



Introduction to Code Parallelization Using MPI

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Outline

- Why parallel programming
- Parallel programming models
 - OpenMP for Shared Memory System
 - MPI for Distributed Memory System
 - MPI+OpenMP for hybrid systems
- Layout of an MPI program
- Compiling and running an MPI program
- Basic MPI concepts
 - size, rank, communicator, message, MPI datatype, tag
- Point-to-point communication
- Collective communication

Why Parallel Programming

- The semiconductor industry has long ago switched from boosting a single core CPU performance to producing multi-core systems
 - Free performance gain for a serial program has come to an end
- Almost all of today's computers are multi-core systems, ranging from desktops to HPC clusters
- A serial code won't automatically benefit from the multiple cores
- Some applications may take years to get a solution if running in serial
- Parallel programming is the key!

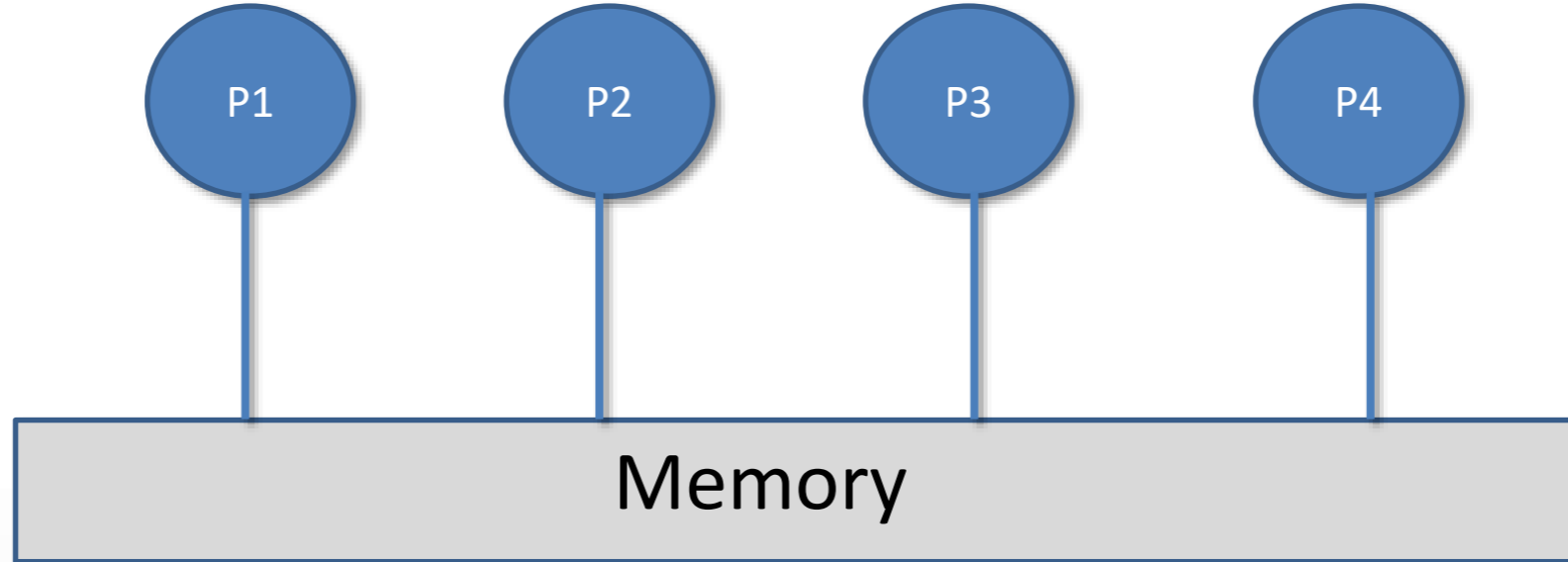
Parallel Computing Systems

We use a **processor** or a CPU **core** to refer to the smallest physical processing unit where a program is executed

- Shared Memory Systems
- Distributed Memory Systems
- Hybrid Systems

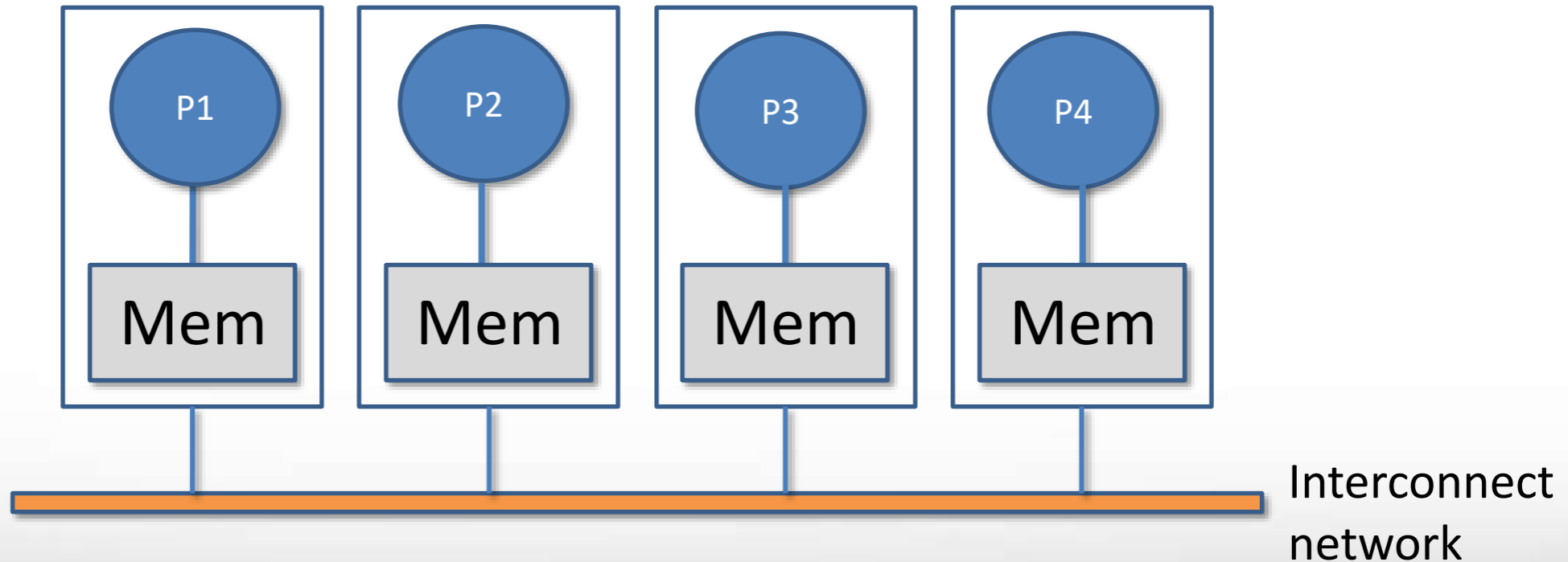
Parallel Computing Systems

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



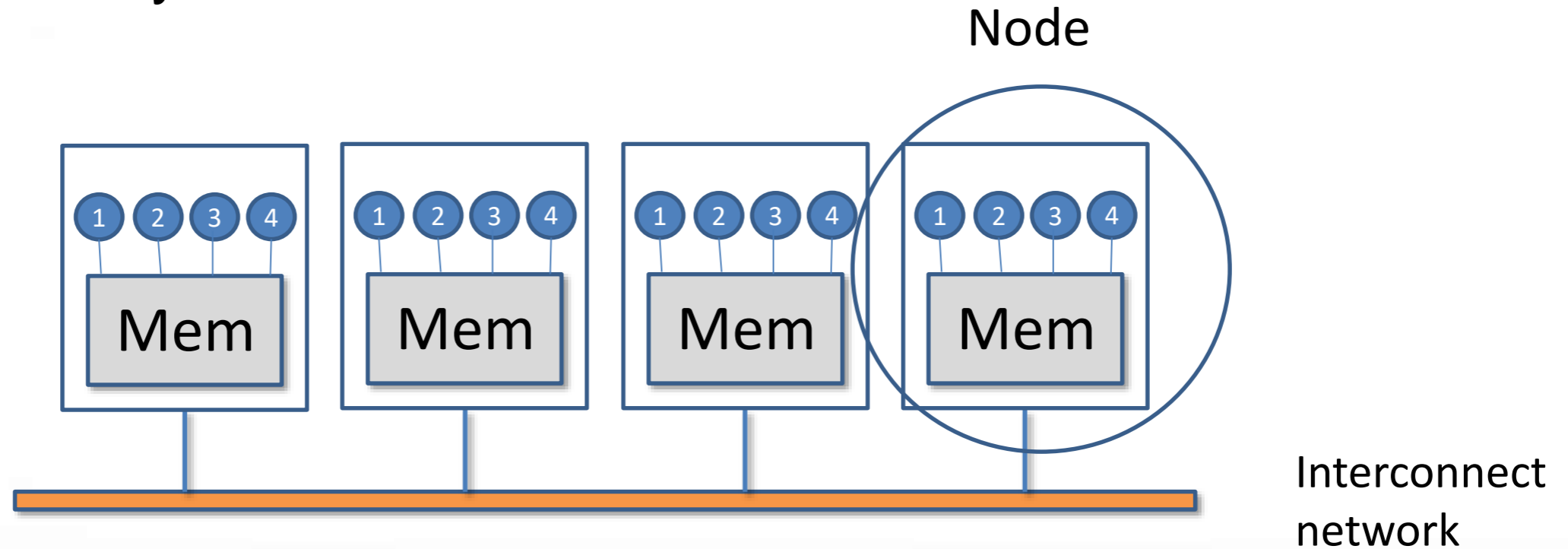
Parallel Computing Systems

- **Distributed Memory System** – an abstraction to a parallel system where each processor has its own local memory and the processors don't share a global memory subsystem.



Parallel Computing Systems

- A Hybrid System



Parallel Programming Models

- Mapping from the parallel programming models to the parallel computing systems

OpenMP

MPI

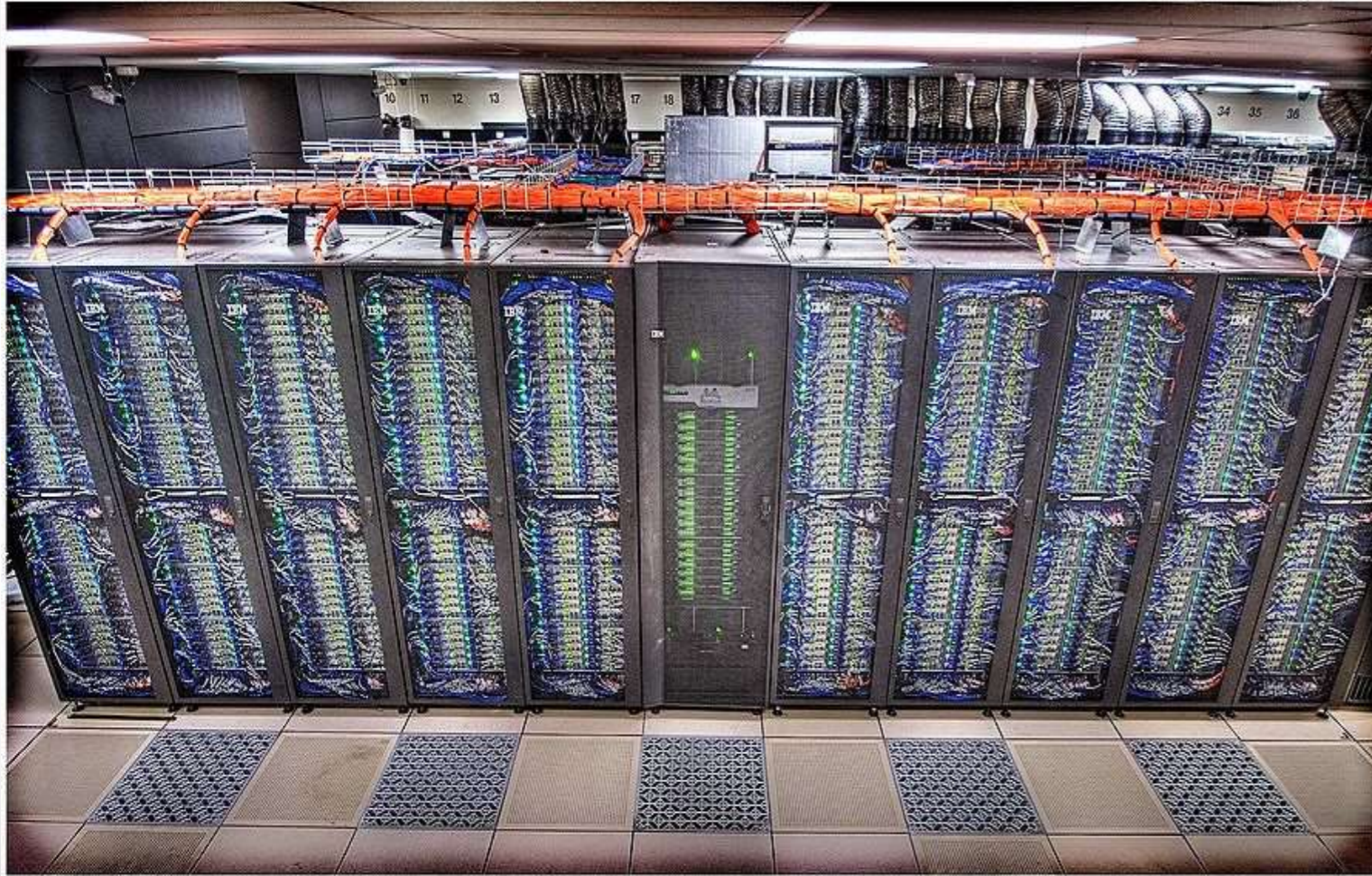
MPI+OpenMP

Shared Memory Systems

Distributed Memory Systems

Hybrid Systems

Ada and Terra

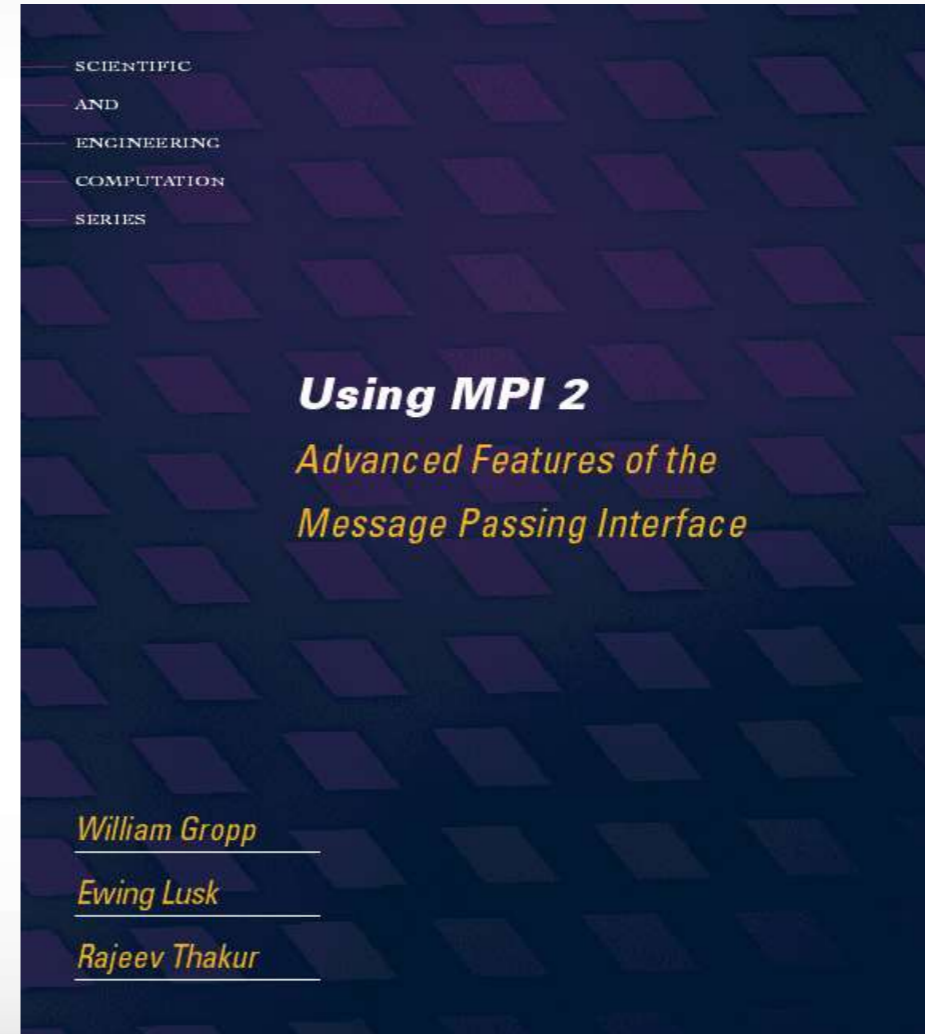
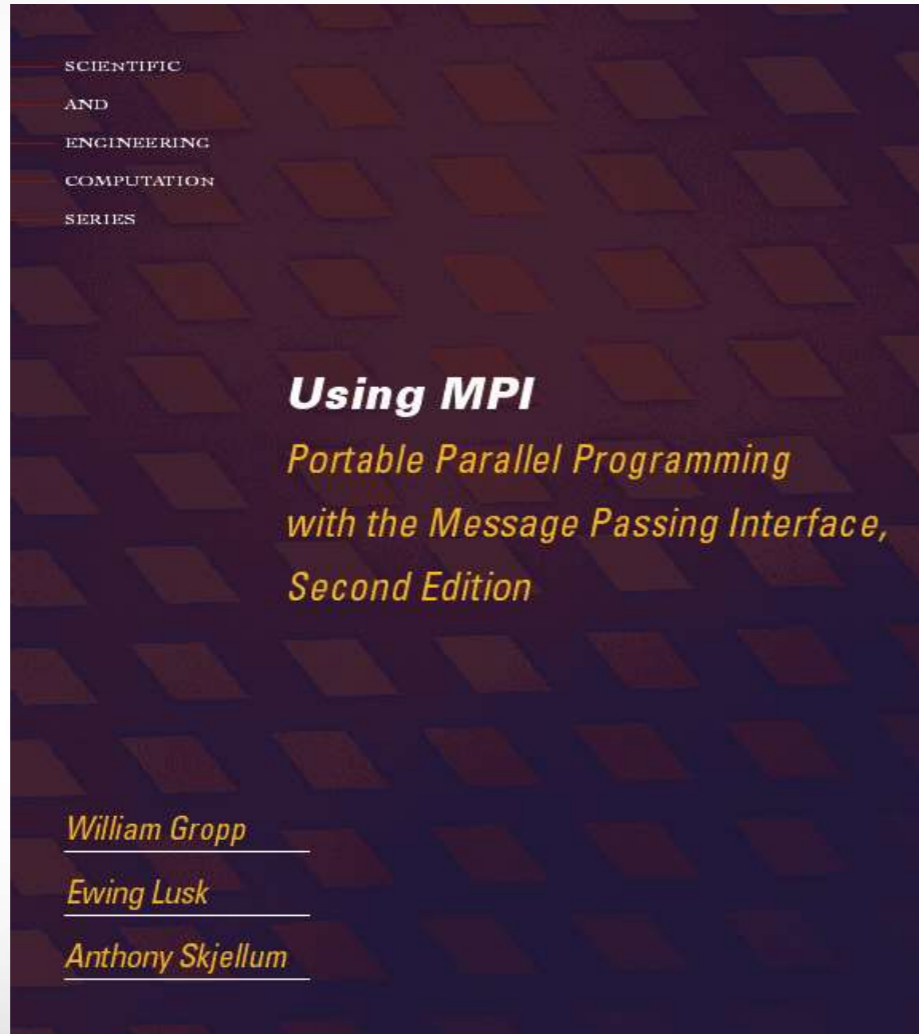


- Ada has 852 nodes and 17340 cores
- Terra has 304 compute nodes and 8512 cores
- Both support all three parallel programming models
 - OpenMP at node level
 - MPI at node and cluster level
 - Hybrid at node and cluster level

Resources

- Two books: <<Using MPI>> and <<Using MPI II>>
- MPI standard: <http://mpi-forum.org/docs/mpi-3.1/mpi31-report.pdf>
- <https://www.mpich.org/static/docs/v3.2/>
- https://www.cac.cornell.edu/education/Training/parallelMay2011/Hybrid_Talk-110524.pdf
- Part of the content is adapted from former Supercomputing Facility staff Mr. Spiros Vellas' introductory MPI short course

Books



Example 1: Hello World

C

```
#include <stdlib.h>

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

    printf("Hello, world\n");

}
```

Fortran

```
program hello
implicit none

print *, "Hello, world"

end program hello
```

Example 1: Hello World

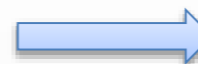
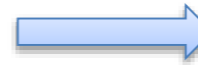
```
C
#include <stdlib.h>

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

Fortran
program hello
implicit none

print *, "Hello, world"

end program hello
```



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

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

Fortran
program hello
use mpi
implicit none

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

Layout of an MPI Program

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

    mpi calls
    happen here

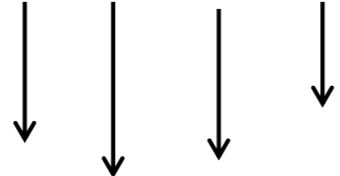
    MPI_Finalize();
    ... no mpi calls
}
```

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

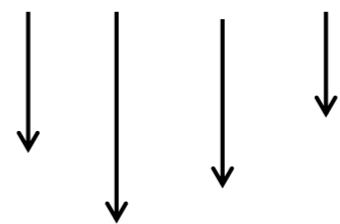
mpi calls
happen here

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

mpi calls
happen here



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



mpi calls
happen here

Compiling and Linking MPI Programs

`module load intel/2017A`

```
mpicc prog.c [options] -o prog.exe (C)
mpicpc prog.cpp [options] -o prog.exe (C++)
mpiifort prog.f [options] -o prog.exe (Fortran)
```

(Intel compilers)

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

(GNU compilers)

Running MPI Programs

- Load the modules first

```
module load intel/2017A
```

- Run the mpi program interactively

```
mpirun -np n [options] prog.exe [prog_args]
```

- Useful options

```
-ppn/-perhost
```

```
-hosts
```

```
-hostfile
```

```
-h
```


Running MPI Programs

- Batch Examples

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/2017A
mpirun prog.exe
```

`bsub < mpibatch.job`

Terra

```
#!/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/2017A
mpirun prog.exe
```

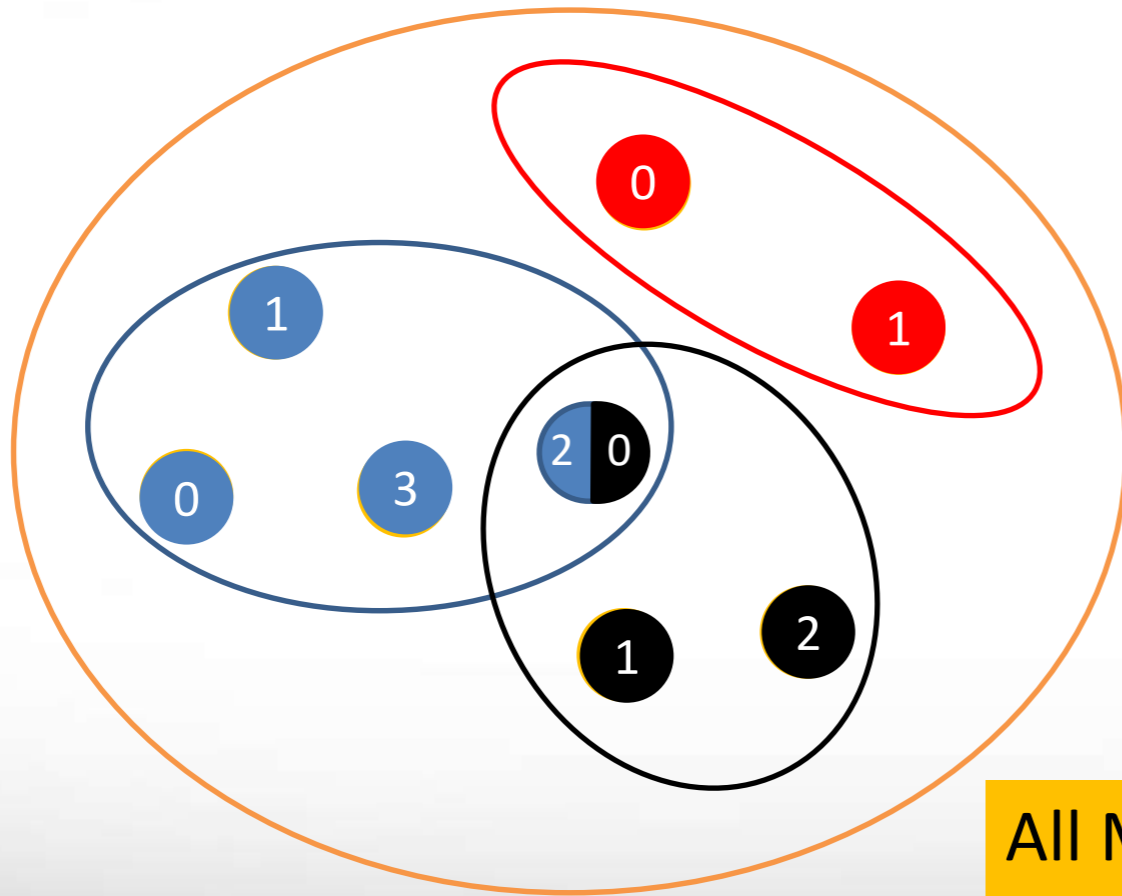
`sbatch mpibatch.job`

What is MPI

- **Message Passing Interface**: a specification for the library interface that implements message passing in parallel programming.
- Is standardized by the MPI forum for implementing portable, flexible, and reliable codes for **distributed memory systems**, regardless of the 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
- 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 programming paradigm for large scale scientific computing.

Basic MPI Concepts

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

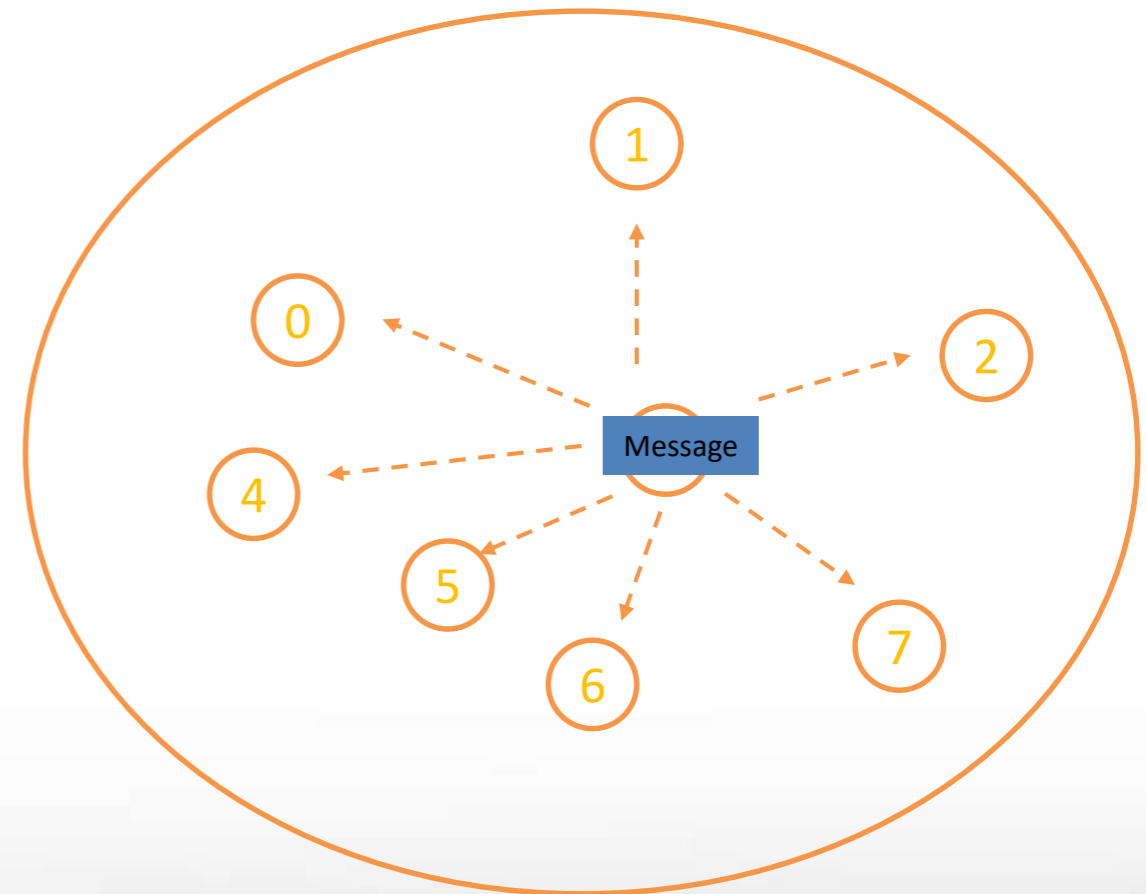
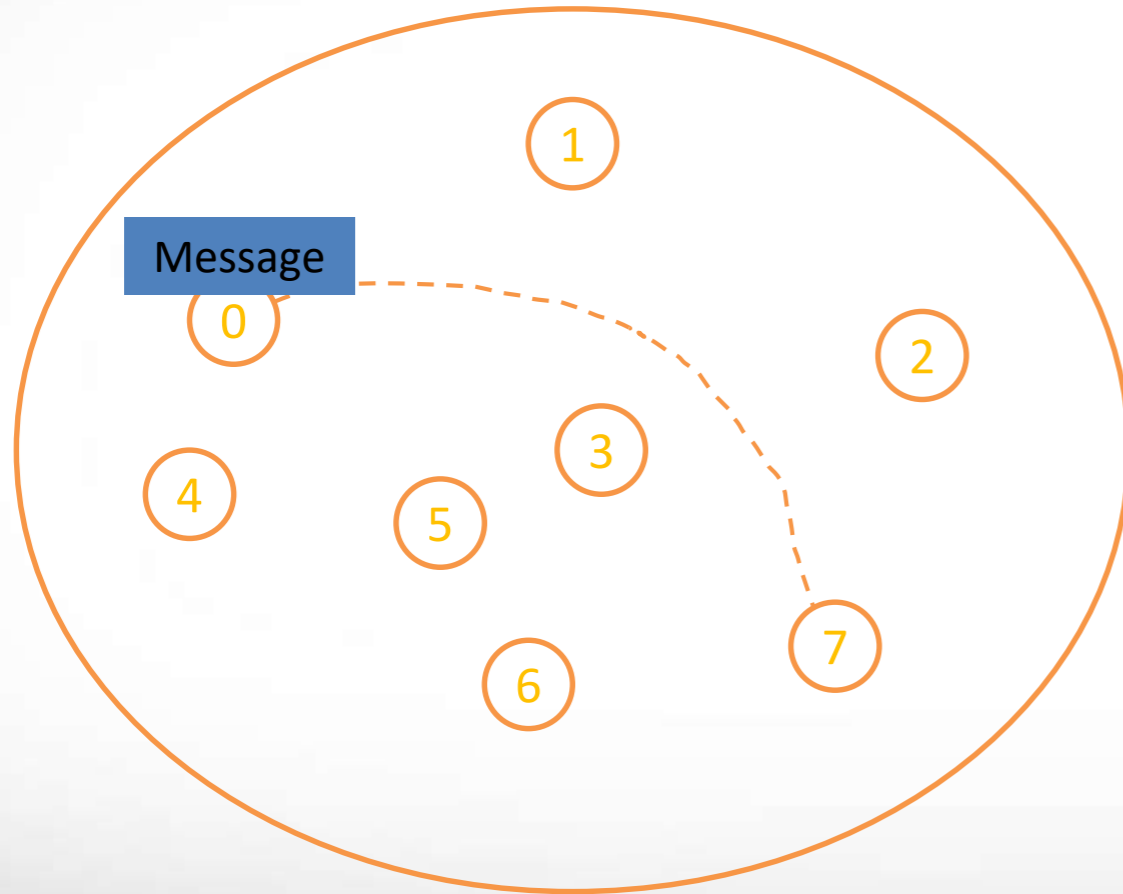
Size: 3

Rank: 0, 1, 2

All MPI communications must specify a communicator.

Basic MPI Concepts

message, point-to-point communication, collective communication



Example 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);

    if (rank == 0){
        number = 1234;
        MPI_Send(&number, 1, MPI_INT, 1, 0, MPI_COMM_WORLD);
        printf("Process %d sends out %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
```

Communicator

- In MPI, a communicator is a software structure through which we specify a group of processes.
- Each process in 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 an initial communicator that includes all the MPI processes activated in the running of a program. MPI_COMM_WORLD is typically the most used communicator.
- Communicators are especially useful in characterizing the tasks that different groups of processes carry out.

Size and Rank

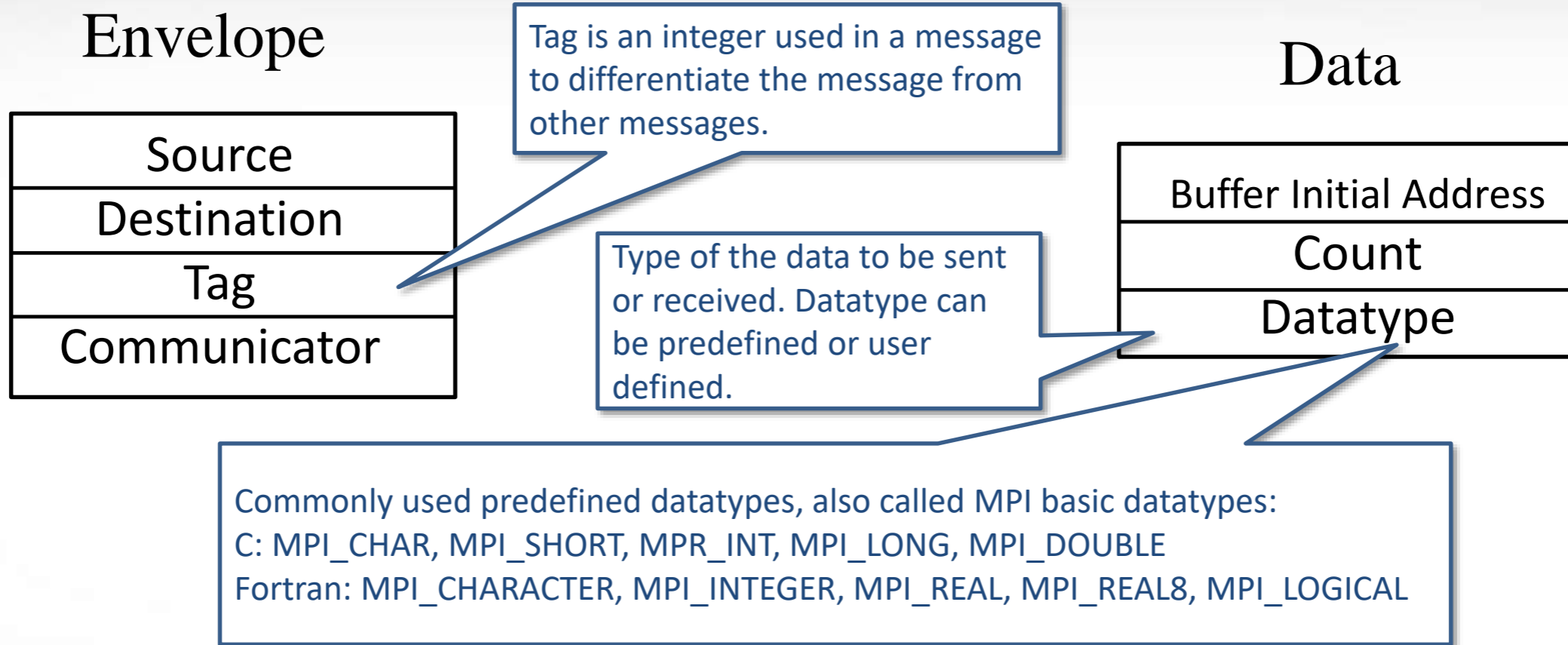
- How many processes in a communicator?

C	<code>int MPI_Comm_size(MPI_Comm comm, int *size)</code>
Fortran	<code>SUBROUTINE MPI_COMM_SIZE(comm, size, ierr)</code> <code>integer comm, size, ierr</code>

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

C	<code>int MPI_Comm_rank(MPI_Comm comm, int *rank)</code>
Fortran	<code>SUBROUTINE MPI_COMM_RANK(comm, rank, ierr)</code> <code>integer comm, rank, ierr</code>

Message



```
MPI_Send(&number, 1, MPI_INT, 1, 0, MPI_COMM_WORLD);
```

Data

Envelope

Send and Receive a Message

C

```
MPI_Send(&number, 1, MPI_INT, 1, 0, MPI_COMM_WORLD);
```

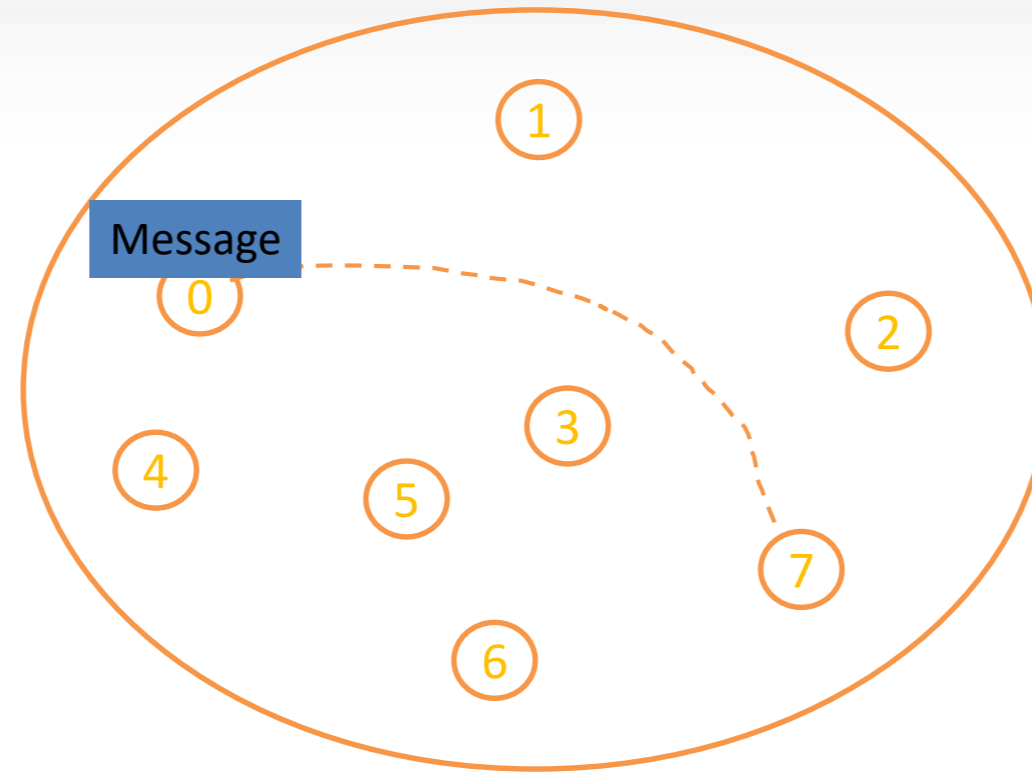
```
MPI_Recv(&number, 1, MPI_INT, 0, 0, MPI_COMM_WORLD, status);
```

Fortran

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

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

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	initial 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

Comments on Blocking Send

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

- The calling process causes **count** many contiguous elements of type **datatype** to be sent, starting from **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.

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 buer
datatype	datatype of each receive buer element
source	rank of source or <code>MPI_ANY_SOURCE</code>
tag	message tag or <code>MPI_ANY_TAG</code>
comm	communicator
status	status object

`MPI_ANY_SOURCE` and `MPI_ANY_TAG` are MPI defined wildcards.

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 in contiguous locations, starting at the address of `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 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)
```


Example 3

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

int main(int argc, char **argv){
    int number, size, rank;
    int i;

    MPI_Init(&argc, &argv);
    MPI_Comm_size(MPI_COMM_WORLD, &size);
    if (size < 2){
        MPI_Abort(MPI_COMM_WORLD, 99);
    }
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    if (rank == 0){
        printf("Type any number from the input: ");
        scanf("%d", &number);
        for (i=1; i<size; i++){
            MPI_Send(&number, 1, MPI_INT, i, 0, MPI_COMM_WORLD);
        }
    }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);
    }
    MPI_Finalize();
}
```

```
program ex3
use mpi
implicit none
integer rank, np, ierr, number, i

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

if (np < 2) then
    call MPI_ABORT(MPI_COMM_WORLD, 99, ierr)
endif
if (rank == 0) then
    print *, "Type an integer from the input"
    read *, number
    do i=1, np-1
        call MPI_SEND(number, 1, MPI_INTEGER, i, 0, MPI_COMM_WORLD, ierr)
    enddo
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
call MPI_FINALIZE(ierr)
end program ex3
```

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)

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

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

MPI_WAIT

MPI_WAIT(request, status)

request	request (handle)
status	status object (Status)

C	Fortran
<pre>MPI_Request request; MPI_Status status; ... MPI_Irecv(recv_buf, count, ..., comm, &request); ...do some computations ... MPI_Wait(&request, &status);</pre>	<pre>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)</pre>

`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

```
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)
```

Fortran

```
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);
```

statuses can be ignored with MPI_STATUSES_IGNORE

Example 4

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]);

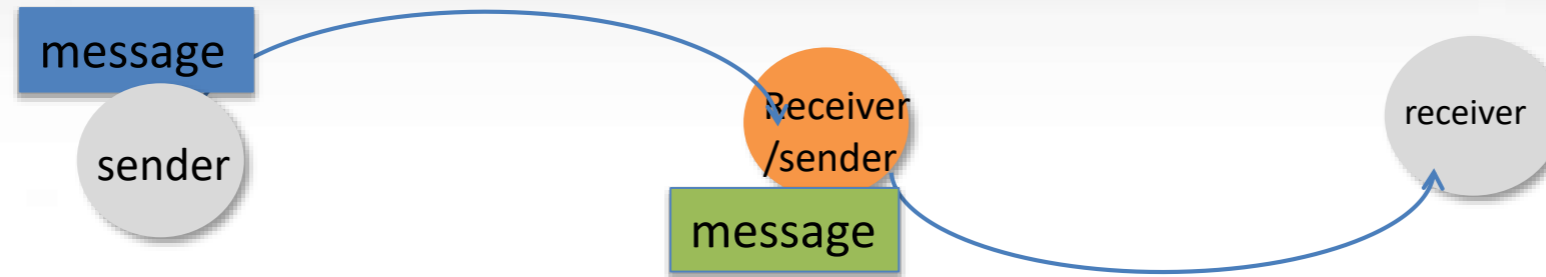
    MPI_Waitall(np-1, requests, MPI_STATUSES_IGNORE);
    free(requests);
}else{
    MPI_Recv(&number, 1, MPI_INT, 0, 0, MPI_COMM_WORLD,
            MPI_STATUS_IGNORE);
    printf("My id is %d. I received %d\n", rank, number);
}
```

Fortran

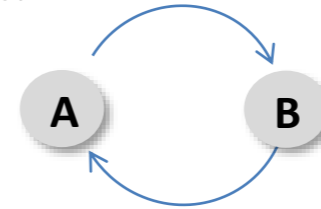
```
integer, allocatable::requests(:)
....
if (rank == 0) then
    print *, "Type an integer from the input"
    read *, number
    allocate(requests(np-1))
    do i=1, np-1
        call MPI_ISEND(number, 1, MPI_INTEGER, i, 0, &
                      MPI_COMM_WORLD, ierr)
    enddo
    call MPI_WAITALL(np-1, 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
```


Send-Receive

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



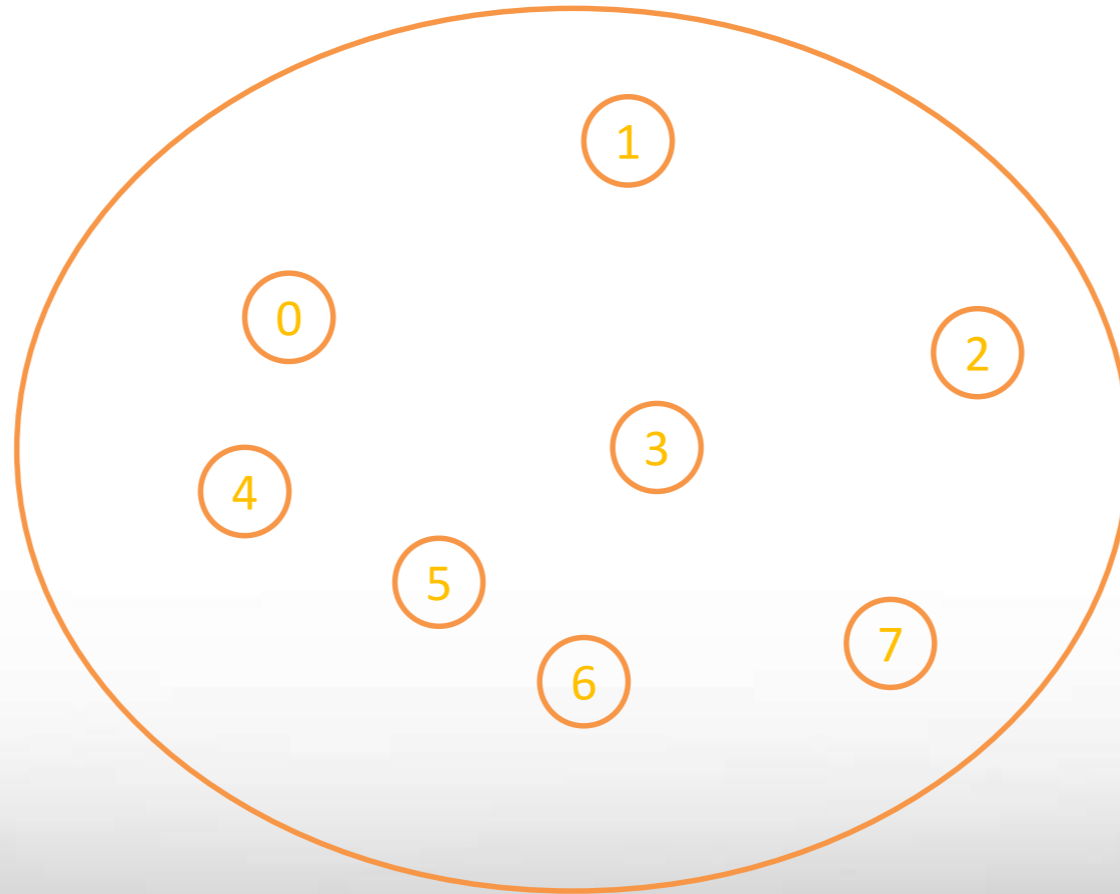
- Combines send and receive operations in one call
- The source and destination can be the same.
- The message sent out by send-receive can be received by blocking/non-blocking receive or another send-receive
- It can receive a message sent by blocking/non-blocking send or another send-receive.
- Useful 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_ALLTOALL	The j-th block of the sendbuf at process i is send to process j and placed in the i-th block of the recvbuf of process j.

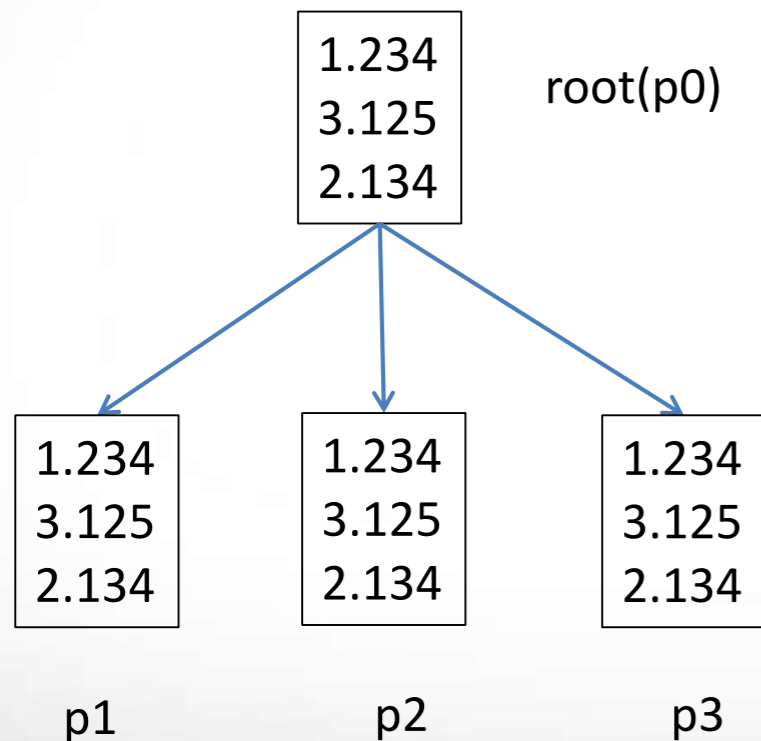
MPI_BARRIER

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_BCAST

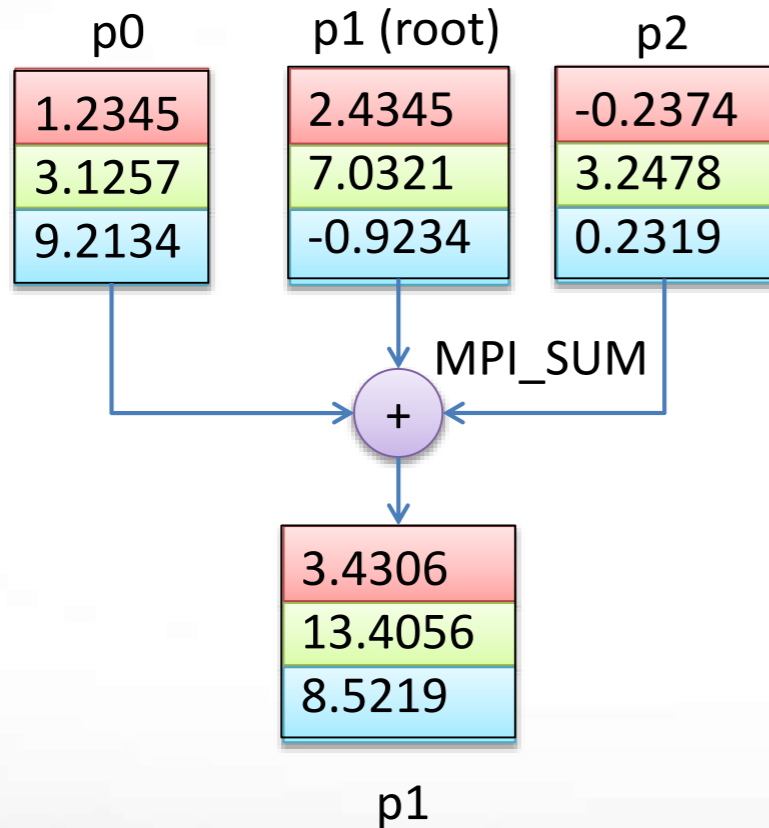
MPI_BCAST(buffer, count, datatype, root, comm)



- Root process: sends a message to all processes (including root) in the communicator **comm**.
- Non-root processes: receives a message from the specified **root**.
- Each receiving process blocks until the message has arrived its **buffer**.
- All processes in **comm** must call this routine.

MPI_REDUCE

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



C: MPI_Op op
Fortran: integer op

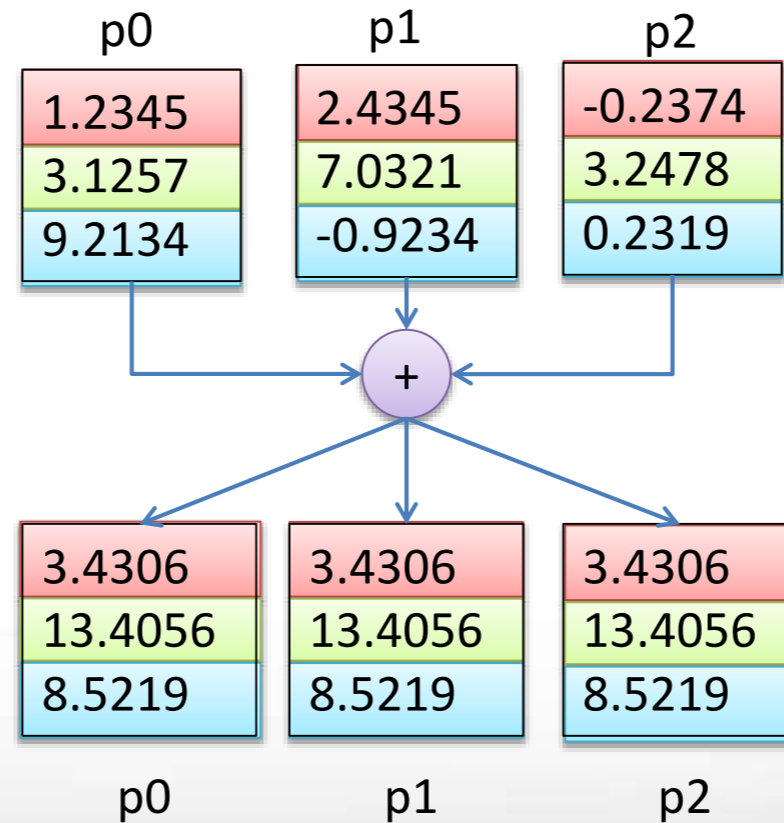
- Performs a reduction operation on all elements with same index in *sendbuf* on all processes and stores results in *recvbuf* of the root process.
- *recvbuf* is significant only at root.
- *sendbuf* and *recvbuf* cannot be the same.
- The size of *sendbuf* and *recvbuf* is equal to **count**.

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

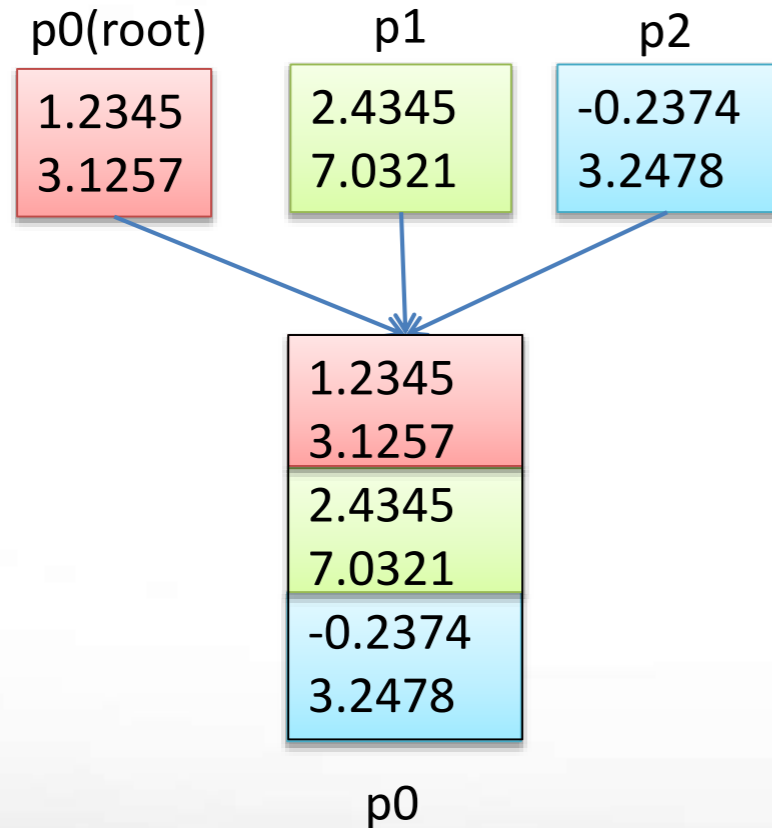
MPI_ALLREDUCE

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



MPI_GATHER

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



- Gathers together data from all process in **comm** and stores in **root** process.
- Data received by root are 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)

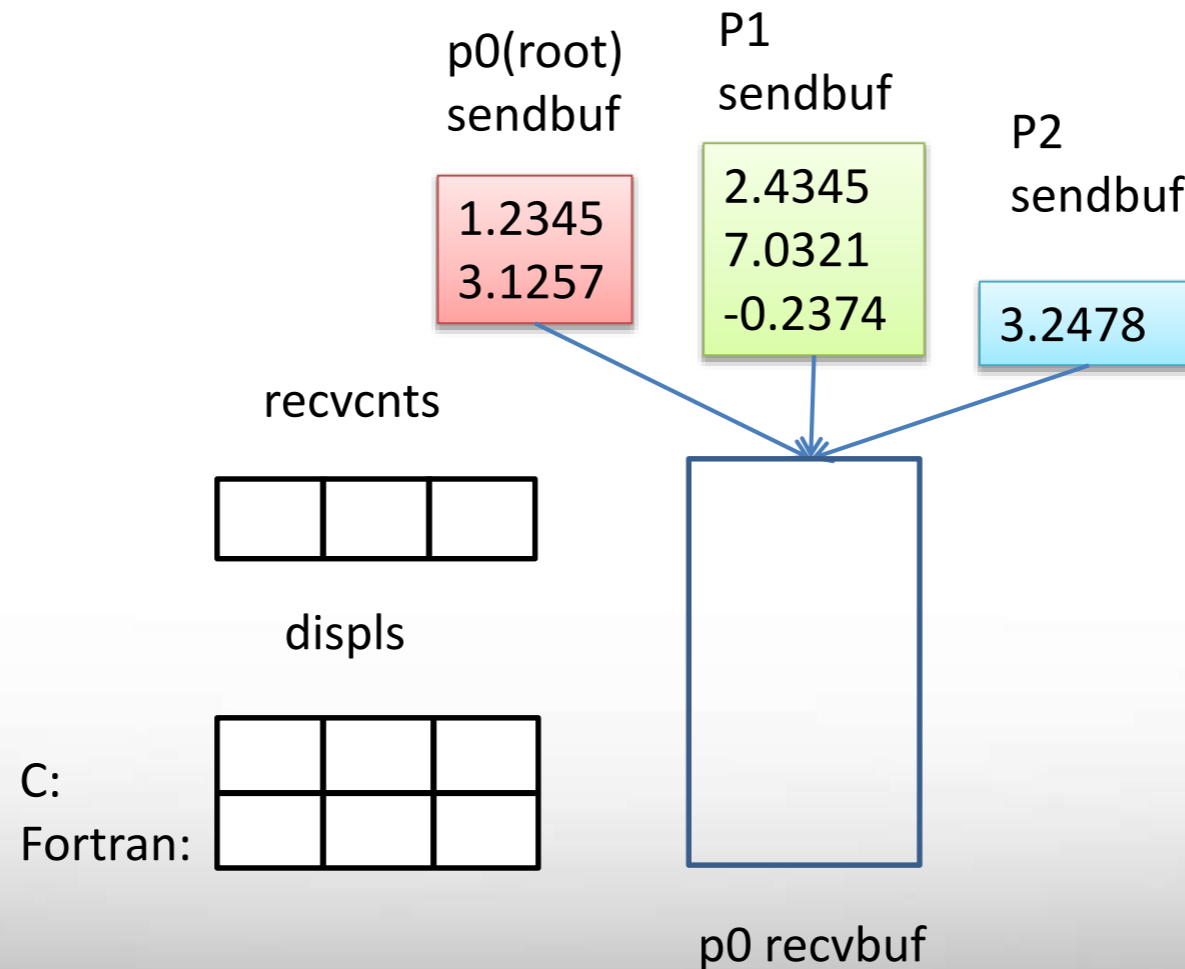
- IN recvcnts an integer array of size of *comm*. recvcnts[i] = number of elements received from process i.
- IN displs an integer array of size of *comm*. displs[i] = displacement from *recvbuf* for process i.

Fortran
integer recvcnts(*), displs(*)

C
int recvcnts[], displs[]

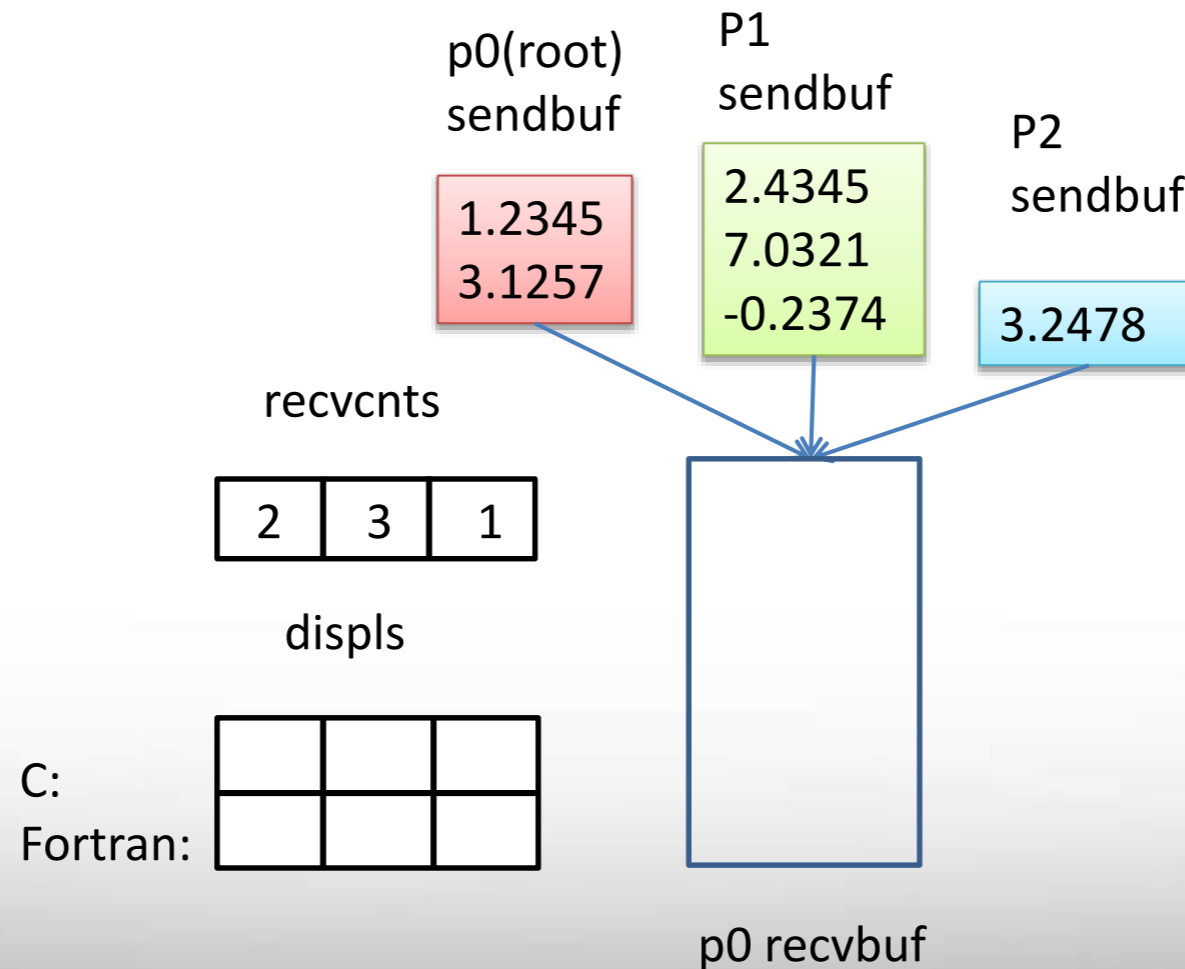
MPI_GATHERV (cont.)

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



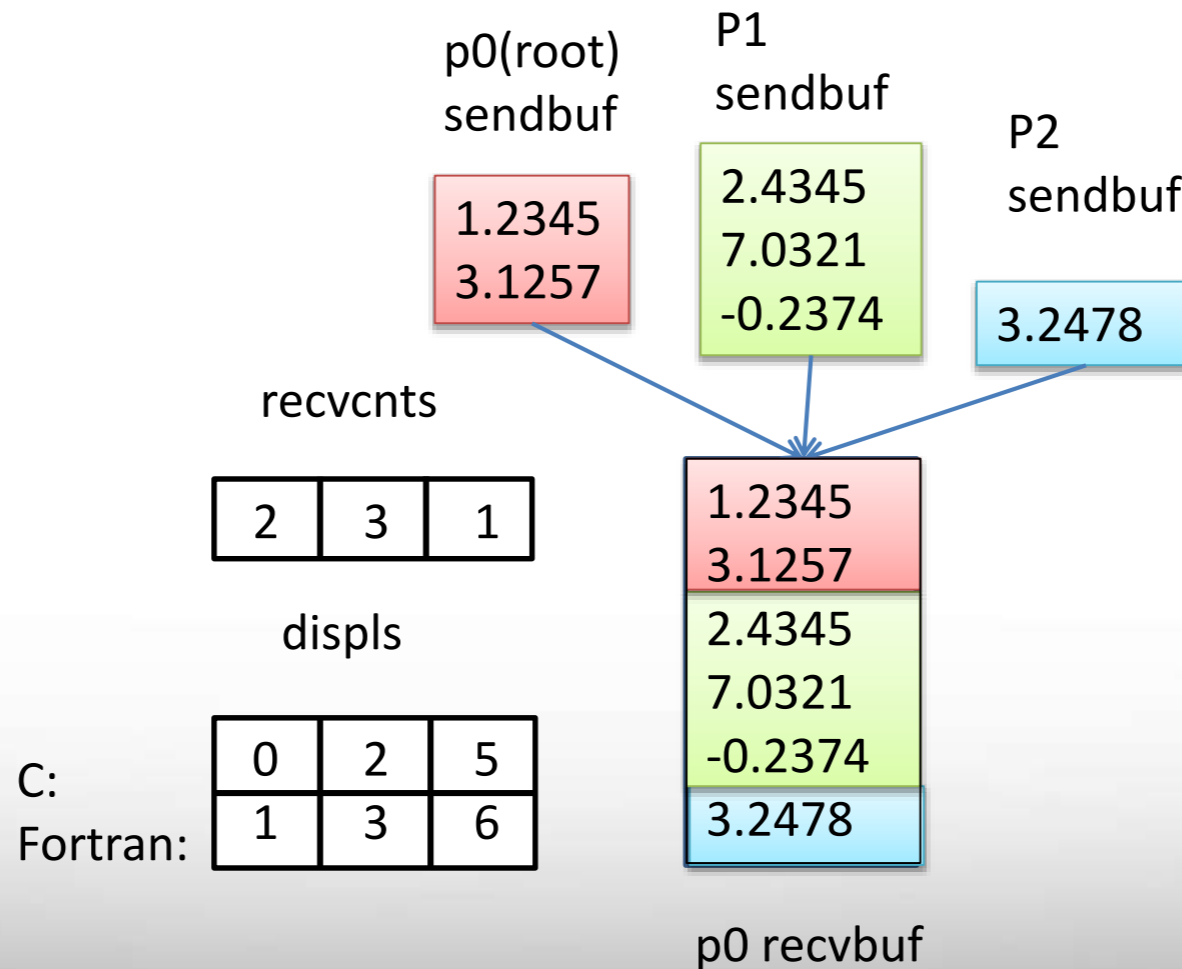
MPI_GATHERV (cont.)

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



MPI_GATHERV (cont.)

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



MPI_ALLGATHER/MPI_ALLGATHERV

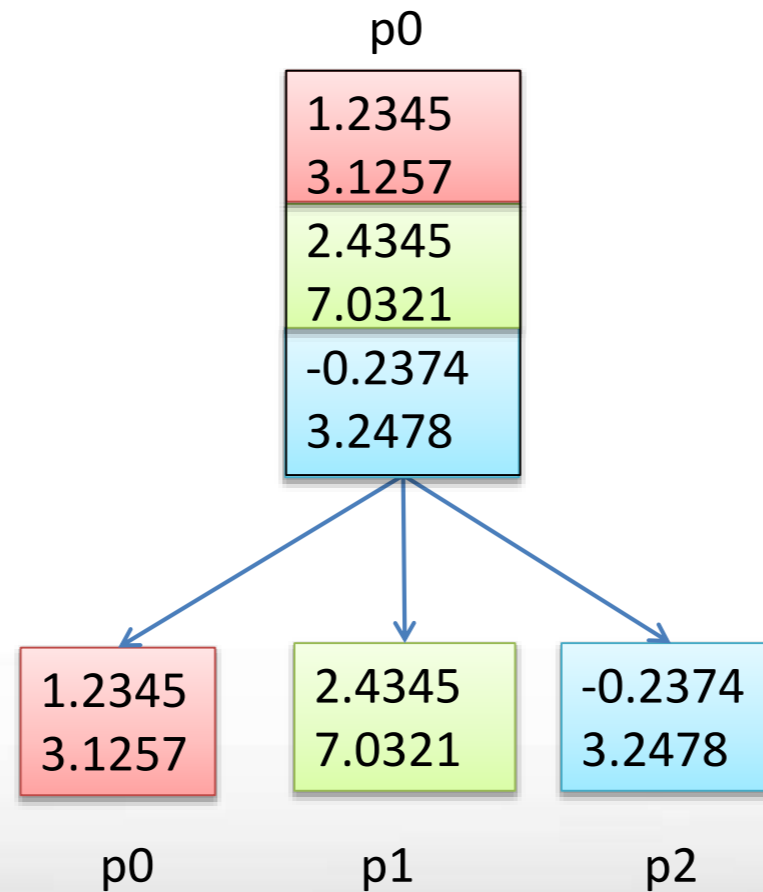
`MPI_ALLGATHER(sendbuf,sendcnt,sendtype,recvbuf,recvcnt,recvtype,comm)`

`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.

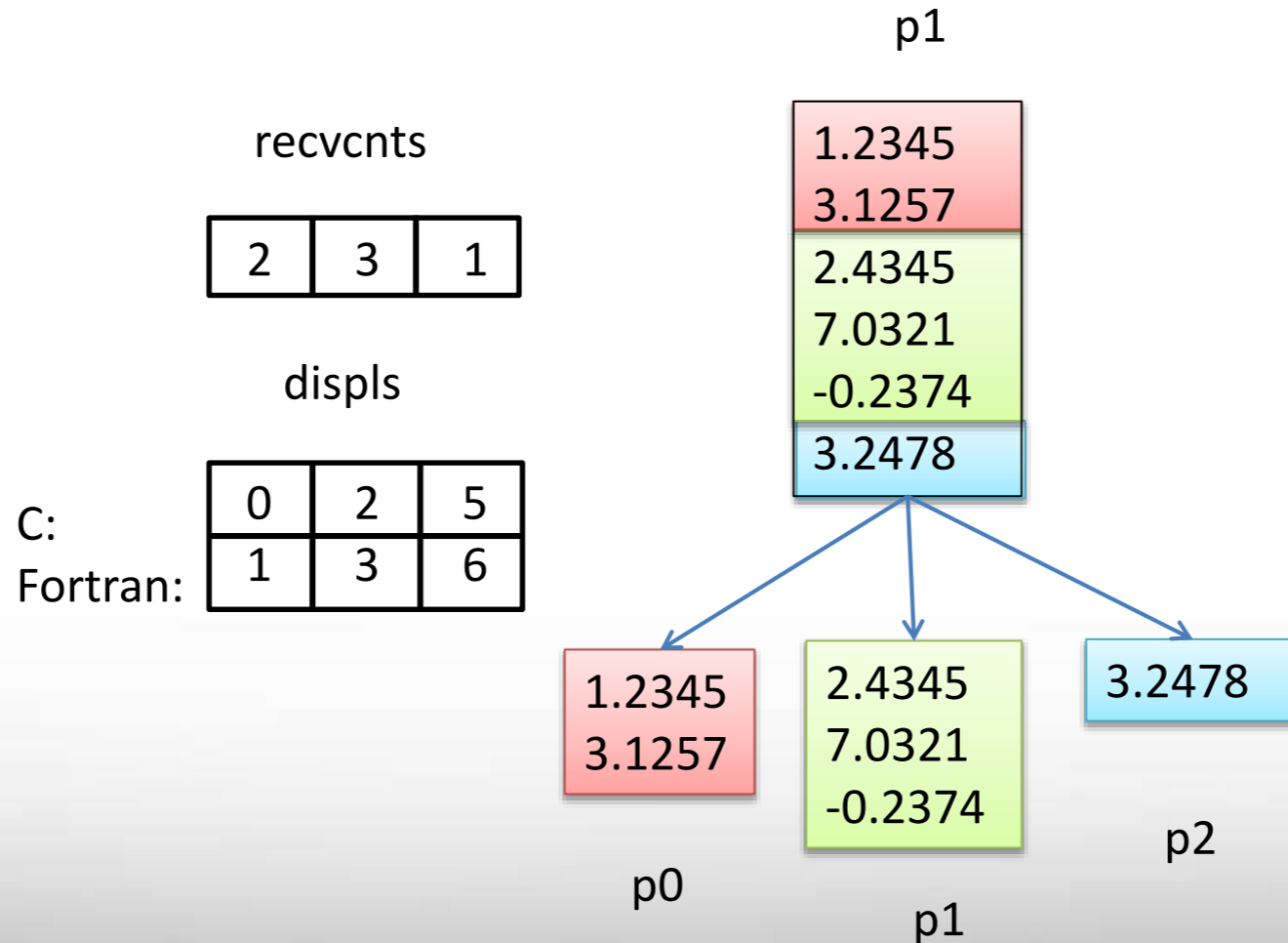
MPI_SCATTER

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



MPI_SCATTERV

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



Timing Routine

MPI_WTIME()

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

C

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

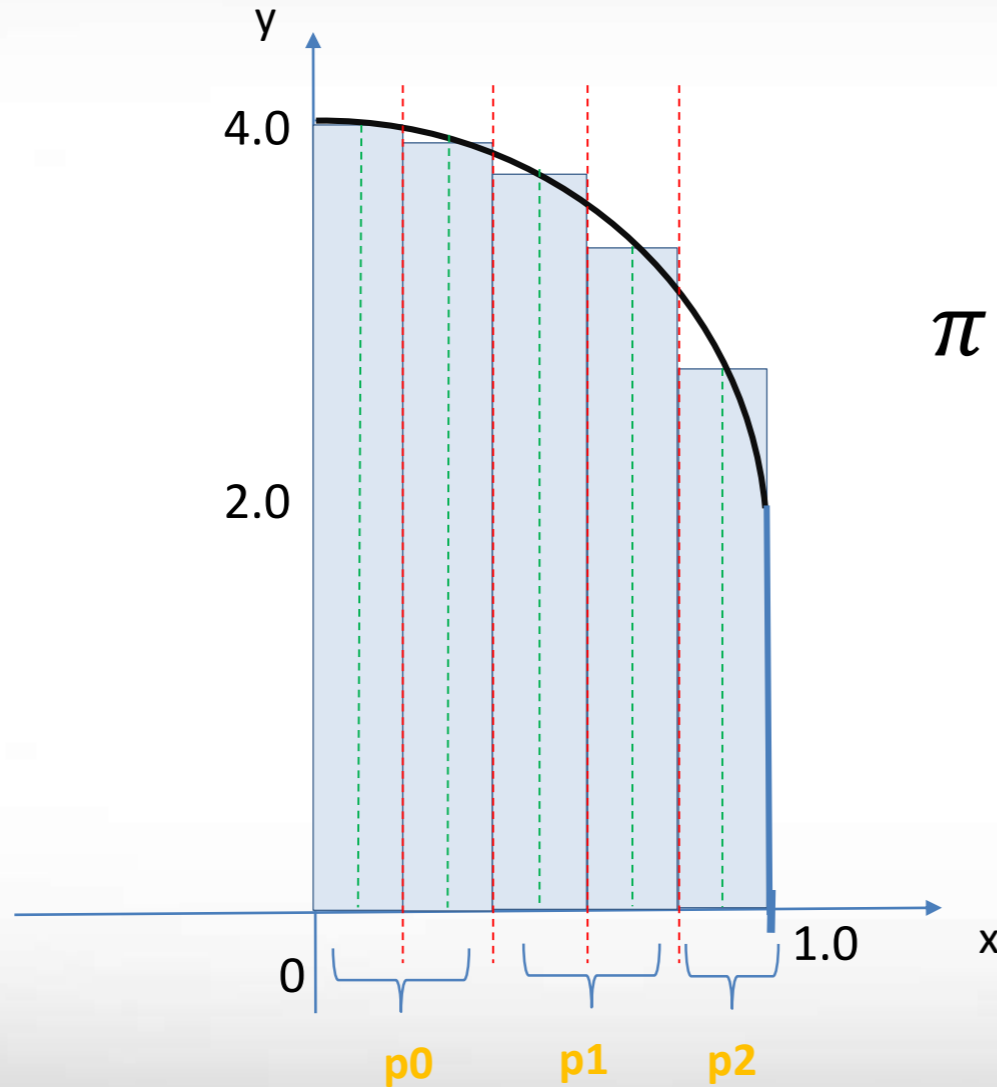
Fortran

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

Important Note On Using MPI

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

Example 5: Calculate PI



$$\pi = \int_0^1 \frac{4.0}{1+x^2} dx$$

Break

Outline for MPI Part II

- Exploring parallelism
 - Task-parallelism
 - Data-parallelism
- Matrix-vector multiplication
- Solving the 2D Poisson equation
- Domain decomposition
- MPI/OMP hybrid programming
- MPI/OMP: A Case Study

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

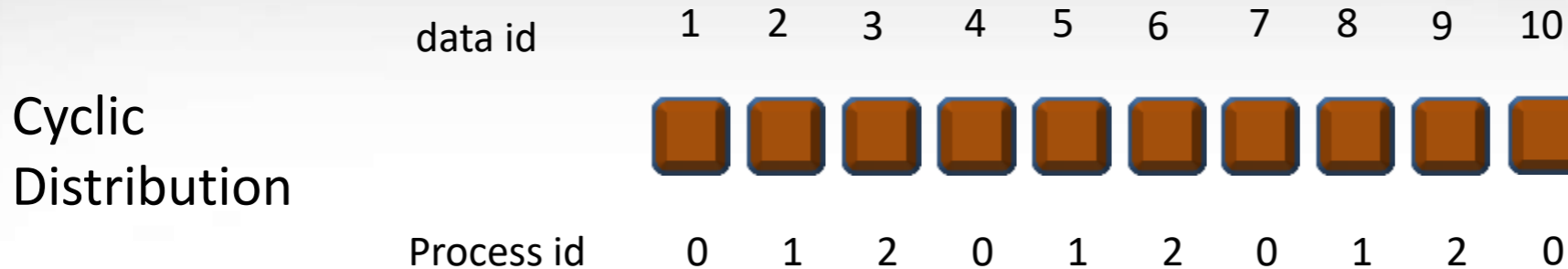


4 meals

salad
steak
desert

Data parallelism

Example 6: Data Distribution



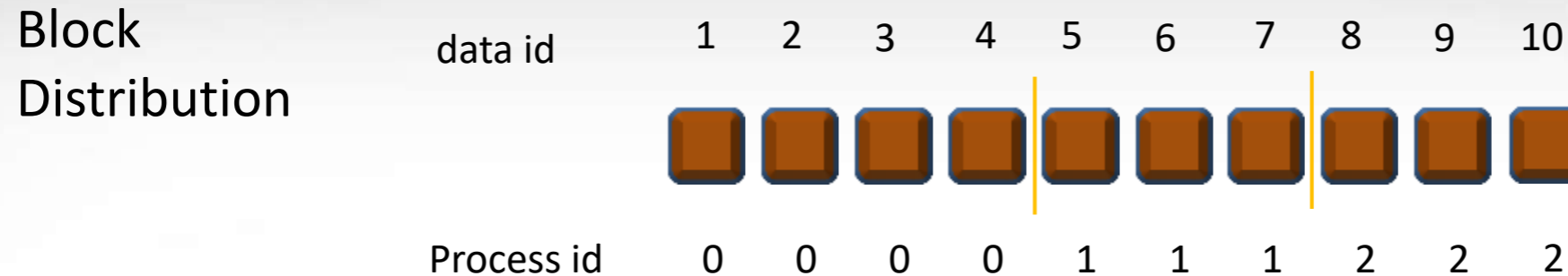
Data is distributed in a round robin manner among the processes.

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

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

calc_PI_cyclic.c

Example 6: Data 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

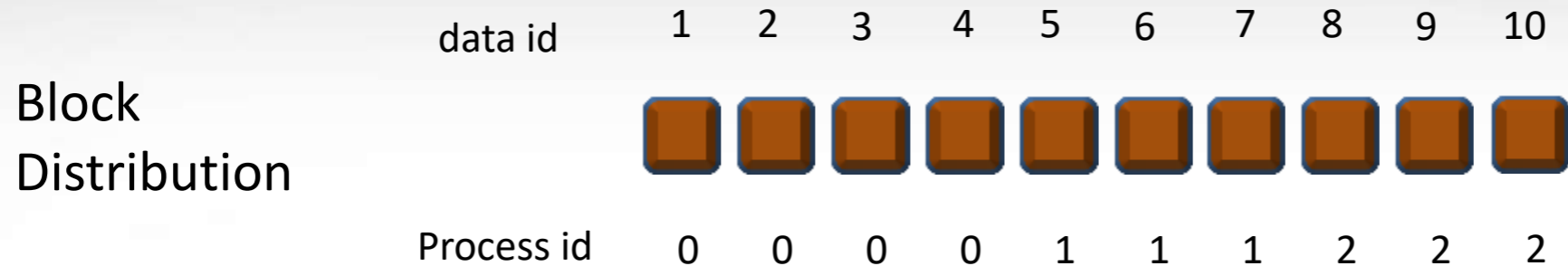
```
block_map(1, N, nprocs, myid, &l1, &l2);  
for (i=l1; i<=l2; i++){  
    x = h*(i-0.5);  
    sum += 4.0/(1.0+x*x);  
}  
sum = sum*h;
```

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
```

calc_PI_block.c

Example 6: Data Distribution



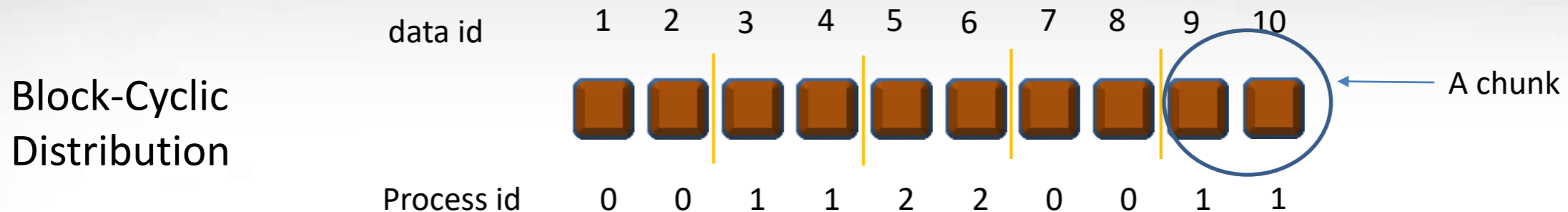
```
C
void block_map(int n1, int n2, int nprocs,
               int myid, int *l1, int *l2)
{
    int block, rem;
    block = (n2-n1+1)/nprocs;
    rem   = (n2-n1+1)%nprocs;
    if (myid < rem) {
        block++;
        *l1 = n1+myid*block;
    } else
        *l1 = n1+rem+block*myid;

    *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
```

Example 6: Data Distribution



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

Loop through chunks

C	Fortran
<pre>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;</pre>	<pre>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</pre>

Loop through blocks inside a chunk

calc_PI_bc.c

Example 7: matvec-scatterv

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

\vec{a}_i is a column vector.

In this program, strips of consecutive columns of A are distributed to all processes. Each process carries out a part of the linear vector sum

$$b_i\vec{a}_i + \dots + b_j\vec{a}_j$$

Example 8: Solving the x-y Poisson Equation

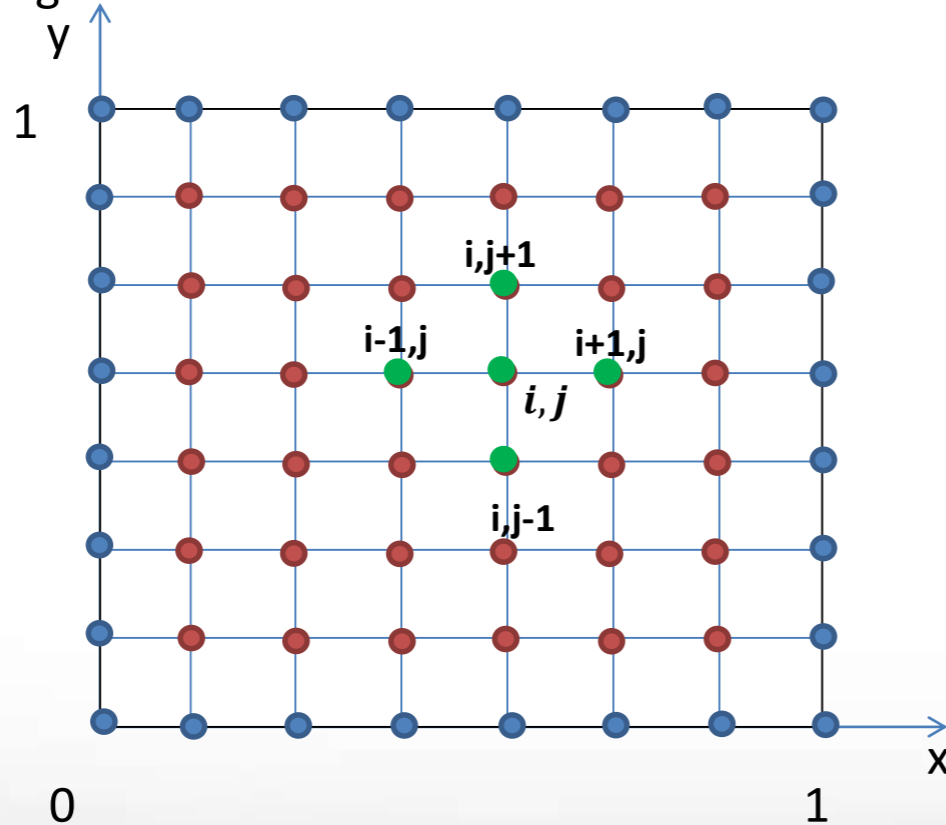
Solve the partial differential equation

$$\frac{\partial^2 u}{\partial^2 x} + \frac{\partial^2 u}{\partial^2 y} = f(x, y)$$

where $x, y \in [0, 1]$

and $u = g(x, y)$ on boundary

using the finite difference method.



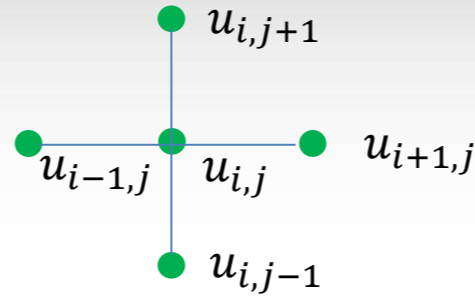
Discretize the domain along x and y using n internal points in each direction.

The increment is
 $h = 1/(n + 1)$

$$x_i = ih, y_j = jh \\ (0 \leq i, j \leq n + 1)$$

$$u_{ij} = u(x_i, y_j) = u(ih, jh) \\ (0 < i, j < n + 1)$$

Example 8: the x-y Poisson Equation



5-point finite difference stencil approximation:

$$u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j} = h^2 f_{i,j} \quad (0 < i, j < n + 1)$$

$$u_{i,j} = 0.25 * (u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - h^2 f_{i,j})$$

k+1 Jacobi iteration step at $x_i = ih$; $y_j = jh$; $i, j = 1:n$

$$u^{k+1}_{i,j} = 1/4(u^k_{i-1,j} + u^k_{i,j+1} + u^k_{i,j-1} + u^k_{i+1,j}) - h^2 f_{i,j}$$

Jacobi iteration across all points:

```
do j=1, n
```

```
  do i = 1, n
```

```
    unew(i, j) = 0.25*(u(i-1,j) + u(i, j+1) + u(i+1,j) + u(i, j-1)) - f(i,j)*h^2
```

```
  end do
```

```
end do
```

Example 8: Solving the x-y Poisson Equation

Boundary conditions (stay fixed):

$$u(x_i, 0) = \frac{\cos(\pi x_i) - \pi^2}{\pi^2} \quad (0 \leq x \leq 1)$$

$$u(x_i, 1) = \frac{\cos(\pi x_i) - \pi^2 \cos(x_i)}{\pi^2} \quad (0 \leq x \leq 1)$$

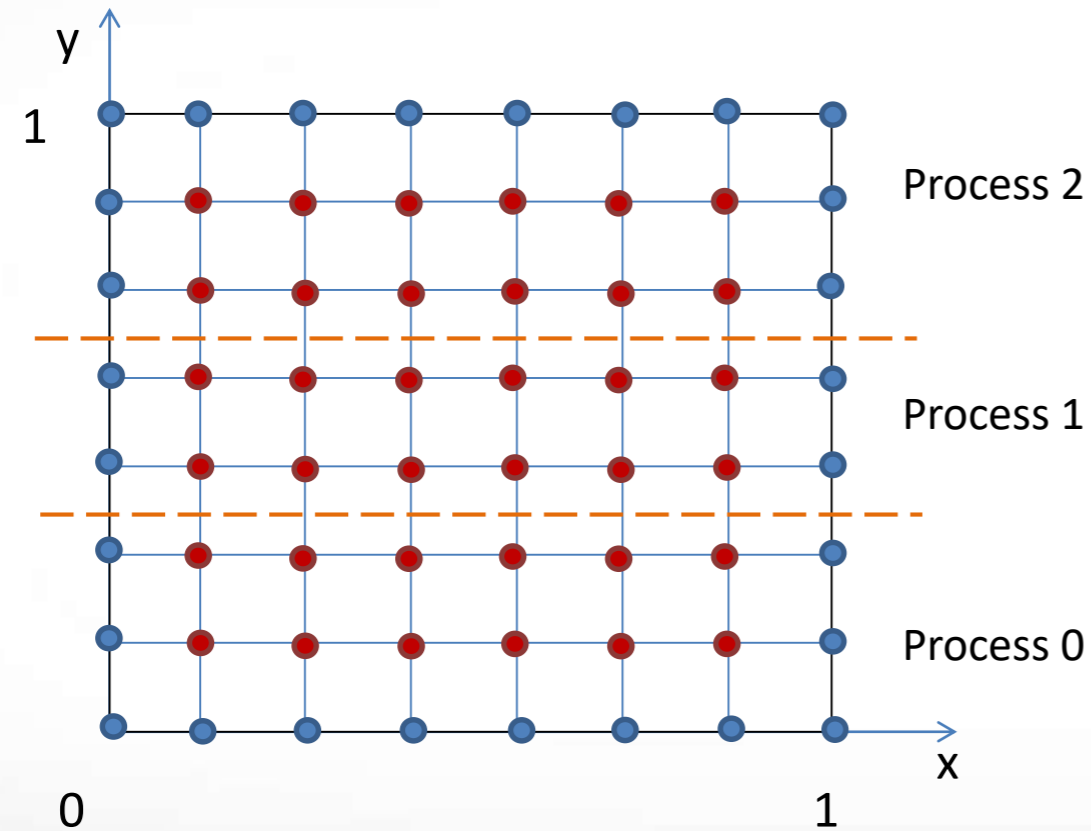
$$u(0, y_j) = \frac{1}{\pi^2} - 1 \quad (0 \leq y \leq 1)$$

$$u(1, y_j) = -\left(\frac{1}{\pi^2} + \cos(y_j)\right) \quad (0 \leq y \leq 1)$$

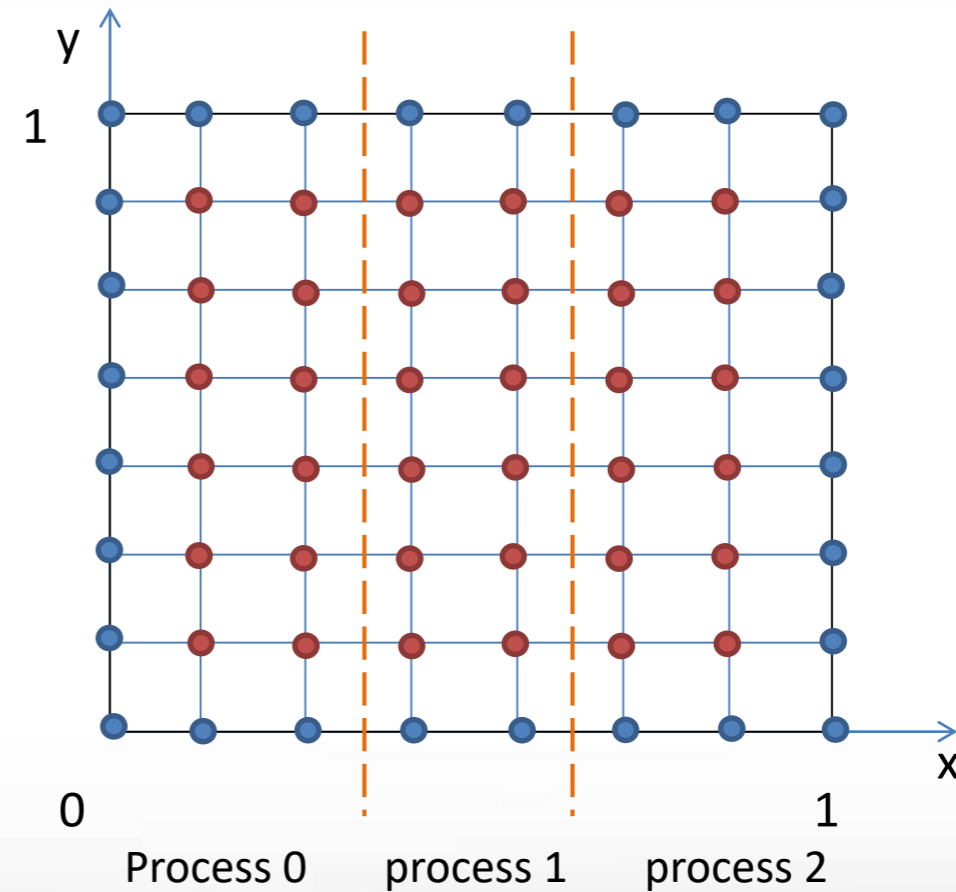
$$\text{RHS: } f(x_i, y_j) = (x_i^2 + y_j^2)\cos(x_i y_j) - \cos(\pi x_i)$$

1d-Domain Decomposition

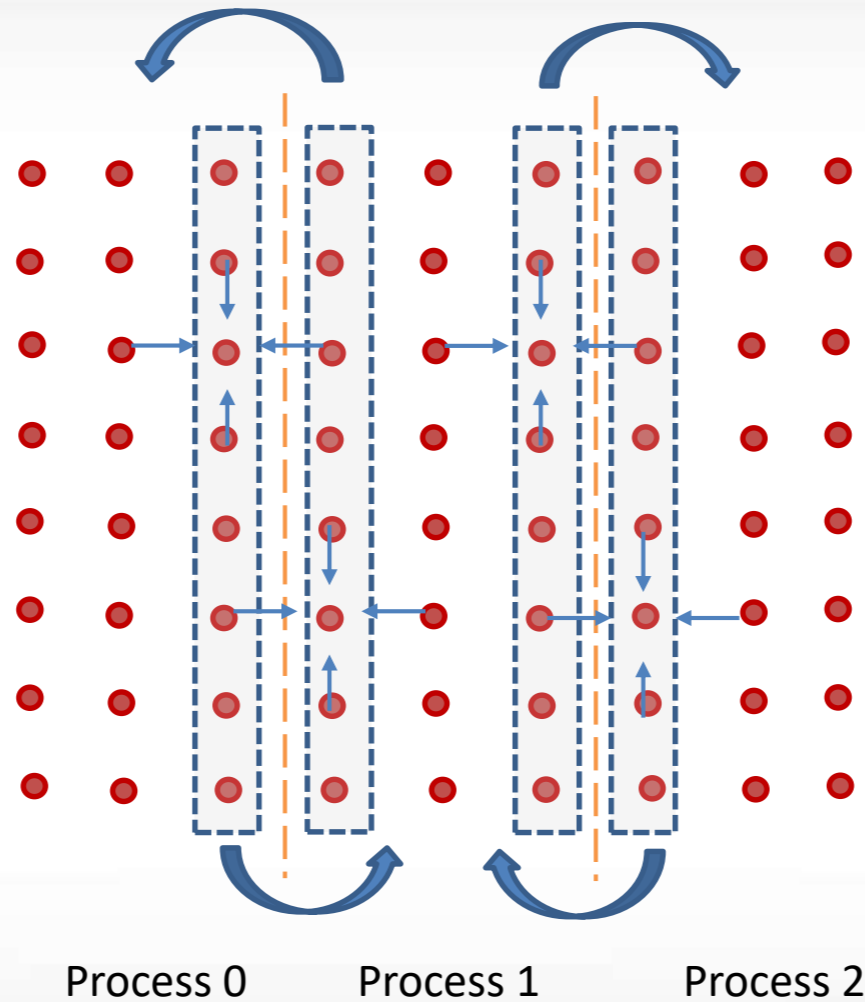
C: decompose along y axis



Fortran: decompose along x axis



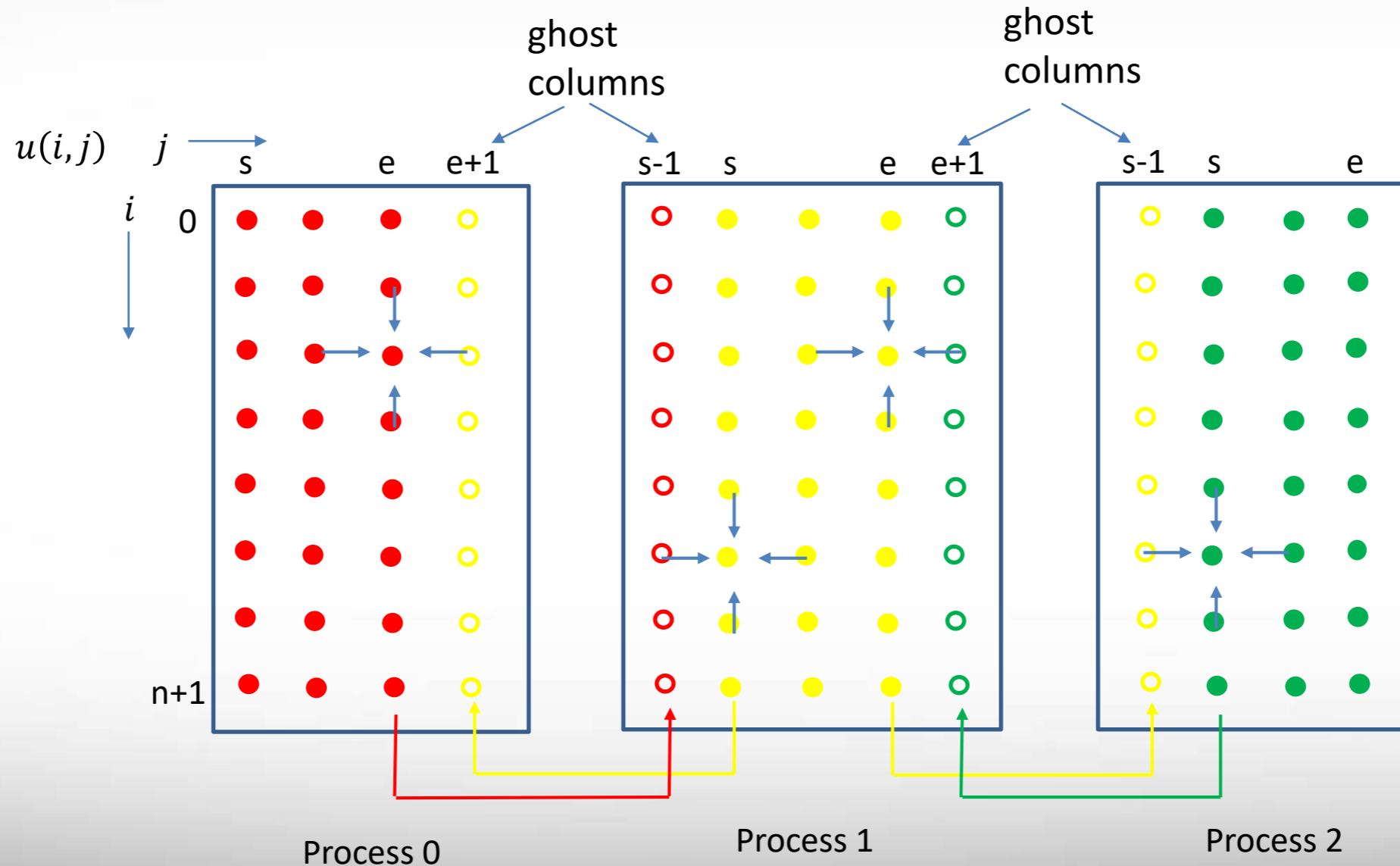
1d-Domain Decomposition



Border columns need to be copied into the memory space of the neighboring processes for the five-point stencil calculation. Same for row-wise decomposition.

1d-Domain Decomposition

Exchanged border columns are stored in 'ghost' columns in each process to be used in five-point stencil calculation



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

ex2_single.c

- MPI_THREAD_FUNNELED

ex2_funnel.c

- MPI_THREAD_SERIALIZED

ex2_serialized.c

- MPI_THREAD_MULTIPLE

ex2_multiple.c

- To compile

```
mpiicc -qopenmp [options] prog.c -o prog.exe
```

```
mpiifort -qopenmp [options] prog.f90 -o prog.exe
```

MPI+OMP Hybrid Programming

- Not all program will benefit from hybrid programming

poisson_1d performance comparison: pure MPI vs hybrid

	Pure MPI Single-node	Pure MPI 4-node	Hybrid OMP_NUM_THREADS=2	Hybrid OMP_NUM_THREADS=4
np=2	22.8697 seconds			
np=4	11.9441 seconds	np=4 13.5297 seconds	np=2 25.0954 seconds	np=1 49.7846 seconds
np=8	6.5824 seconds	np=8 7.7067 seconds	np=4 13.3360 seconds	np=2 25.0660 seconds
np=16	3.6141 seconds	np=16 4.6635 seconds	np=8 7.5272 seconds	np=4 13.3054 seconds

Hybrid is worse

example8/poisson_1d.c (.f90)

example9-hybrid/poisson_1d_hybrid.c

Acknowledgement

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