

## MPI Programming Part 1

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### Outline

- Why MPI
- MPI programing basics
- Point-to-point communications





# Why Parallel Computing

As computing tasks get larger and larger, may need to enlist more computer resources

- Bigger: more memory and storage
- Faster: each processor is faster
- More: do many computations simultaneously





# Memory System Models for Parallel Computing

Different ways of sharing data among processors

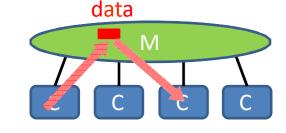
- Shared Memory
- Distributed Memory
- Hybrid (shared + distributed)
- PGAS (Partitioned Global Address Space)





# **Shared Memory Model**

- All threads/processes have access to global address space
- Data sharing achieved via read/ write to the same memory location



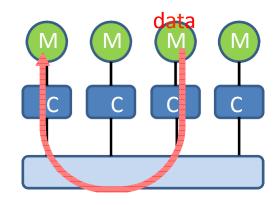
Within single computer
 e.g., OpenMP





# Distributed Memory Model

- Each process has its own address space locally
- Data sharing achieved via explicit message passing (through network)
- Inter- and intra computers
- Example: MPI (Message Passing Interface)

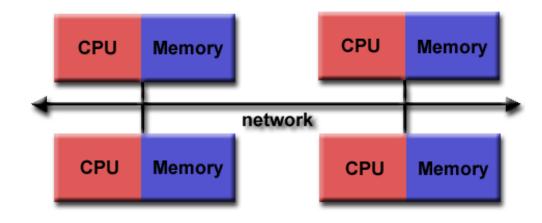




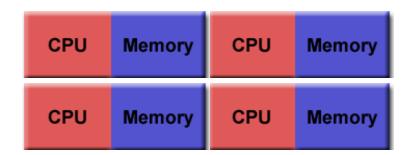


# MPI Programming Models

Distributed



Single node

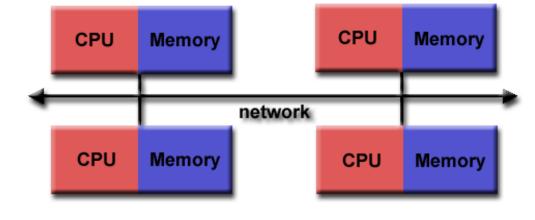




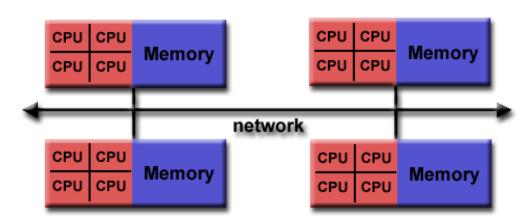


## MPI Programming Models





HybridMPI+OpenMP

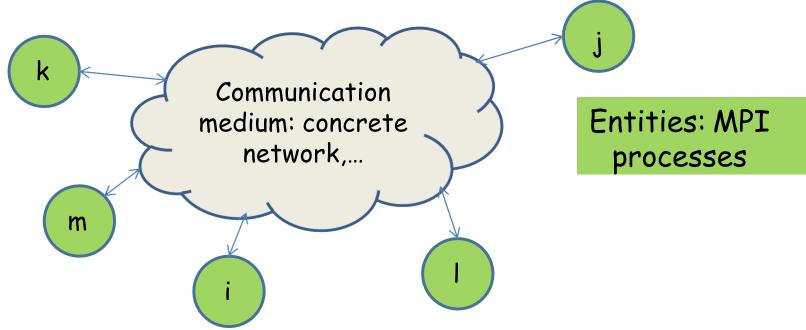






## Message Passing

Any data to be shared must be explicitly transferred from one to another







# Why MPI?

- Universality:
  - Works on separate processors connected by any network or shared memory systems
  - Most modern parallel supercomputers have right hardware
  - Most useful on distributed memory machines
- Performance:
  - Scalability keeps MPI as a permanent component of HPC
  - Each message passing process only directly uses its local data, avoiding complexity of process-shared data, cache contention



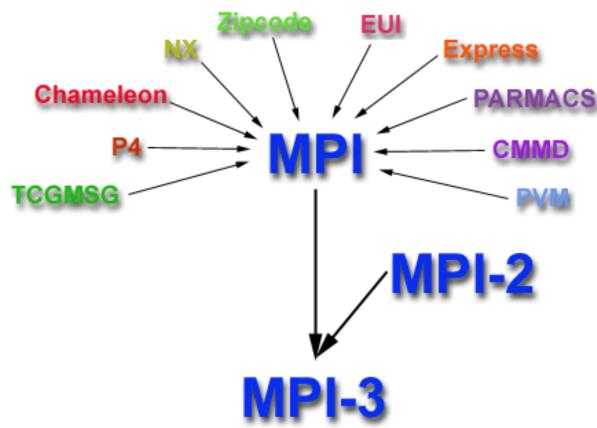
## **MPI** History

• 1980-1990

• 1994:MPI-1

• 1998:MPI-2

• 2012:MPI-3







### **MPI Standards**

- MPI defines the portable message-passing standard designed by a group of researchers from academia and industry to function on a wide variety of parallel computing architectures
- MPI defines standard APIs for message passing
  - The standard includes
    - What functions are available
    - The syntax of those functions
    - What outcome to expect from those functions
  - The standard does NOT include
    - Implementation details (e.g. how the data transfer occurs)
    - Runtime details (e.g. how many processes the code run with etc.)
- MPI provides C/C++ and Fortran bindings
- Several third-party bindings for Python, R and more other languages



## Various MPI Implementations

- OpenMPI: open source, portability and simple installation and configuration
- MPICH: open source, portable
- MVAPICH2: MPICH derivative InfiniBand, iWARP and other RDMA-enabled interconnects (GPUs)
- Intel MPI (IMPI): vendor-supported MPICH from Intel





### More about MPI

- A MPI Program launches separate processes (tasks)
- Each task has its own address space
  - Requires partitioning data across tasks
  - Without data decomposition, the same task run N times
  - Data is explicitly moved from task to task by message passing
- Two classes of message passing
  - Point-to-Point communication: involving only two tasks
  - Collective communication: involving many tasks simultaneously





# Let's try it

- \$ whoami
- \$mpirun —np 4 whoami





## What just happened?

- mpirun launched 4 processes
- Each process ran `whoami`
- Each process ran independently
- Usually launch no more MPI processes than #processors
- Use multiple nodes:

```
mpirun —hostfile machine.lst
-np/-npp 4 app.exe
```





# Outline of a MPI Program

- Initialize communications
   MPI\_INIT initializes the MPI environment
   MPI\_COMM\_SIZE returns the number of processes
   MPI\_COMM\_RANK returns this process's index (rank)
- Communicate to share data between processes
   MPI\_SEND sends a message
   MPI\_RECV receives a message
- 3. Exit in a "clean" fashion when MPI communication is done MPI\_FINALIZE



# Hello World (C)

```
include "mpi.h"

int main(int argc, char* argv[]){
int nprocs, myid;
...

MPI_Init(&argc, &argv);

MPI_Comm_size(MPI_COMM_WORLD, &nprocs);

MPI_Comm_rank(MPI_COMM_WORLD, &myid);
printf("Hi %s, Hello World from process %d/%d
\n", name, myid, nprocs);

MPI_Finalize();
...
}
Header file

Initialization

Communication

Termination
```





# Hello World (C)

```
include "mpi.h"

int main(int argc, char* argv[]){
  int nprocs, myid;
...

MPI_Init(&argc,
MPI_Comm_size(M)
MPI_Comm_rank(M)
    Dear dear, Hello World from process 3/4
    printf("Hello W)
    \n", myid, npro
    Dear dear, Hello World from process 2/4
    Dear dear, Hello World from process 1/4

MPI_Finalize();
...
}
```





## Hello World (Fortran)

include "mpif.h"

Header file

integer::nprocs, ierr, myid

integer::status(mpi\_status\_size)

call mpi\_init(ierr)
call mpi\_comm\_size(mpi\_comm\_world, nprocs, ierr)
call mpi\_comm\_rank(mpi\_comm\_world, myid, ierr)

Initialization

Computation &

communication

write(\*, '("Hello World from process ",I3," /",I3)') myid, nprocs

**Termination** 

call mpi\_finalize(ierr)

•••





## Hello World (Fortran)

#### include "mpif.h"

Header file

integer::nprocs, ierr, myid

integer::status(mpi\_status\_size)

```
call mpi_init(ierr)

call mpi_comr [wfeinste@shelob1 hello]$ mpif90 hello.f90

call mpi_comr [wfeinste@shelob1 hello]$ mpirun -np 4 ./a.out

Hello World from process 3 / 4

nprocs

Hello World from process 0 / 4

Hello World from process 1 / 4

Hello World from process 2 / 4

call mpi_finalize(ierr)
```

•••





# Naming Signature (C/Fortran)

- Function name convention
  - C: MPI\_Xxxx(arg1,...)MPI Comm size(MPI COMM WORLD, &nprocs)
  - Fortran: mpi\_xxx(): not case sensitive
     mpi\_comm\_size(mpi\_comm\_world, nprocs, ierr)
- Error handles
   If rc/ierr == MPI\_SUCCESS, then the call is successful.
  - C: int rc = MPI Xxxx(arg1,...)
  - Fortran: call mpi\_some\_function(arg1,...,ierr)





### What is a MPI Communicator?

```
MPI_Comm_size(MPI_Com MPI_COMM_WORLD, int &nprocs)
MPI_Comm_rank(MPI_Com MPI_COMM_WORLD, int &myid)
```



 A group identifier of MPI processes that can send and receive messages to each other





### Communicators

- MPI\_COMM\_WORLD: the default communicator contains all processes running a MPI program
  - Point-point and collective communication
  - When a function is called to send data to all processes, MPI needs to understand what "all" means
- A process can belong to multiple communicators
- There can be many communicators

```
e.g., MPI_Comm_split(MPI_Comm comm, int color, int, kye, MPI_Comm* newcomm)
```





### Ranks and Size

- Rank: unique process id within a communicator (start from 0)
  - C: MPI\_Comm\_Rank(MPI\_Comm comm, int \*rank)
  - Fortran: MPI COMM RANK (COMM, RANK, ERR)
- Size: total process # within a communicator
  - C: MPI Comm Size (MPI Comm comm, int \*size)
  - Fortran: MPI COMM SIZE (COMM, SIZE, ERR)





### **Compiling MPI Programs**

#### Not a part of the standard

- Could vary from platform to platform
- Or even from implementation to implementation on the same platform
- mpicc/mpicxx/mpif77/mpif90: wrappers to compile MPI code and auto link to startup and message passing libraries.





# **MPI Compilers**

Language	Script Name	<b>Underlying Compiler</b>
С	mpicc	gcc
	mpigcc	gcc
	mpiicc	icc
	mpipgcc	pgcc
C++	mpiCC	g++
	mpig++	g++
	mpiicpc	icpc
	mpipgCC	pgCC
Fortran	mpif90	f90
	mpigfortran	gfortran
	mpiifort	ifort
	mpipgf90	pgf90





### Compiling and Running MPI Programs

- Compile
- C: mpicc -o <executable name> <source file>
- Fortran: mpif90 -o <executable name> <source file>
- Run

```
mpirun -hostfile $PBS_NODEFILE -np <number of
procs> <executable name> <input parameters>
```

Compile: mpicc -o hello hello.c

Run: mpirun -np 16 hello Marry





### In Class Exercises

- Exercises
  - Track a: Process color
  - Track b: Matrix multiplication
  - Track c: Laplace solver
- Your tasks:
  - Fill in blanks to make MPI code work under /exercise directory
  - Solutions are provided in /solution directory





## Request an Interactive Node

- Never run your jobs on a cluster head node
- qsub -I -A hpc\_training\_2018 -I walltime=4:0:0
   -I nodes=1:ppn=16





### Exercise a1: Process Color

### mpi\_part1\_2018/color/exercise

- Compile and run ex0a.c (C) or ex0a.f90 (Fortran)
- What do you get?
- Processes with odd rank print to screen "Process x has the color green"
- Processes with even rank print to screen "Process x has the color red"
- Modify ex1a.c (C) or ex1a.f90 (Fortran)



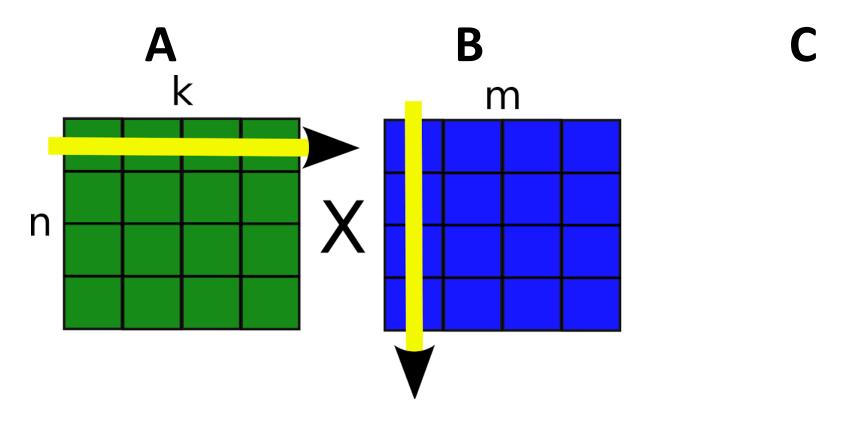


### Exercise a1: Process Color

```
MPI Init(&argc,&argv);
MPI Comm size(MPI COMM WORLD, &nprocs);
MPI Comm rank(MPI COMM WORLD, &myid);
char host[10];
gethostname(host, 255);
if (myid % 2 == 0) // myid with even numbers
    printf("Process %d from %s has color red\n", myid, host);
else
                 // myid with odd numbers
    printf("Process %d from %s has color green\n", myid, host);
MPI Finalize();
 mpicc exla solution.c
 mpirun —np 24 —hostfile $PBS NODEFILE a.out
```



## Exercise b1: Matrix Multiplication







### Exercise b1: Matrix Multiplication





### Exercise b1: Matrix Multiplication

- Goal: Distribute the work load among processes in 1-d manner
  - Each process initializes its own copy of A and B
  - Each process computes part of the workload
    - Determine how to decompose (which process deals which rows or columns)
    - Make sure dimensions of A and B can be evenly divided by number of MPI processes
  - Validate the result C[rpeek][cpeek]

```
mpicc ex1a_solution.c
mpirun -np 16 a.out
```





### Workload non-sharing vs. sharing

```
int rows_per_process = nra/nprocs;
Int r_start = myrank * rows_per_process
Int r_end = (myrank+1)* rows_per_process - 1;

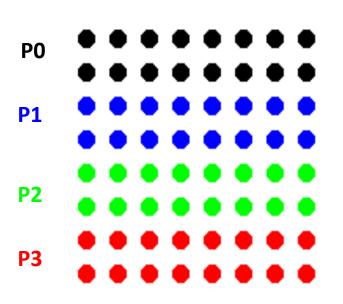
for (i=r_start; i<=r_end; i++)
    for (j=0; j<ncb; j++)
        for (k=0; k<nca; k++)
        C[i][j] += A[i][k]*B[k][j];</pre>
```

mpirun —np 16 a.out 100 200





#### How to divide workload among ranks/processes



```
int nra = 8; // 8x8 matrix
int nprocs = 4; //by colors
int r_per_prc = nra/nprocs; //rows per rank
//starting point per rank
int ira start = myrank*r per prc;
//end point per rank
int ira end = (myrank+1)*r_per_prc-1;
for (i=ira start; i<=ira end; i++)</pre>
   for (j=0;j<ncb;j++){
      for (k=0; k < nca; k++) {
          C[i][j] += A[i][k]*B[k][j];
```



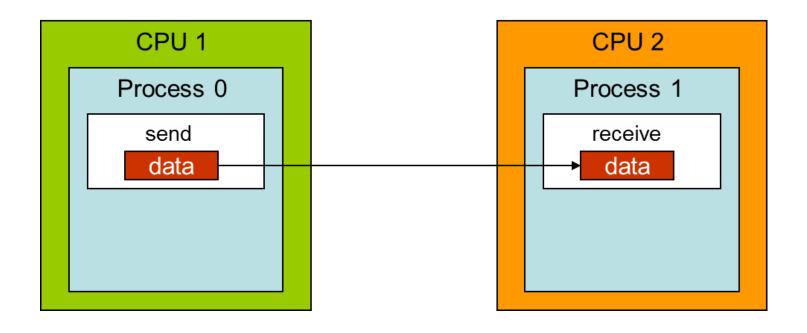
#### **MPI** Data Communication

- Environment management functions
  - Initialization and termination
- Point-to-point communication functions
  - Message transfer from one process to another
- Collective communication functions
  - Message transfer involving all processes in a communicator





### Point-to-point Communication







## Blocking vs. non-blocking

- Communication between a pair of processes
  - Blocking: not return until conditions met
    - Send: when buffer is available for reuse
    - Receive: returns only after it contains the data in its buffer
  - Non-blocking:
    - Create request for send/receive, get back a handle and terminate.
    - Returns from call without waiting for task to complete
    - Sender side allows overlapping computation with communication





## Send/Receive Modes (blocking)

- Standard: message sent (no guarantee that the receive has started). It is up to MPI to decide what to do
- Buffered: int MPI\_Bsend(const void \*buf, int count, MPI\_Datatype datatype, int dest, int tag, MPI\_Comm comm)
- Synchronous: A send will not complete until a matching receive has been posted int MPI\_Ssend(const void \*buf, int count, MPI\_Datatype datatype, int dest, int tag, MPI\_Comm comm)
- Ready: int MPI\_Rsend(const void \*buf, int count, MPI\_Datatype datatype, int dest, int tag, MPI\_Comm comm)

#### One blocking receive:

int MPI\_Recv(void \*buf, int count, MPI\_Datatype dtype, int source, int tag, MPI\_Comm comm, MPI\_Status \*status)



#### Blocking send/receive

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





#### Blocking send/receive

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

- A MPI message consists of two parts
  - Message itself: data body





#### Blocking send/receive

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

- A MPI message consists of two parts
  - Message itself: data body
  - Message envelope: routing infomation
- status: information about received message





#### What is A Message?

- Collection of data (array) of MPI data types
  - Basic data types such as int /integer, float/real
  - Derived data types
- Message "envelope" source, destination, tag, communicator





### Standard send/receive (Blocking)

```
int MPI_Send(void *buf, int count, MPI_Datatype dtype,
int dest, int tag, MPI_Comm comm);
int MPI_Recv(void *buf, int count, MPI_Datatype dtype,
int source, int tag, MPI Comm comm, MPI Status *status)
```

- buf address of sending/receive buffer
- count maximum number of elements in receive buffer
- datatype datatype of each sending/receive buffer element
- dest/source rank of dest / source
- tag message tag
- comm communicator
- status status object,
   e.g., status.MPI\_SOURCE, status.MPI\_TAG)





### Standard send/receive (Blocking)

- The sending process calls the MPI\_SEND function
  - C: int MPI\_Send(void \*buf, int count, MPI\_Datatype dtype, int dest, int tag, MPI Comm comm)
  - Fortran:

```
MPI SEND (BUF, COUNT, DTYPE, DEST, TAG, COMM, IERR)
```

- The receiving process calls the MPI\_RECV function
  - C: int MPI\_Recv(void \*buf, int count, MPI\_Datatype dtype, int source, int tag, MPI Comm comm, MPI Status \*status)
  - Fortran:

```
MPI_RECV(BUF, COUNT, DTYPE, SOURCE, TAG, COMM, STATUS, IERR)
```





### MPI Data Types (C)

```
MPI_CHAR
MPI_SHORT
MPI_INT
MPI_LONG MPI_UNSIGNED_CHAR
MPI_UNSIGNED_SHORT MPI_UNSIGNED_LONG
MPI_UNSIGNED MPI_FLOAT MPI_DOUBLE
MPI_LONG_DOUBLE MPI_BYTE
MPI_PACKED
```





## MPI Data Types (Fortran)

- MPI INTEGER INTEGER
- MPI\_REAL REAL
- MPI\_DOUBLE\_PRECISION DOUBLE PRECISION
- MPI\_CHARACTER CHARACTER(1)
- MPI\_COMPLEX COMPLEX
- MPI\_LOGICAL LOGICAL

• . . .





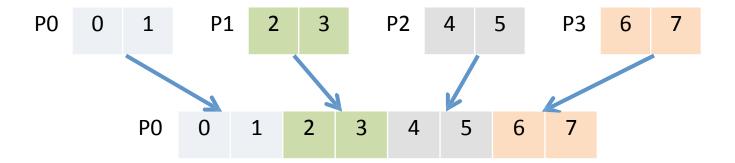
#### Example 1

```
MPI Status Stat;
MPI Init(&argc,&argv);
MPI Comm size(MPI COMM WORLD, &numtasks);
MPI Comm rank(MPI COMM WORLD, &rank);
if (rank == 0) {
   dest = 1; source = 1;
   rc = MPI Send(&outmsg,1,MPI CHAR,dest,tag,MPI COMM WORLD);
   rc = MPI Recv(&inmsg,1,MPI CHAR, source, tag, MPI COMM WORLD, &Stat);
else if (rank == 1) {
   dest = 0; source = 0;
   rc = MPI Recv(&inmsg,1,MPICHAR, source, tag, MPI COMM WORLD, &Stat);
   rc = MPI Send(&outmsg,1,MPI CHAR,dest,tag,MPI COMM WORLD);
rc = MPI Get count(&Stat, MPI CHAR, &count);
printf("Task %d: Received %d char(s) from task %d with tag %d \n",
rank, count, Stat.MPI SOURCE, Stat.MPI TAG);
MPI Finalize(); }
```



## **Example 2: Gathering Array Data**

Gather some array data from each process and place it in the memory of the root process







#### **Example: Gathering Array Data**

```
integer,allocatable :: array(:)
! Initialize MPI
call mpi init(ierr)
call mpi comm size (mpi comm world, nprocs, ierr)
call mpi comm rank(mpi comm world, myid, ierr)
! Initialize the array
allocate(array(2*nprocs))
array(1) = 2 * myid array(2) = 2 * myid + 1
! Send data to the root process
if (myid.eq.0) then do
 i=1,nprocs-1
   call mpi recv(array(2*i+1),2,mpi integer,i,i,status,ierr)
 enddo
 write(*,*) "The content of the array: Source
 write(*,*) array
                                                    tag
                                        dest
else
 call mpi send(array,2,mpi integer,0,myid,ierr)
endif
```



#### MPI\_Barrier

MPI\_Barrier(MPI\_COMM\_WORLD)

- Force all the processes within a communicator to wait for each other
- All processes halt until every single one has reached the barrier





#### MPI\_Wtime()

MPI\_Wtime()

Returns an elapsed time on the calling processor Time in seconds since an arbitrary time in the past





#### MPI\_Get\_count()

```
MPI_Status: Information about status e.g., status.MPI_SOURCE, status.MPI_TAG
```





#### MPI\_Probe()

- Similar to MPI\_Recv() without receiving
- Used to allocate receiving memory dynamically





### **Blocking Operations**

- MPI\_SEND and MPI\_RECV are blocking operations
  - They will not return from the function call until the communication is completed
  - When a blocking send returns, the value(s) stored in the variable can be safely overwritten
  - When a blocking receive returns, the data has been received and is ready to be used





## Deadlock (1)

Deadlock occurs when both processes await each other to make progress

- Guaranteed deadlock!
- Both receives wait for data, but no send can be called until the receive returns





## Deadlock (2)

How about this one?

- No deadlock!
- P0 receives the data first, then sends the data to P1
- There will be performance penalty due to serialization of potentially concurrent operations.





## Deadlock (3)

And this one?

- It depends
- If one send returns, then we are OKAY most MPI implementations buffer the message, so a send could return even before the matching receive is posted.
- If the message is too large to be buffered, deadlock will occur.





## Blocking vs. Non-blocking

- Blocking operations are data corruption proof
- Until a matching receive has signaled that it is ready to receive, a blocking send may continue to wait
  - Possible deadlock
  - Performance penalty
- Non-blocking operations allow overlap of completion and computation
  - The sender process can work on other tasks between the initialization and completion
  - Should be used whenever possible





# Non-blocking Operations (asynchronous)

- Separate initialization of a send or receive from its completion
- Two calls are required to complete a send or receive
  - Initialization
    - Send: MPI ISEND
    - Receive: MPI IRECV
  - Completion: MPI WAIT or MPI TEST





#### Non-blocking Isend and Irecv

#### ♦ MPI\_ISEND function

- C: int MPI\_Isend(void \*buf, int count, MPI\_Datatype dtype, int dest, int tag, MPI\_Comm comm, MPI\_Request \*request)
- Fortran: MPI\_ISEND (BUF, COUNT, DTYPE, DEST, TAG, REQ, COMM, IERR)

#### ♦ MPI\_IRECV function

- C: int MPI\_Irecv(void \*buf, int count, MPI\_Datatype dtype,
  int source, int tag, MPI\_Comm comm, MPI\_Status\*status,
  MPI\_Request \*request)
- Fortran: MPI\_IRECV(BUF, COUNT, DTYPE, SOURCE, TAG, COMM, STATUS, REQ, IERR)



#### Waiting for Completion: MPI\_Wait

int MPI\_Wait(MPI\_Request \*request, MPI\_Status \*status)

- request: communication request
- Status: status object
- Force the process in "blocking mode" waiting to finish on a given request
- As soon as the request is complete, a status instance is returned in status.





#### Non-blocking Example (C)

```
if (myrank == 0) {
   MPI Isend(&x, 1, MPI INT, 1, tag1, MPI COMM WORLD, &send reg);
   printf("Process %d receiving from process 1\n", me);
   MPI Irecv(&x, 1, MPI INT, 1, tag2, MPI COMM WORLD, &recv reg);
// do computations here while waiting for communication
   MPI Wait(&send req, &status);
   MPI Wait(&recv req, &status);
   printf("Process %d ready\n", myrank);
else if (myrank == 1) {
   MPI Irecv(&y, 1, MPI INT, 0, tag1, MPI COMM WORLD, &recv reg);
   MPI Isend(&y, 1, MPI INT, 0, tag2, MPI COMM WORLD, &send req);
   MPI Wait(&recv req, &status)
   MPI Wait(&send req, &status);
```



#### Non-blocking Example (Fortran)

```
integer reqids,reqidr
integer status(mpi_status_size)
if (myid.eq0) then
    call mpi_isend(to_p1,n,mpi_integer,1,100,mpi_comm_world,reqids,ierr)
    call mpi_irecv(from_p1,n,mpi_integer 1,101,mpi_comm_world,reqidr,ierr)
else if (myid.eq.1) then
    call mpi_isend(to_p0,n,mpi_integer,0,101,mpi_comm_world,reqids,ierr)
    call mpi_irecv(from_p0,n,mpi_integer,0,100,mpi_comm_world,reqidr,ierr)
endif

call mpi_wait(status, reqids, ierr)
Call mpi_wait(status, reqidr, ieer)
```





#### Test for Completion: MPI\_Test

- request: communication request
- flag: true if operation completed
- status: status object
- Check if the request can be completed.
- If it can, the request is automatically completed and data is transferred





#### Example: MPI\_Test





#### Exercise a2: Find Global Maximum

- Goal: Find the global maximum
  - Each process (myrank) randomly generate 10 numbers
  - Each process (myrank) finds its own max\_local
  - Root (rank=0) collects max\_local from each process to get the max\_global





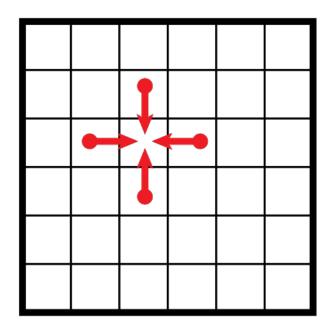
#### Exercise b2: Matrix Multiplication

- Modify b1 so that each process sends its partial results to the root process
  - The root process should now have the whole matrix
  - Note: b1: each process holds its own part of calculation locally
- Validate the result at the root process





### Last Exercise: Laplace Solver



$$\begin{array}{c|c}
D \\
(x,y-1)
\end{array}$$

$$\begin{array}{c|c}
D & P & D \\
(x-1,y) & (x,y) & (x+1,y)
\end{array}$$

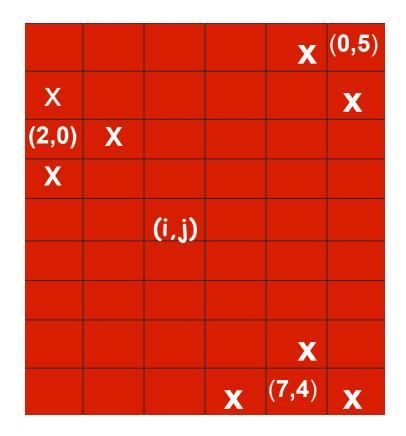
$$\begin{array}{c|c}
D \\
(x,y+1)
\end{array}$$

$$P_{x,y} = (D_{x-1,y} + D_{x,y-1} + D_{x+1,y} + D_{x,y+1}) / 4$$





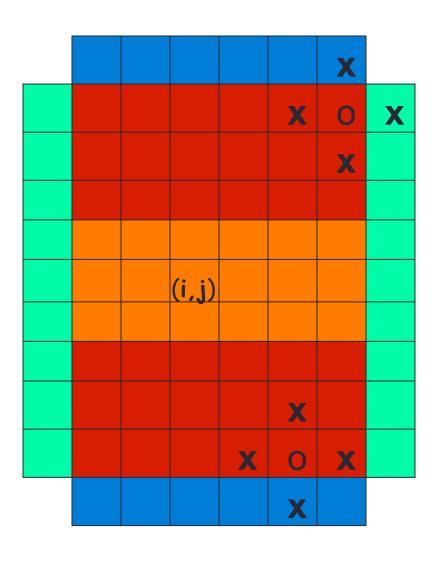
#### Five-point Finite-Difference Stencil (border cells)







#### **Domain Decomposition**



thread 0

thread 1

thread 2

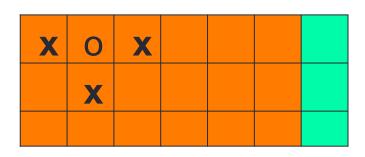




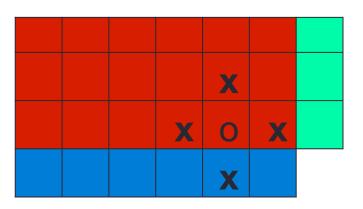
## Unknowns at Border Cells – 1D

Thread 0

Five-point finite-difference stencil applied at thread domain border cells require cells from neighboring threads and/or boundary cells.



thread 1



Thread 2



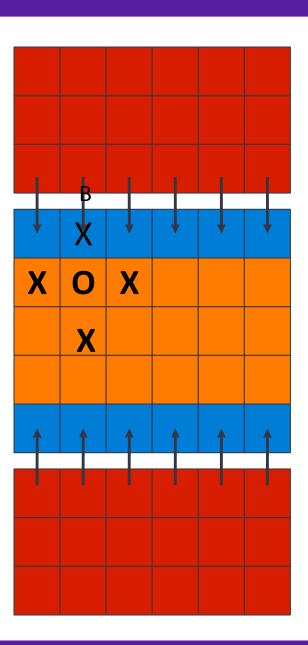


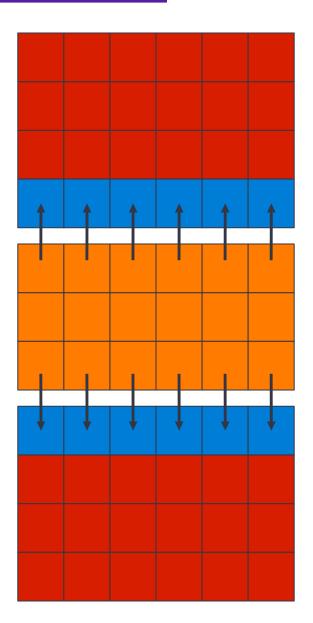
thread 0

thread 1

current thread

thread 2









#### Exercise c: Laplace Solver

- Goal: develop a working MPI Laplace solver
  - Distribute the workload in 1D manner
  - Initialize the sub-matrix at each process and set the boundary values
  - Calculate new values
  - At the end of each iteration
    - Exchange boundary data with neighbors
    - Find the global convergence error and distribute to all processes
    - Update entire matrix using new values





#### **Conclusions**

- Standardized
  - With efforts to keep it evolving (MPI 3.0)
- Portability
  - MPI implementations are available on almost all platforms
- Scalability
  - In the sense that it is not limited by the number of processors that can access the their local memory space
- Popularity
  - De Facto programming model for distributed memory machines
- Nearly every big academic or commercial simulation or data analysis running on multiple nodes uses MPI directly or indirectly





#### Continue...

- MPI Part 2: Collective communications
- MPI Part 3: Understanding MPI applications

