Introduction to MPI Programming – Part 1

CENTER FOR COMPUTATION & TECHNOLOGY

Outline

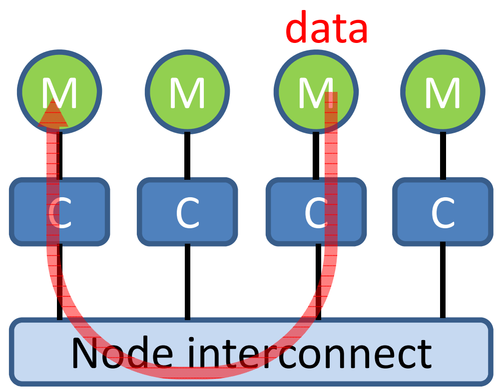
- Introduction – what is MPI and why MPI
- MPI program basics
- Point-to-point communication

Memory system models

- Different ways of sharing data among processors
  - Distributed Memory
  - Shared Memory
  - Other memory models
    - Hybrid model
    - PGAS (Partitioned Global Address Space)

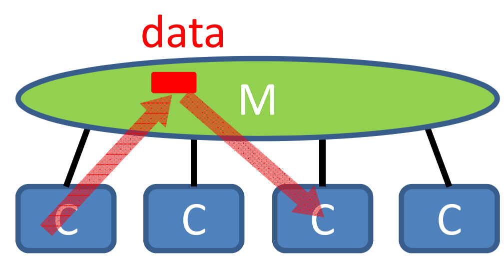
Distributed memory model

- 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)



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



Message Passing

- Context: distributed memory parallel computers
  - Each processor has its own memory space and cannot access the memory of other processors
  - Any data to be shared must be explicitly transferred from one to another

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)
      - Many different implementations out there: MPICH, MVAPICH, OpenMPI, Intel MPI etc.
    - Runtime details (e.g. how many processes the code with run with etc.)
- MPI provides C/C++ and Fortran bindings

Why MPI?

- Standardized
  - With efforts to keep it evolving (MPI 3.0 draft came out in 2010)
- 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

When NOT to use MPI

- Not suitable for fine, inner loop level parallelization
  – Shared memory programming model (e.g. OpenMP) and accelerators (e.g. GPU, Xeon Phi) are better suited for this purpose

MPI Functions

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

MPI Program Structure

```
program hello
…
include "mpif.h"
integer :: nprocs,myid,ierr
…
call mpi_init(ierr)
…
call mpi_comm_size(mpi_comm_world,nprocs,ierr)
call mpi_comm_rank(mpi_comm_world,myid,ierr)
Write(*,'("There are",I3," processes")') nprocs
write(*,'("Process",I3," says Hello World!")') myid
…
call mpi_finalize(ierr)
…
```

Header file
Initialization
Computation and communication
Termination

MPI Program Structure

```
program hello
…
include "mpif.h"
integer :: nprocs,myid,ierr
…
call mpi_init(ierr)
…
call mpi_cc
call mpi_cc
Write(*,'("
write(*,'("
…
call mpi_fi
…
```

```
[lyan1@qb563 ex]$ mpirun -np 4 ./a.out
There are  4 processes.
There are  4 processes.
There are  4 processes.
There are  4 processes.
Process  3 says Hello World!
Process  1 says Hello World!
Process  0 says Hello World!
Process  2 says Hello World!
```

Header file
Initialization
Computation and communication
Termination

C vs. Fortran

- Not too much difference
- Header file
  - C: `mpi.h`
  - Fortran: `mpif.h`
- Function names
  - C: `MPI_Some_Function`
  - Fortran: `mpi_some_function` (not case sensitive)
- Error handles
  - C returns the error value, while Fortran passes it as an argument
    - C: `int err = MPI_Some_Function(arg1,arg2,…,argN)`
    - Fortran: `call mpi_some_function(arg1,arg2,…,argN,ierr)`

Initialization and Termination

- Initialization
  - Must be called before any other MPI calls
  - C: `MPI_Init()`
  - Fortran: `MPI_INIT(ierr)`
- Termination
  - Clean up data structures, terminate incomplete calls etc.
  - C: `MPI_Finalize()`
  - Fortran: `MPI_FINALIZE(ierr)`

Communicators (1)

- 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 (2)

- MPI_COMM_WORLD: the default communicator that contains all processes running the MPI program
  - This is the only one we will use for this workshop
- There can be many communicators
- A process can belong to multiple communicators
  - The rank is usually different

Getting Communicator Information

- Get the rank of a communicator
  - C: `MPI_Comm_Rank(MPI_Comm comm, int *rank)`
  - Fortran: `MPI_COMM_RANK(COMM,RANK,ERR)`
- Get the size in a communicator
  - C: `MPI_Comm_Size(MPI_Comm comm, int *size)`
  - Fortran: `MPI_COMM_SIZE(COMM,SIZE,ERR)`

Compiling and Running MPI Programs

- Not a part of the standard
  - Could vary from platform to platform
  - Or even from implementation to implementation on the same platform
- 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: Miscellaneous exercises
  - Track B: Matrix multiplication
  - Track C: Laplace solver
  - Located at: /home/lyan1/loniworkshop2014/<problem>/mpi
- For most exercises, a serial program will be provided and your task is to parallelize it with MPI
  - You can start from the serial program, or
  - You can fill the blanks in the provided MPI programs

Exercise 1a: 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 1b: Matrix Multiplication version 1

- 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 1c: Laplace Solver version 0

- 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)

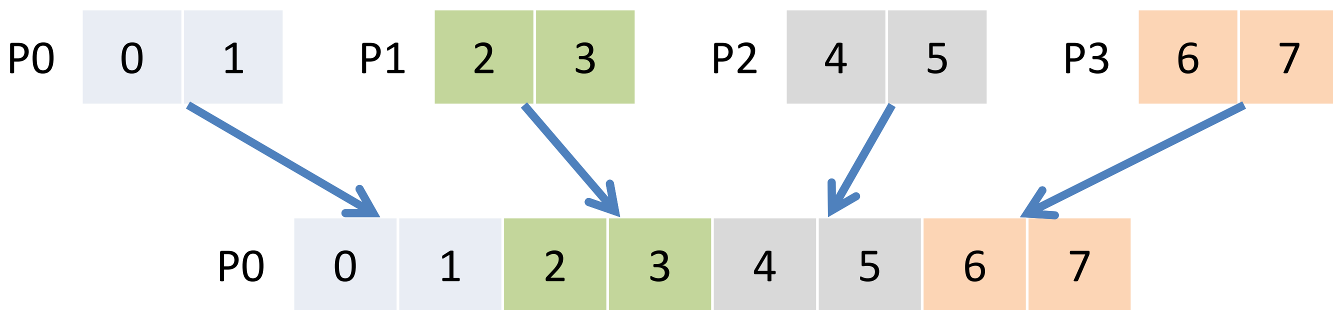
Point-to-point Communication

- Communication between a pair of processes, so two functions calls are required
  - 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)`
- The function arguments characterize the message being transferred

MPI Message

- A MPI message consists of two parts
  - Message body
    - Buffer: starting location in memory for outgoing data (send) or incoming data (receive)
    - Data type: type of data to be sent or received
    - Count: number of items of type datatype to be sent or received
  - Message envelope
    - Destination (source): rank of the destination (source) of the message
    - Tag: what MPI uses to match messages between processes
    - Communicator
- The `status` argument contains information on the message that is received
  - Only for MPI_RECV

Example: Gathering Array Data



- Goal: 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:”
  write(*,*) array
else
  call mpi_send(array,2,mpi_integer,0,myid,ierr)
endif
```

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
```

```
[lyan1@qb563 ex]$ mpirun -np 4 ./a.out
The content of the array:
           0           1           2           3           4           5
           6           7
```

```
  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:"
  write(*,*) array
else
  call mpi_send(array,2,mpi_integer,0,myid,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
```

This is a guaranteed deadlock because both receives will be waiting 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
```

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 will occur – process 0 will receive the data first, then send the data to process 1; However, there will be performance penalty because we serialize potential 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
```

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 of the sends returns, then we are OKAY - most MPI implementations buffer the message, so a send could return even before the matching receive is posted. However, if this is not the case or the message is too large to be buffered, deadlock will occur.

Non-blocking Operations (1)

- Non-blocking operations separate the 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 Operations (2)

- MPI_ISEND
  - 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
  - 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, `**`REQUEST`**`, 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)
```

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 things between the initialization and completion
  - Should be used whenever possible

Exercise 2a: 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
  - This can be done in two steps
    - 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 2b: Matrix Multiplication Version 2

- Modify version 1 so that each process sends its partial results to the root process
  - The root process should have the whole matrix of C
- Then validate the result at the root process

Exercise 2c: Laplace Solver Version 1

- Goal: develop a working MPI Laplace solver
  - Distribute the workload in a one-dimensional 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