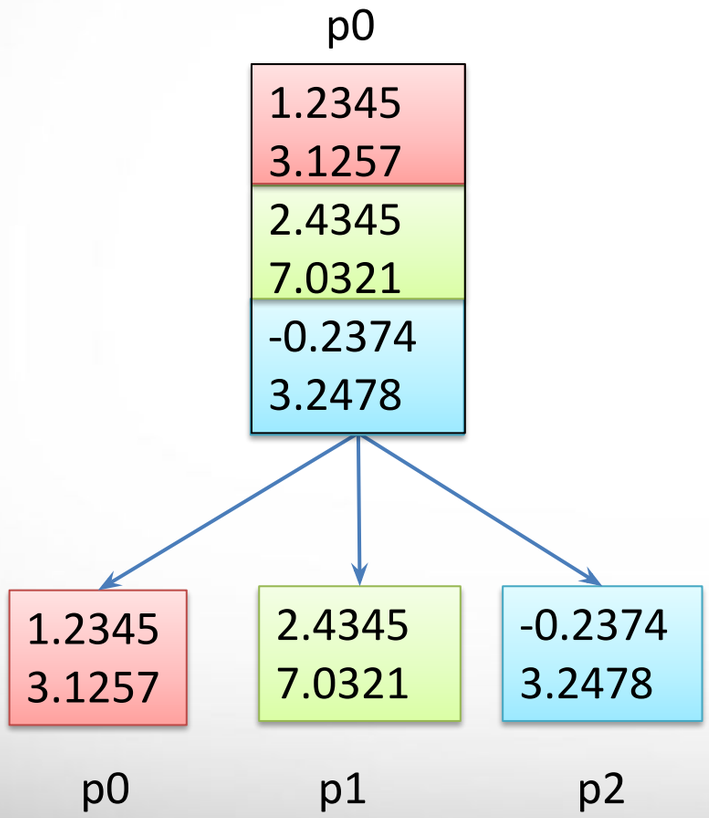
MPI_BARRIER

MPI_BARRIER(comm)

- Blocks all processes in comm until all processes have called it.
- Is used to synchronize the progress of all processes in comm.

MPI_SCATTER

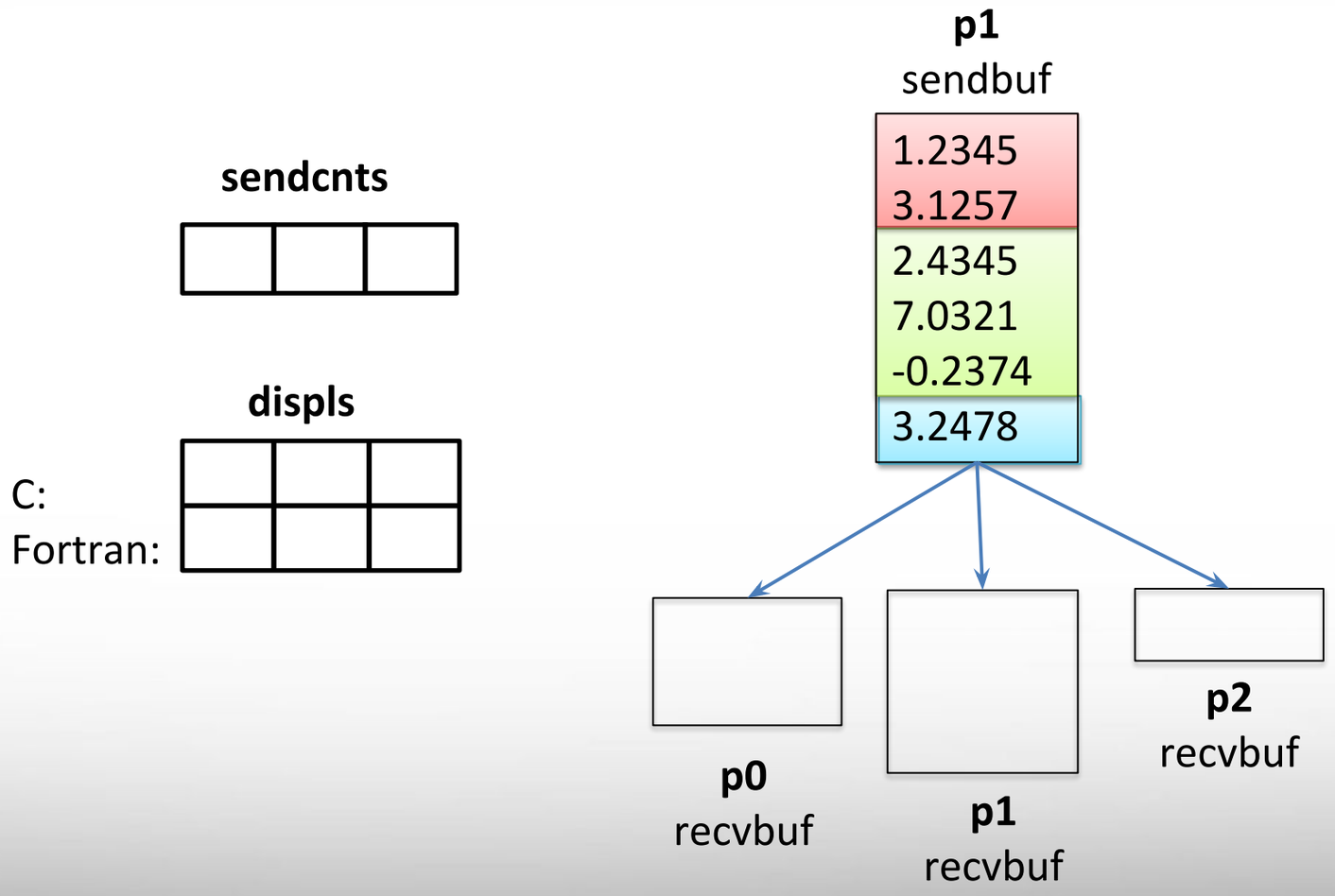
MPI_SCATTER(sendbuf, sendcnt, sendtype, recvbuf, recvcnt, recvtype, root, comm)



- Scatters data from root to all tasks in comm
- Data Sent by root is assigned by rank order.
- sendcnt is number of elements send to each task
- sendbuf, sendcnt, sendtype are significant only at root.

MPI_SCATTERV

MPI_SCATTERV(sendbuf, sendcnts, displs, sendtype, recvbuf, recvcnt, recvtype,root,comm)



MPI_SCATTERV

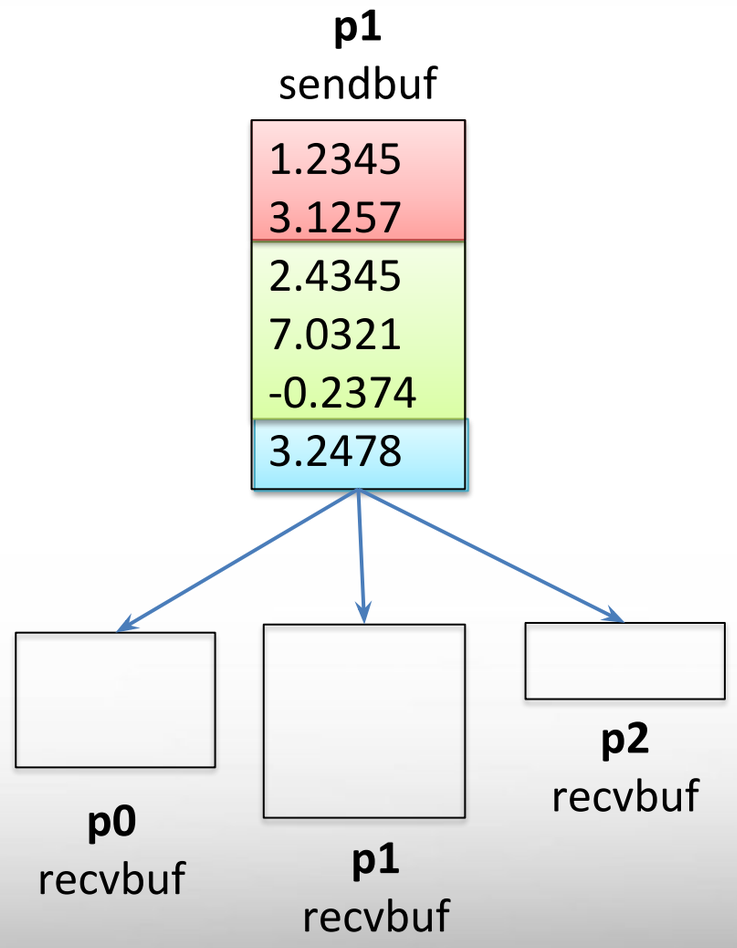
MPI_SCATTERV(sendbuf, sendcnts, displs, sendtype, recvbuf, recvcnt, recvtype,root,comm)

sendcnts

2	3	1

displs

C:	0	2	5
Fortran:	1	3	6



MPI_SCATTERV

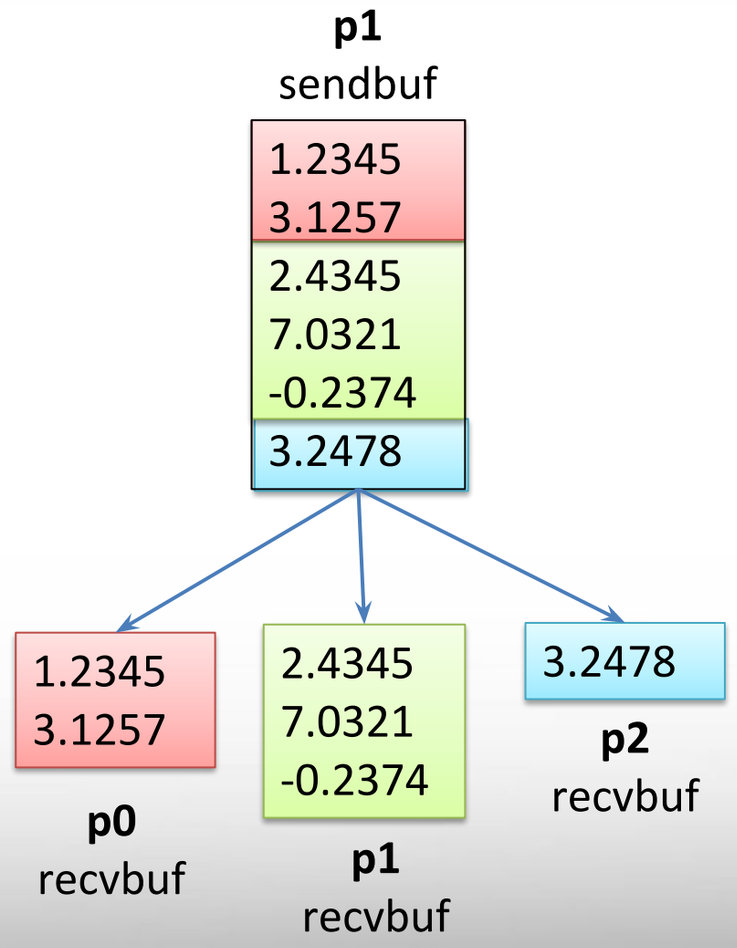
MPI_SCATTERV(sendbuf, sendcnts, displs, sendtype, recvbuf, recvcnt, recvtype,root,comm)

sendcnts

2	3	1

displs

C:	0	2	5
Fortran:	1	3	6

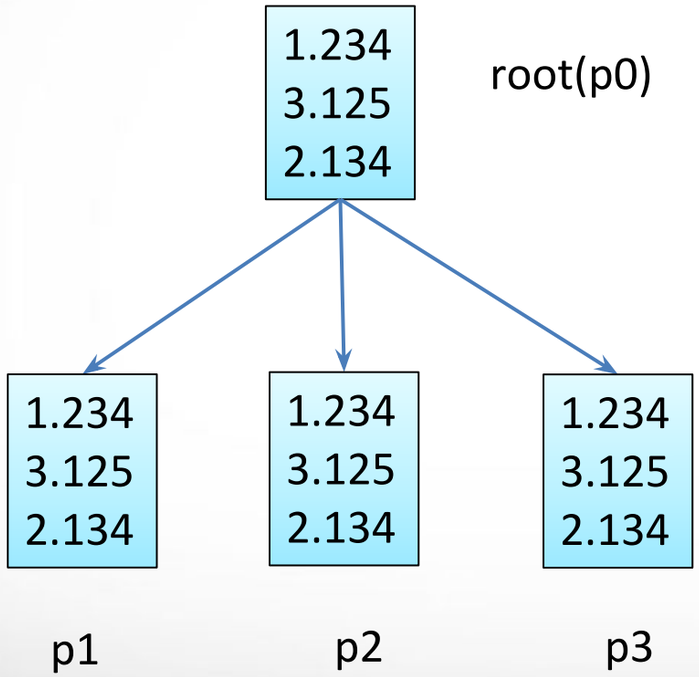


Case Study: Computing Pi (2)

In the first version, the root distributed all the random points one by one among all the tasks. In this exercise, instead of sending all the random points, we will use the MPI_SCATTER function to distribute the input

MPI_BCAST

MPI_BCAST(buf, count, datatype, root, comm)



- root sends count elements of type datatype, starting at buf to all tasks (including root) in communicator comm.
- Non-root tasks receive data from root.
- Each receiving task blocks until the message has arrived in its buffer.
- **All tasks in comm must call this routine.**

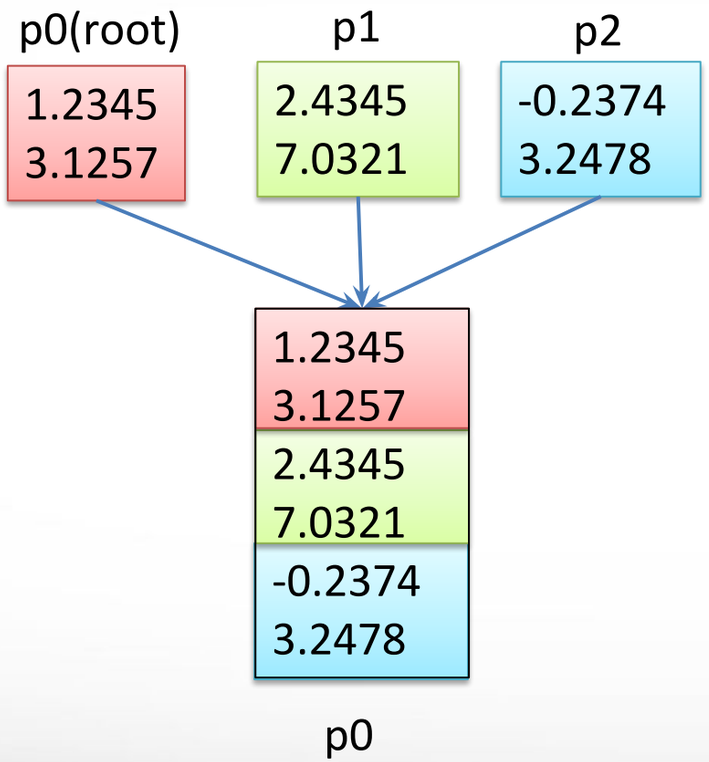
Case Study: Computing Pi (3)

Lets adjust the compute_pi program. Instead of the root sending (or scattering) all the random points, root will only broadcast the total number of points. Every task will generate the random points themselves.

(shows overhead of excessive communication)

MPI_GATHER

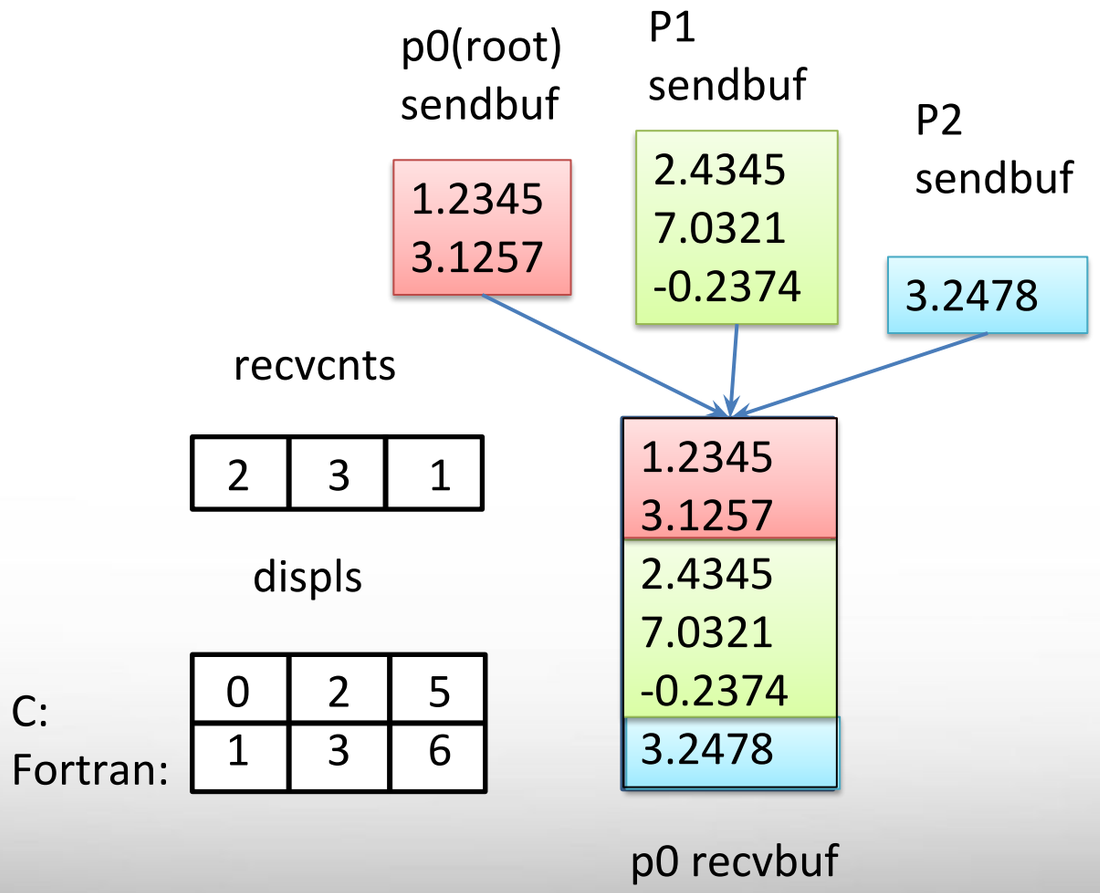
MPI_GATHER(sendbuf, sendcnt, sendtype, recvbuf, recvcnt, recvtype, root, comm)



- Gathers data from all tasks in comm and stores them in task root.
- Data received by root is stored in rank order.
- recvcnt is number of elements received per process
- recvbuf, recvcnt, recvtype are significant only at root.

MPI_GATHERV

MPI_GATHERV(sendbuf, sendcnt, sendtype, recvbuf, recvcnts, displs, recvtype, root, comm)



MPI_ALLGATHER/MPI_ALLGATHERV

MPI_ALLGATHER(sendbuf,sendcnt,sendtype,recvbuf,recvcnt,recvtype,comm)

MPI_ALLGATHERV(sendbuf,sendcnt,sendtype,recvbuf,recvcnts,displs,recvtype,comm)

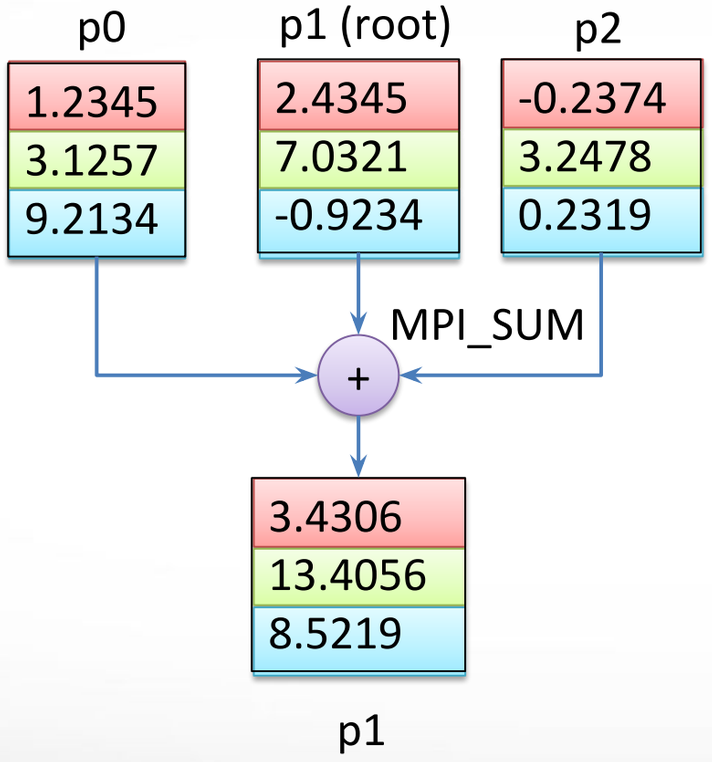
- Same as MPI_GATHER/MPI_GATHERV, except no root.
- Root is not needed since every process in the communicator stores the data gathered in its recvbuff.

Case Study: Computing Pi (4)

In the previous version, all the tasks sent their results back to the root and the root received them one by one and combined (i.e. reduced) the results. In this exercise we will use MPI_GATHER to collect the results

MPI_REDUCE

MPI_REDUCE(sendbuf, recvbuf, count, datatype, op, root, comm)



C: MPI_Op op

Fortran: integer op

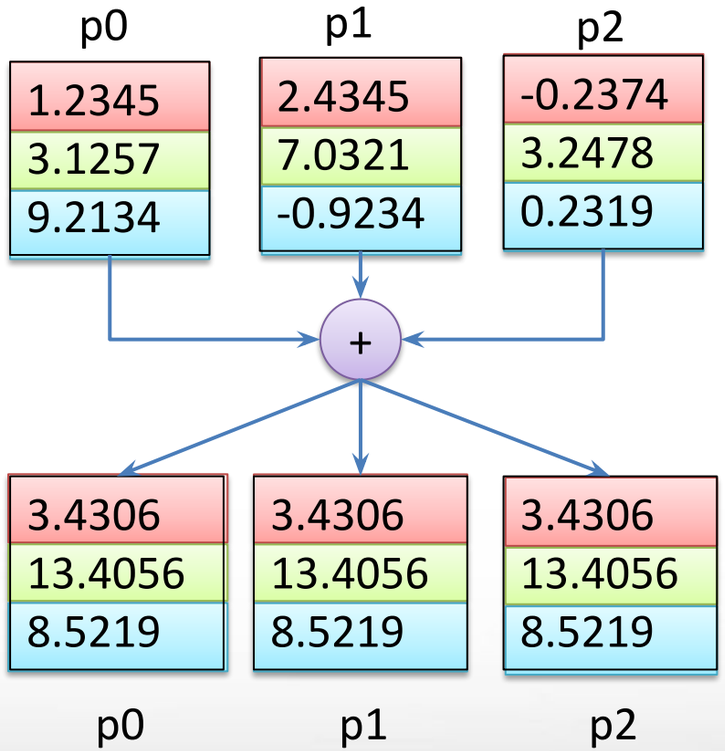
- Performs a reduction operation on all elements with same index in *sendbuf* on all tasks and stores results in *recvbuf* of the root process.
- *recvbuf* is significant only at root.
- *sendbuf* and *recvbuf* cannot be the same.
- The size of *sendbuf* and *recvbuf* is equal to count.

Predefined Reduction Operations

PREDEFINED OPERATIONS	MPI DATATYPES
MPI_SUM, MPI_PROD	MPI_REAL8, MPI_INTEGER, MPI_COMPLEX, MPI_DOUBLE, MPI_INT, MPI_SHORT, MPI_LONG
MPI_MIN, MPI_MAX	MPI_INTEGER, MPI_REAL8, MPI_INT, MPI_SHORT, MPI_LONG, MPI_DOUBLE
MPI_LAND, MPI_LOR, MPI_LXOR	MPI_LOGICAL, MPI_INT, MPI_SHORT, MPI_LONG
MPI_BAND, MPI_BOR, MPI_BXOR	MPI_INTEGER, MPI_INT, MPI_SHORT, MPI_LONG

MPI_ALLREDUCE

MPI_ALLREDUCE(sendbuf, recvbuf, count, datatype, op, comm)



Case Study: Computing Pi (5)

In the previous version, root gathered the partial results and combined (i.e. reduced) the results manually. Let's use MPI_REDUCE to do the last step.

DEMO: matvec

$$A\vec{b} = (\vec{a}_1 \quad \dots \quad \vec{a}_n)\vec{b} = b_1\vec{a}_1 + b_2\vec{a}_2 + \cdots + b_n\vec{a}_n = \vec{c}$$

$\vec{a}_i$ is a column vector.

Use the following steps to calculate the matrix vector multiplicaton:

1. Distribute the columns of matrix A among all the tasks
2. Distribute vector b among all the tasks
3. Each task computes partial mat-vec multiplication ($b_i\vec{a}_i + \cdots + b_j\vec{a}_j$)
4. Root will collect the partial results and combine them to complete the multiplication

What MPI functions do we use to distribute the data and collect the results?

Some final Considerations

- Exploring parallelism
  - Task-parallelism
  - Data-parallelism
- MPI/OMP hybrid programming

Important Note On Using MPI

- All parallelism is explicit: the programmer is responsible for correctly identifying parallelism and implementing parallel algorithms using MPI constructs

Exploring Parallelism

- Task-parallelism: The programmer identifies different tasks of a program and distribute the tasks among different processors
- Data-parallelism: The programmer partitions the data used in a program and distribute them among different processors, each performing similar operations on the subset of data assigned.

3 chefs need to prepare a three-course menu for 12 guests

salad steak desert

Preparing 12 salads

Task 1

Preparing 12 steaks

Task 2

Preparing 12 deserts

Task 3

Task parallelism

4 meals

salad steak desert

4 meals

salad steak desert

4 meals

salad steak desert

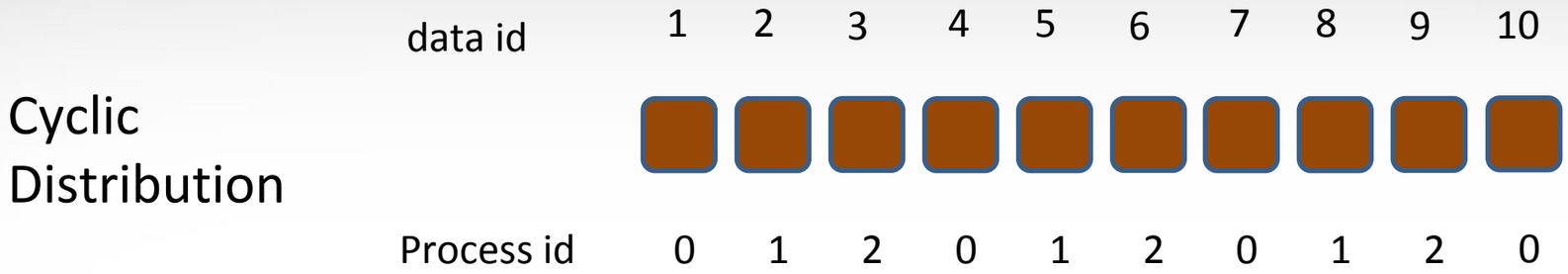
Data parallelism

https://101clipart.com/wp-content/uploads/02/Clipart%20Chef%20Cooking%2012.jpg

https://classroomclipart.com/images/gallery/Clipart/Culinary/chef-thumbs-up-holding-plate-hot-food-clipart-622.jpg

http://www.marbellafamilyfun.com/images/chef-and-waiter-wanted-for-summer-job-from-14th-august-for-2-weeks-21516737.jpg

Data Distribution: cyclic



Data is distributed in a round robin manner among the processes.

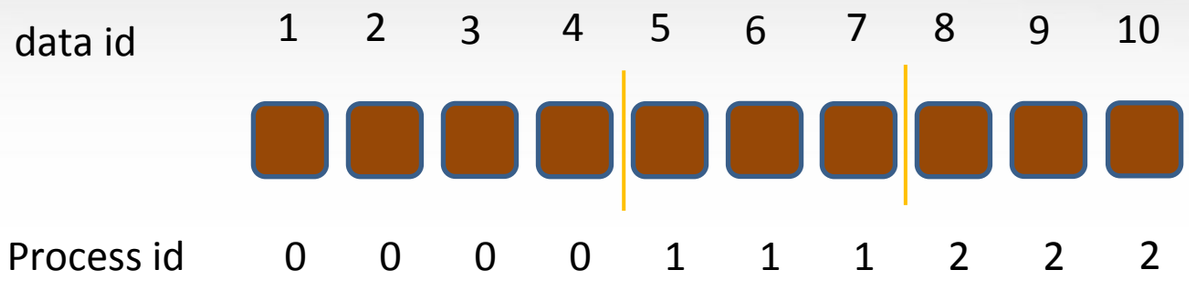
C	Fortran

`for (i=myid+1; i<=N; i+=nprocs){`
`  x = h*(i-0.5);`
`  sum += 4.0/(1.0+x*x);`
`}`
`sum = sum*h;`
	`do i=myid+1, N, nprocs`
	`  x = h*(i-0.5d0)`
	`  sum = sum+4.0d0/(1.0d0+x*x)`
	`enddo`
	`sum = sum*h;`

example6-data_distribution/calc_PI_cyclic

Data Distribution: block

Block Distribution



Data is partitioned into *n* contiguous parts, where *n* is equal to the number of processes. Each process will take one part of the data.

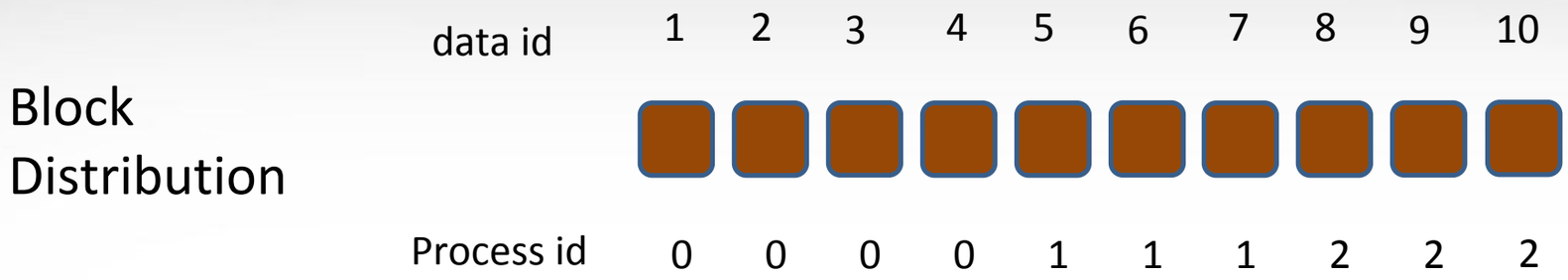
C

```
block_map(1,N,nprocs,myid,&l1,&l2);
for (i=l1; i<=l2; i++){
   x = h*(i-0.5);
   sum += 4.0/(1.0+x*x);
}
sum = sum*h;
```

Fortran

```
call block_map(1,N,nprocs,myid,l1,l2)
do i=l1, l2
   x = h*(i-0.5d0)
    sum = sum + 4.0d0/(1.0d0+x*x)
enddo
sum = sum*h
```

Data Distribution: block



C

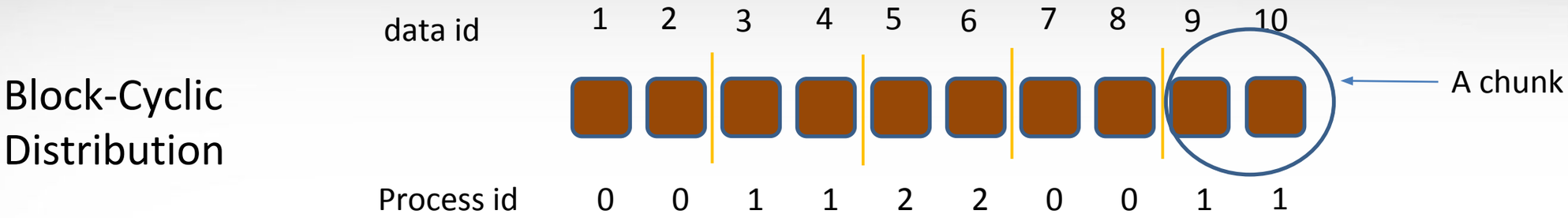
```
void block_map(int n1, int n2,int nprocs,
               int myid, int *l1, int *l2)
{
  int block, rem;
  block = (n2-n1+1)/nprocs;
  rem   = (n2-n1+1)%nprocs;
  if (myid < rem){
    block++;
    *l1 = n1+myid*block;
  }else
    *l1 = n1+rem+block*myid;

  *l2 = *l1+block-1;
}
```

Fortran

```
subroutine block_map(n1,n2, nprocs, myid, l1, l2)
Integer n1, n2, nprocs, myid, l1,l2

integer block, rem
block = (n2-n1+1)/nprocs
rem = mod(n2-n1+1, nprocs)
if (myid < rem) then
    block = block+1
    l1 = n1+myid*block
else
    l1 = n1+rem+block*myid
end if
l2 = l1+block-1
end subroutine block_map
```

example6-data_distribution/calc_PI_block

Data Distribution: block cyclic



Data is divided into chunks of contiguous blocks and the chunks are distributed in a round-robin manner

Loop through chunks

Loop through blocks inside a chunk

C

```
for (i=myid*BLK+1; i<=N; i+=nprocs*BLK){
    for (j=i; j<=MIN(N,i+BLK-1); j++){
        x = h*(j-0.5);
        sum += 4.0/(1.0+x*x);
    }
}
sum = sum*h;
```

Fortran

```
do i=myid*BLK+1, N, nprocs*BLK
   do j=i, MIN(N,i+BLK-1)
       x = h*(j-0.5d0)
       sum = sum+4.0d0/(1.0d0+x*x)
  enddo
enddo
sum = sum*h
```

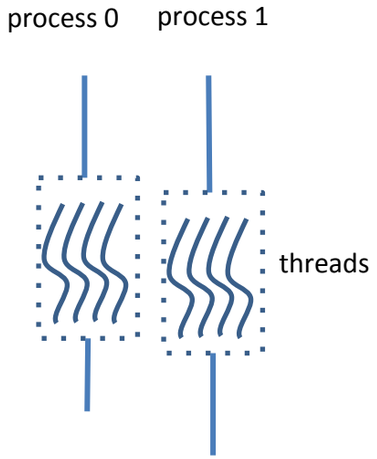
example6-data_distribution/calc_PI_bc

MPI/OpenMP Hybrid Programming

- Simplest and intuitive form:
  master-only: only master thread can execute MPI calls

```
Call MPI_INIT(ierr)
...
Call MPI_SEND(...)
...
!$OMP DO
DO i=1, N
...
ENDDO
!$OMP END DO
...
CALL MPI_FINALIZE(ierr)
```

(no MPI calls in the openMP parallel region)



- Starting MPI-2, the standard provides guidelines on how to interact MPI with threads
- Four levels of thread support
  - MPI_THREAD_SINGLE: Only one thread will execute
  - MPI_THREAD_FUNNELED: Only master thread will make MPI-calls
  - MPI_THREAD_SERIALIZED: Multiple threads may make MPI-calls, but only one at a time
  - MPI_THREAD_MULTIPLE: Multiple threads may call MPI, with no restrictions

MPI_INIT_THREAD(required, provided, ierr)

mpiifort –qopenmp [options] prog.f90 –o prog.exe

Example 9: Hybrid Programming

Int MPI_Init_thread(int *argc, char **argv, int required, int *provided)

MPI_INIT_THREAD(required, provided, ierr)

- Four possible values for the parameter required:
  - MPI_THREAD_SINGLE
  - MPI_THREAD_FUNNELD
  - MPI_THREAD_SERIALIZED
  - MPI_THREAD_MULTIPLE

ex2_single.c

ex2_funnel.c

ex2_serialized.c

ex2_multiple.c

Acknowledgement

- Part of the content is adapted from former Supercomputing Facility staff Mr. Spiros Vellas' introductory MPI short course

Questions?

You can always reach us at help@hprc.tamu.edu