Introduction to MPI Programming – Part 1

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Outline

- Introduction
- MPI program basics
- Point-to-point communication

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

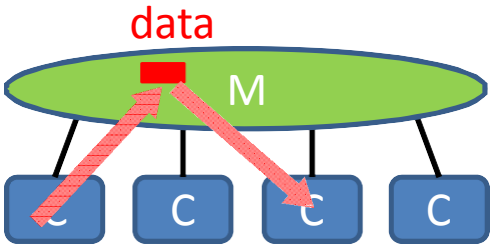
Memory system models for parallel computing

Different ways of sharing data among processors

- Shared Memory
- Distributed Memory
- Other memory models
  - Hybrid model
  - PGAS (Partitioned Global Address Space)

Shared memory model

- All threads can access the global address space
- Data sharing achieved via writing to/reading from the same memory location
- Example: OpenMP

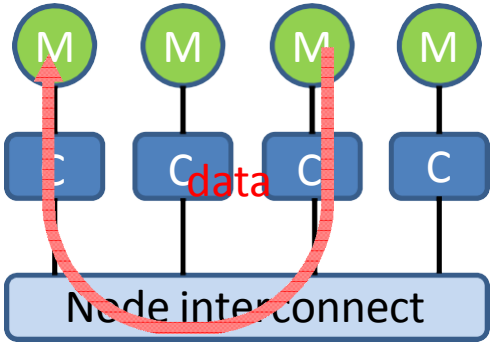


Distributed memory model

- Each process has its own address space

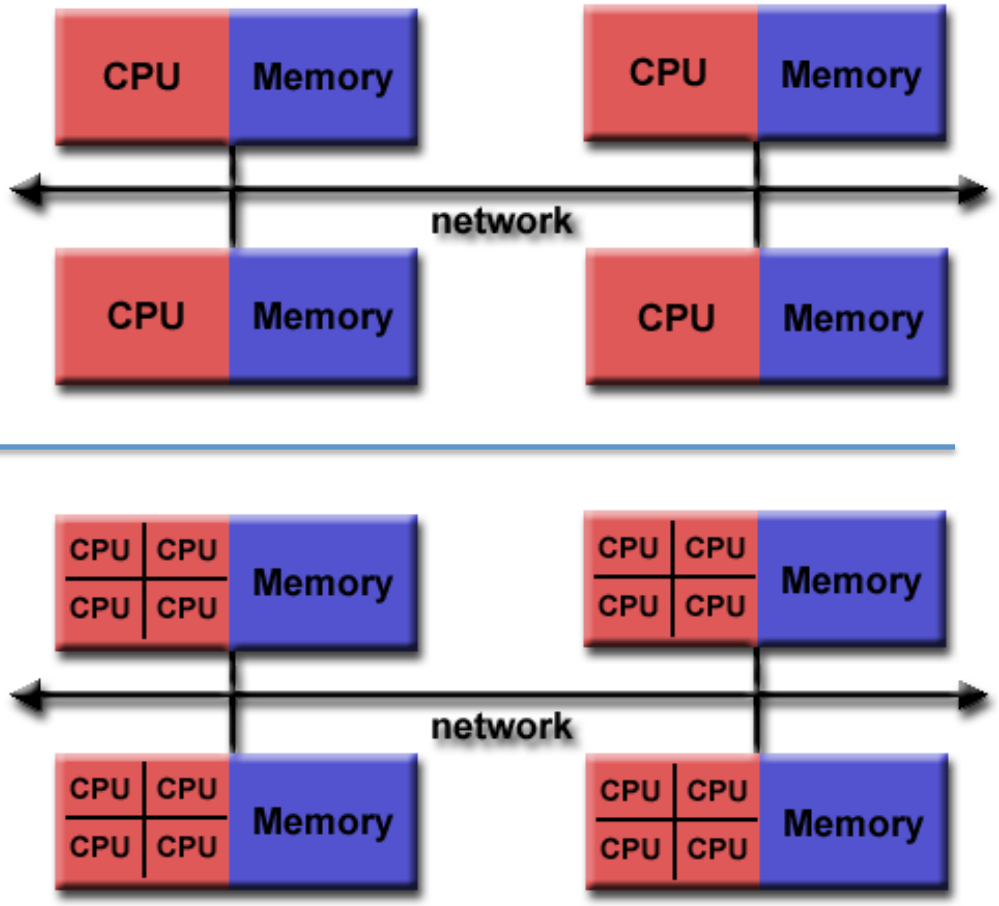
  Data is local to each process

- Data sharing achieved via explicit message passing (through network)
- Example: MPI (Message Passing Interface)



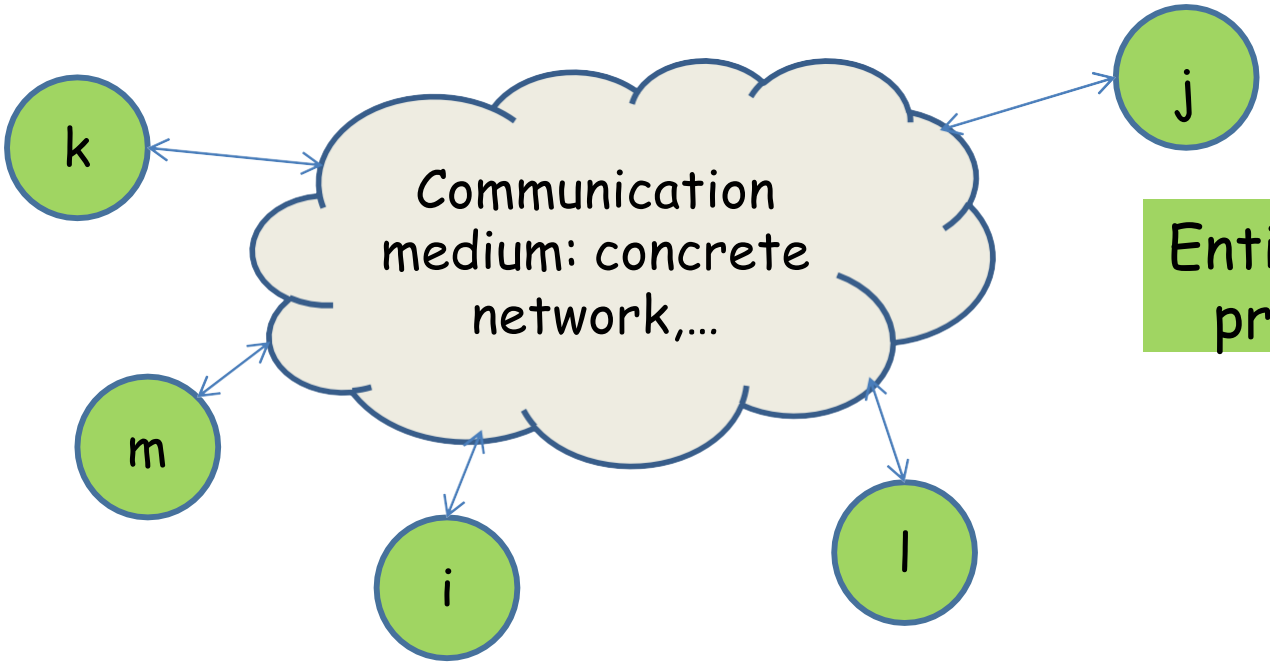
MPI Programming Models

- Distributed



Message Passing

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



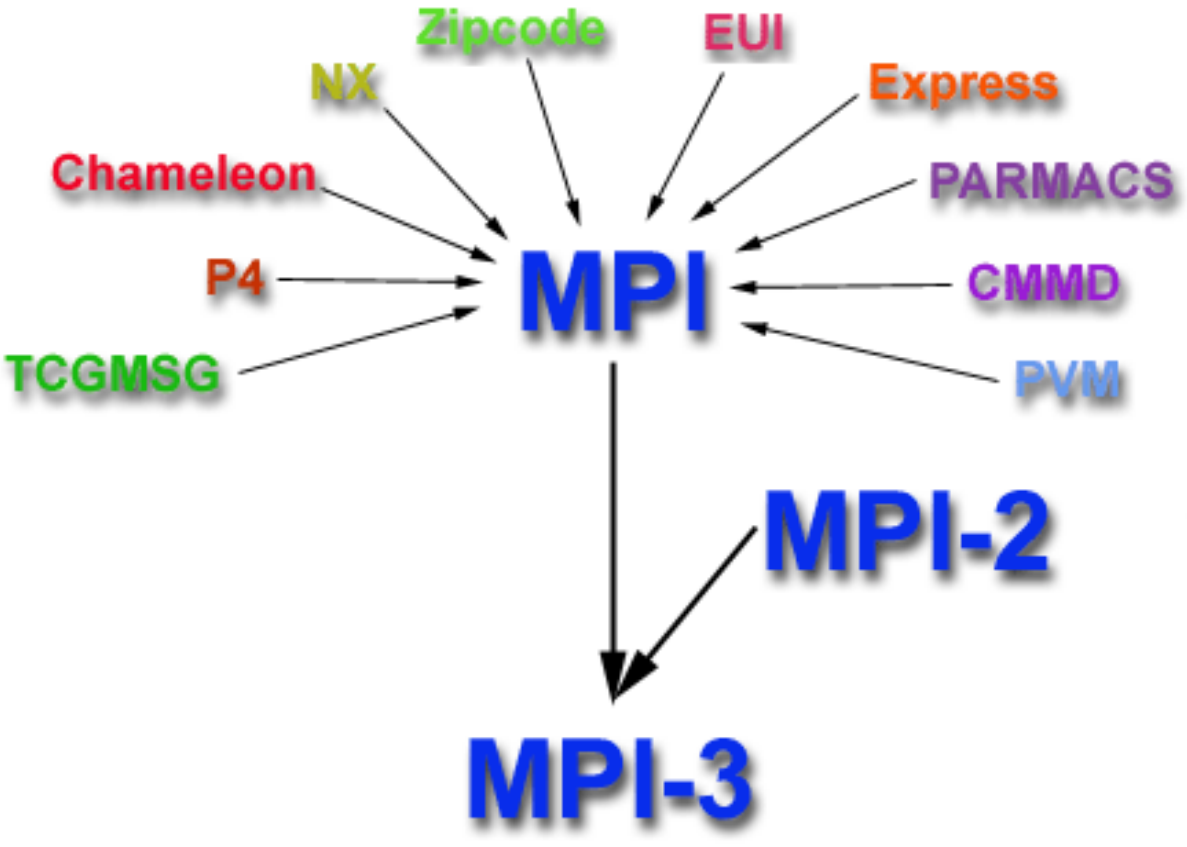
Entities: MPI processes

Why MPI?

- There are already network communication libraries
- Optimized for performance
- Take advantage of faster network transport
  - Shared memory (within a node)
  - Faster cluster interconnects (e.g. InfiniBand)
  - TCP/IP if all else fails
- Enforces certain guarantees
  - Reliable messages
  - In-order message arrival
- Designed for multi-node technical computing

MPI History

- 1980-1990
- 1994:MPI-1
- 1998:MPI-2
- 2012:MPI-3



Message Passing Interface

- MPI defines a standard API for message passing
  - The standard includes
    - What functions are available
    - The syntax of those functions
    - What the expected outcome is when calling 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

Various MPI Implementations

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

High or low level programming?

- High level compared to other network libraries
  - Abstract transport layer
  - Supply higher-level operations
- Low level for scientists
  - Handle problem decomposition
  - Manually write code for every communications among processes

More about MPI

- MPI provides interface to libraries
  - APIs and constants
  - Binding to Fortran/C
  - Several third-party bindings for Python, R and more other languages
  - Run MPI programs (e.g. mpiexec)

Let's try it

- `$whoami`
- `$mpiexec –np 4 whoami`

What just happened?

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

```
mpiexec –hostfile machine.lst –
np/-npp 4 app.exe
```

Outline of a MPI Program

1. 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)

2. 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_Status status;

MPI_Init(&argc, &argv);
MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
MPI_Comm_rank(MPI_COMM_WORLD, &myid);
printf("Hello World from process %d/%d
\n", myid, nprocs);

MPI_Finalize();
…
}
```

Header file

Initialization

Computation and communication

Termination

Hello World (C)

```
include “mpi.h”

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

MPI_Init(&arg
MPI_Comm_size
MPI_Comm_rank
printf("Hello
\n", myid, np

MPI_Finalize();
…
}
```

```
[wfeinste@shelob1 hello]$ mpicc hello.c
[wfeinste@shelob1 hello]$ mpirun -np 4 ./a.out
Hello World from process 3/4
Hello World from process 0/4
Hello World from process 2/4
Hello World from process 1/4
```

Header file

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Termination

Hello World (Fortran)

```
include "mpif.h"

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)

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

call mpi_finalize(ierr)

….
```

Header file

Initialization

Computation and communication

Termination

Hello World (Fortran)

```
include "mpif.h"

integer::nprocs, ierr, myid
integer::status(mpi_status_size)

call mpi_init(ierr)
call mpi_comm
call mpi_comm

write(*, '("Hel
nprocs

call mpi_finalize(ierr)

….
```

Header file

Initialization

utation and
nunication

Termination

```
[wfeinste@shelob1 hello]$ mpif90 hello.f90
[wfeinste@shelob1 hello]$ mpirun -np 4 ./a.out
Hello World from process   3 /  4
Hello World from process   0 /  4
Hello World from process   1 /  4
Hello World from process   2 /  4
```

Naming Signature (C/Fortran)

- Function name convention
  - C: `MPI_Xxxx(arg1,…)`
  - Fortran: `mpi_xxx` (not case sensitive)
- 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)`

Communicators (1)

- A communicator is an identifier associated with a group of processes


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

Communicators (2)

- A communicator is an identifier associated with a group of processes
  - Can be regarded as the name given to an ordered list of processes
  - Each process has a unique rank, which starts from 0 (usually referred to as "root")
  - It is the context of MPI communications and operations
    - For instance, when a function is called to send data to all processes, MPI needs to understand what "all" means

Communicators (3)

- MPI_COMM_WORLD: the default communicator contains all processes running a MPI program
- There can be many communicators

  `e.g., MPI_Comm_split(MPI_Comm comm, int color, int, kye, MPI_Comm* newcomm)`
- A process can belong to multiple communicators
  - The rank is usually different

Communicator Information

- Rank: unique id of each process
  - C: `MPI_Comm_Rank(MPI_Comm comm, int *rank)`
  - Fortran: `MPI_COMM_RANK(COMM,RANK,ERR)`
- Get the size/processes of 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	Underlying Compiler
C	mpicc	gcc
	mpiicc	icc
	mpipgcc	pgcc
C++	mpiCC	g++
	mpiicpc	icpc
	mpipgCC	pgCC
Fortran	mpif90	f90
	mpigfortran	gfortran
	mpiifort	ifort
	mpipgf90	pgf90

Compiling and Running MPI Programs

- On Shelob:
  - 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>`

About Exercises

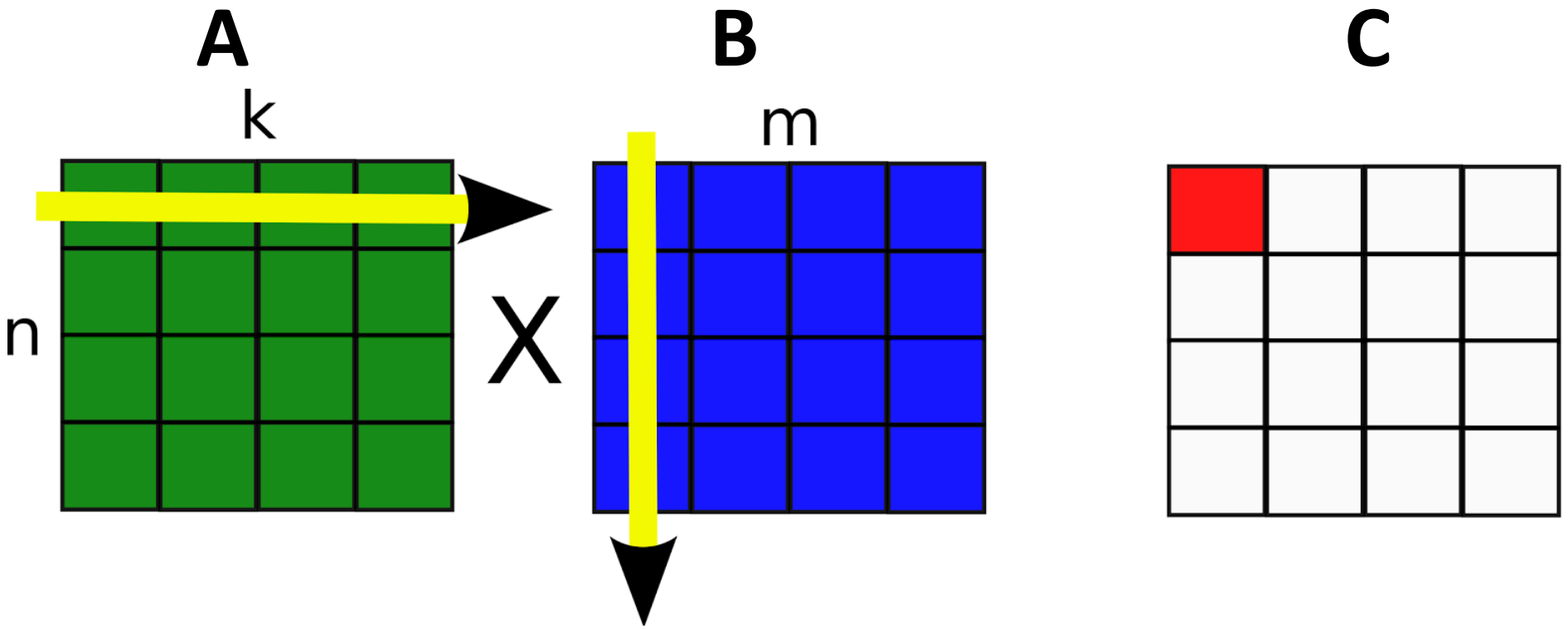
- Exercises
  - Track a: Process color
  - Track b: Matrix multiplication
  - Track c: Laplace solver

- Your tasks:
  - Fill in blanks to make MPI programs work under /exercise directory
  - Solutions are provided in /solution directory

Exercise a1: Process Color

- Write a MPI program where
  - 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”

Exercise b1: Matrix Multiplication



$$C_{1,1} = \sum_{i=n}^{i=1} (A_{1,i} \times B_{i,1})$$

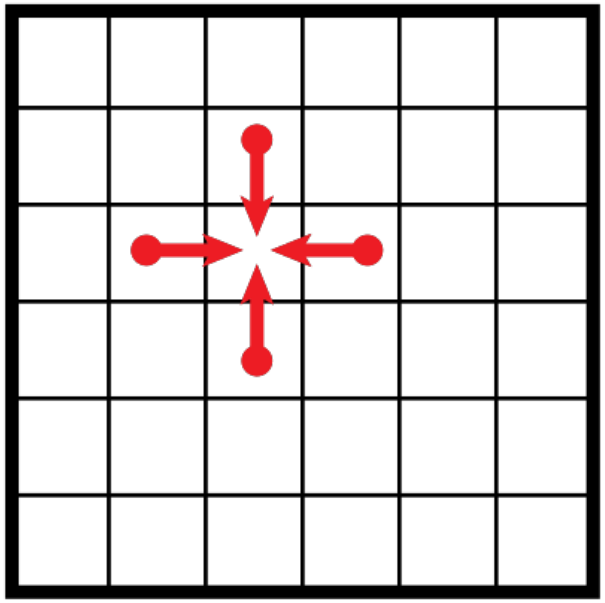
Exercise b1: Matrix Multiplication

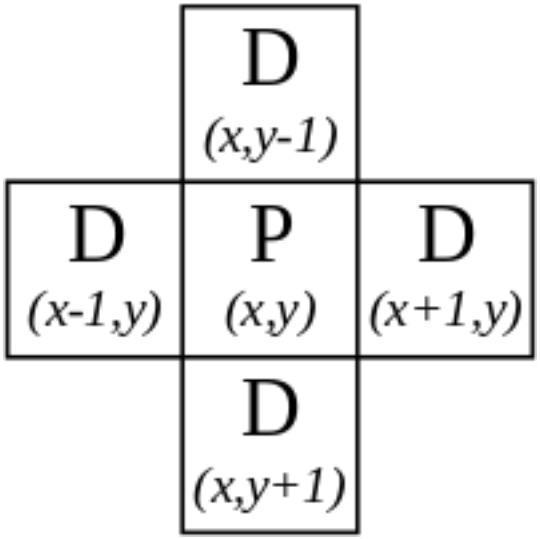
```
for(i=0;i<row;i++){          //row of first matrix
    for(j=0;j<col;j++){      //column of second matrix
        sum=0;
        for(k=0;k<n;k++)
            sum=sum+a[i][k]*b[k][j];
        c[i][j]=sum;         //final matrix
    }
}
```

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
  - Then processes part of the workload
    - Need to determine how to decompose (which process deals which rows or columns)
    - Assume that the dimension of A and B is a multiple of the number of processes (need to check this in the program)
  - Validate the result at the end

Exercise c1: Laplace Solver version 1





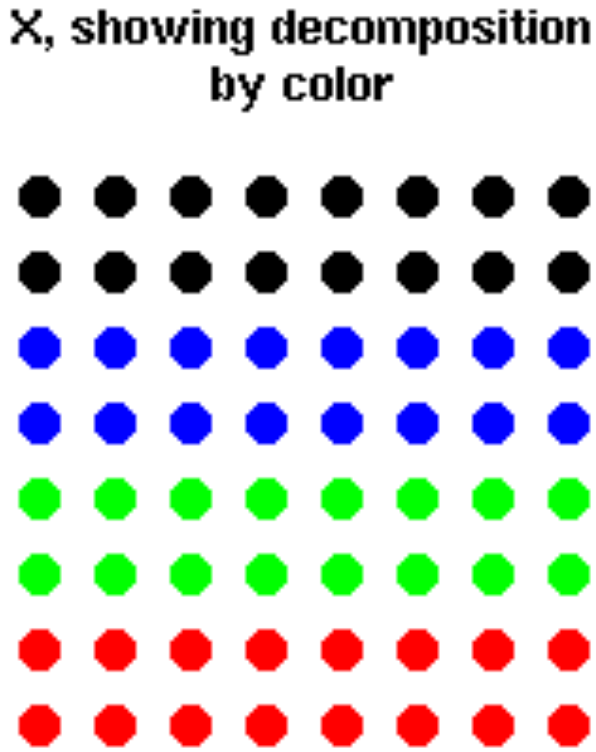
$$P_{x,y} = (D_{x-1,y} + D_{x,y-1} + D_{x+1,y} + D_{x,y+1}) / 4$$

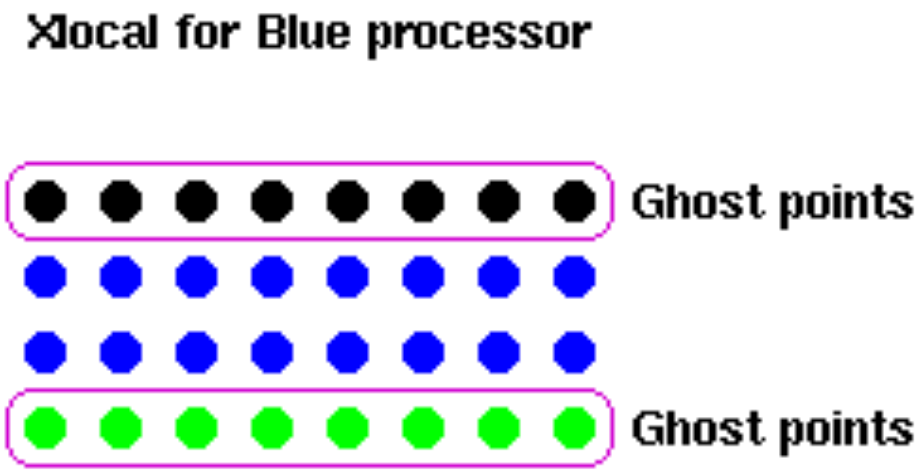
Exercise c1: Laplace Solver version 1

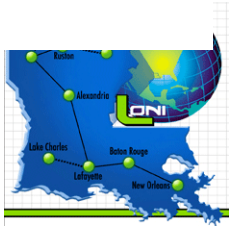
- Goal: Distribute the work load among processes in 1-d manner

  e.g. 4 MPI processes (color coded) to share the work load

Exercise c1: Laplace Solver version 1







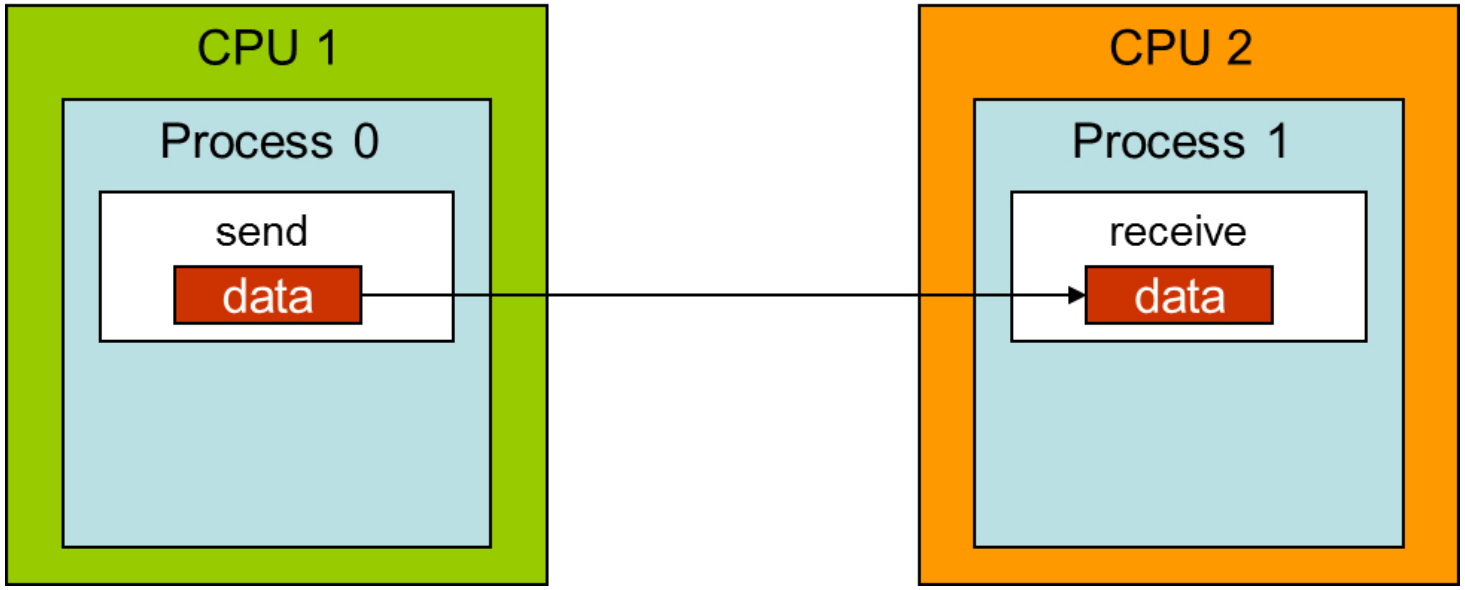
Exercise c1: Laplace Solver version 1

- Goal: Distribute the work load among processes in 1-d manner
  - Find out the size of sub-matrix for each process
  - Let each process report which part of the domain it will work on, e.g. “Process x will process column (row) x through column (row) y.”
    - Row-wise (C) or column-wise (Fortran)

MPI Functions

- 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



Point-to-point Communication

- Blocking send/receive
  - 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)`

Send/Receive

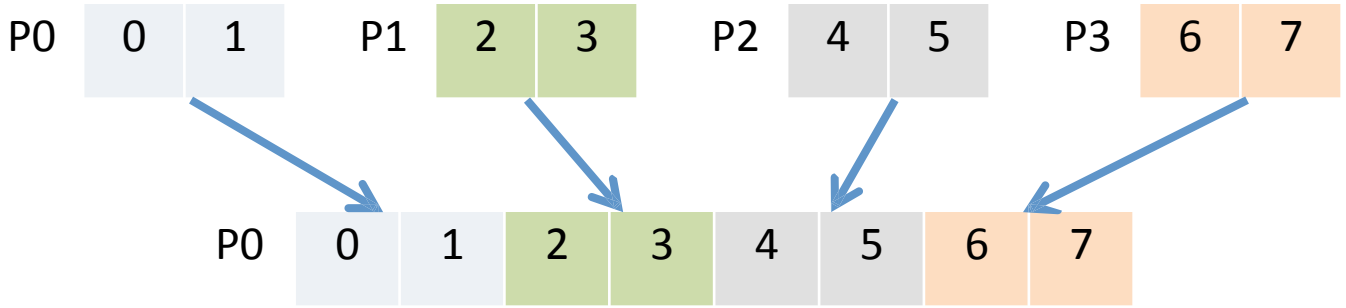
```
int MPI_Send(void *buf, int count, MPI_Datatype  dtype,
int dest, int tag, MPI_Comm comm);

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 info
- **`status`**: information of the message that is received

Example: 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, 0,mpi_comm_world,status,ierr)
  enddo
  write(*,*) "The content of the array:"  write(*,*) array
else
  call mpi_send(array,2,mpi_integer,0,0, mpi_comm_world,ierr)
  endif
```

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 awaits the other to make progress

```
//    Exchange data   between two processes
If  (process 0)
          Receive data from process 1
          Send data to process 1
If  (process 1)
          Receive data from process 0
          Send data to process 0
```

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

Deadlock (2)

- How about this one?

```
//   Exchange data  between two processes
If  (process 0)
       Receive data from process 1
       Send data to process 1
If  (process 1)
       Send data to process 0
       Receive data from process 0
```

- 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?

```
//    Exchange data  between two processes
If  (process 0)
        Send data to process 1
        Receive data from process 1
If  (process 1)
        Send data to process 0
        Receive data from process 0
```

- 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, but
  - Possible deadlock
  - Performance penalty
- Non-blocking operations allow overlap of completion and computation
  - The 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`

Non-blocking Point-to-point Communication

- 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, COMM, REQ, IERR)`
- MPI_IRECV function
  - C: `int MPI_Irecv(void *buf, int count, MPI_Datatype dtype, int source, int tag, MPI_Comm comm, MPI_Request *request)`
  - Fortran: `MPI_IRECV(BUF, COUNT, DTYPE, SOURCE, TAG, COMM, REQ, IERR)`
- MPI_WAIT
  - C: `int MPI_Wait( MPI_Request *request, MPI_Status *status);`
  - Fortran: `MPI_WAIT(REQUEST, STATUS, IERR)`

Example: Exchange Data with Non-blocking calls

```
integer reqids,reqidr
integer status(mpi_status_size)

if (myid.eq.0) 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)
elseif (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,ierr)
```

Exercise a2: Find Global Maximum

- Goal: Find the maximum in an array
  - Each process handle part of the array
  - Every process needs to know the maximum at the end of program
- Hints
  - Step 1: each process send the local maximum to the root process to find the global maximum
  - Step 2: the root process send the global maximum to all other processes

Exercise b2: Matrix Multiplication

- Modify b1 so that each process sends its partial results to the root process
  - The root process should have the whole matrix
- Validate the result at the root process

Exercise c2: Laplace Solver

- Goal: develop a working MPI Laplace solver using c1
  - Distribute the workload in 1D manner
  - Initialize the sub-matrix at each process and set the boundary values
  - At the end of each iteration
    - Exchange boundary data with neighbors
    - Find the global convergence error and distribute to all processes

Why MPI?

- 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 same 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