Parallel Programming with MPI (Message Passing Interface)

Distributed Memory Programming Model



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- Parallel Programming models
- Introduction to MPI
- Structure of MPI and Simple MPI program
- Point to point communication calls
- Collective Communication calls



Sample Parallel Programming Models



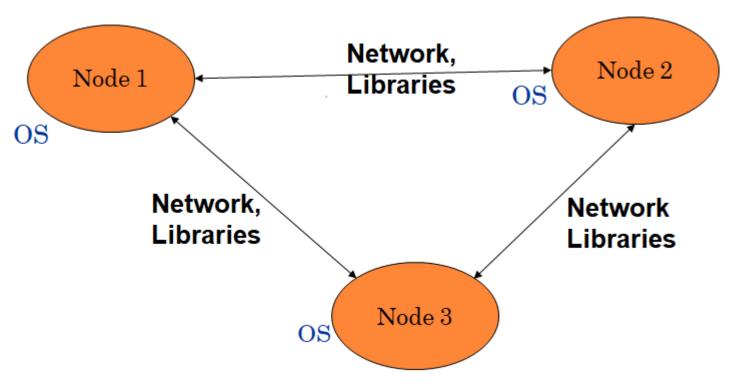
- Shared Memory Programming
 - Processes share memory address space (threads model)
- Transparent Parallelization
 - Compiler works magic on sequential programs
- Directive-based Parallelization
 - Compiler needs help (e.g., OpenMP)
- Message Passing
 - Explicit communication between processes (like sending and receiving emails)



Distributed Architecture



- What differentiates a Supercomputer from a normal computer network



Multiple Nodes connected together to form a Computer Cluster



Distributed Architecture...



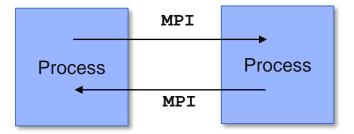
- Each node may have many processor cores
- High Speed Network
- Parallel Programming Libraries
- Simplified Operating System mostly Unix flavors



Introduction to MPI



- A message passing library specification
- Message passing among processes in parallel computing
- Meant for clusters and network of workstations
- Message Passing Standard for Parallel Programs
 - MPI Implementation left to individual vendors.
 - Most commonly supports C, Fortran, C++ and Python programs
- Inter-process communication consists of
 - Synchronization
 - movement of data from one process's address space to another's.





MPI – Characteristics



- Separate memory address spaces Message passing among processes in parallel computing
- Explicit data and work allocation by the user
- Asynchronous parallelism
- Explicit interaction



MPI – How it works?



- A parallel computation consists of no. of processes
- Each process has its local variables
- No mechanism for any process to directly access the memory of another
- Sharing the data among the process through message passing
- Data transfer requires cooperative operations by each process
- Different processes need not be running on different processors



Requisites for MPI Implementations



The Following features are needed in MPI Implementations

- Allow efficient Communication between processes.
- Allow overlap of computation and communication

Important considerations while using MPI

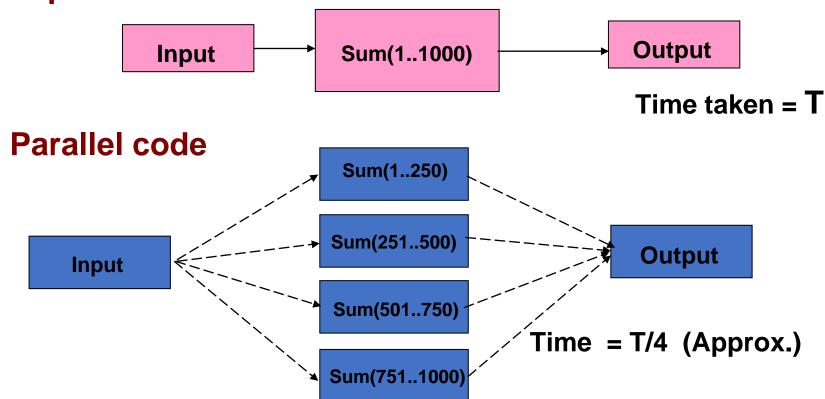
 All parallelism is explicit: the programmer is responsible for correctly identifying parallelism and implementing parallel algorithms using MPI constructs



Why Parallelization of codes?



Sequential code





Structure of MPI Program



MPI include file

Initialize MPI environment

Do work and make message passing calls

Terminate MPI Environment



BASIC MPI Calls



- Many parallel programs can be written using just these six mpi calls,
 - MPI_INIT initialize the MPI library
 - MPI_COMM_SIZE get the size of a communicator
 - MPI_COMM_RANK get the rank of the calling process in the communicator
 - MPI_SEND send a message to another process
 - MPI_RECV receive a message to another process
 - MPI_FINALIZE clean up all MPI state (must be the last MPI function called by a process)



Simple MPI Program



```
#include <stdio.h>
#include <mpi.h>
main(int argc, char *argv[]) {
        int rank, size;
        MPI_Init(&argc, &argv);
        MPI_Comm_rank(MPI_COMM_WORLD, &rank);
        MPI_Comm_size(MPI_COMM_WORLD, &size);
        printf("Process:%d out of %d\n", rank, size);
        MPI_Finalize();
```



Compiling and Running MPI Programs



C program compilation

• \$ mpicc filename.c

Fortran program compilation

•\$ mpiifort filename.f90 (Fortran)

Running C and Fortran mpi applications

- \$ mpirun -np <np> <exe-name>
- \$ mpirun -np <np> -machinefile <hostfilesname> <exe-name>

Where

-np: No. of processes to run on

-machinefile: List of possible machines to run the executable



Only 5 things to know before learning MPI function calls



- Communications
 - Point to point communication
 - Collective communication
- MPI Data types
- Format of MPI Calls
- Communicator
- Rank



MPI Communications



Point-to-Point Communication

- Blocking
- Non Blocking

Collective Communication

- Synchronization
- Collective computation
- Data Movement



MPI Basic Data types- C Programs



MPI Datatype	C Datatype
MPI_CHAR	Signed char
MPI_SHORT	Signed short int
MPI_INT	Signed int
MPI_LONG	Signed long int
MPI_UNSIGNED_CHAR	Unsigned char
MPI_UNSIGNED_SHORT	Unsigned short int
MPI_UNSIGNED	Unsigned int
MPI_UNSIGNED_LONG	Unsigned long int
MPI_FLOAT	Float
MPI_DOUBLE	Double
MPI_LONG_DOUBLE	Long double
MPI_BYTE	



MPI Basic Data types – Fortran programs



MPI Datatype	Fortran Datatype
MPI_INTEGER	INTEGER
MPI_REAL	REAL
MPI_DOUBLE_PRECISION	DOUBLE PRECISION
MPI_COMPLEX	COMPLEX
MPI_LOGICAL	LOGICAL
MPI_CHARACTER	CHARACTER(1)
MPI_BYTE	



Format of MPI Calls - C Language



Format	Rc = MPI_Xxxxx(parameter,)
Ex	Rc = MPI_Send(&buf,count,type,dest,tag,comm)

- All MPI Functions are case sensitive.
- All MPI calls begin with MPI_ followed by actual function name.
- C programs should include the file mpi.h
- Return_integer Rc is of type integer. It is set to MPI_SUCCESS upon success.



Format of MPI Calls- Fortran



	CALL MPI_XXXXX(parameter,, ierr)
Ex	CALL MPI_SEND(buf,count,type,dest,tag,comm,ierr)

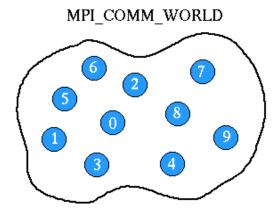
- Case insensitive.
- Fortran programs should include the file mpif.h
- Additional parameter ierr to take care of the function status



Communicator



- The communicator is Communication Universe.
 - Processes that are allowed to communicate
- Messages are sent / received within a given Universe.
- MPI_COMM_WORLD is the default communicator.



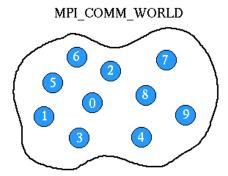


What is 'Rank' in Communicator?



Rank:

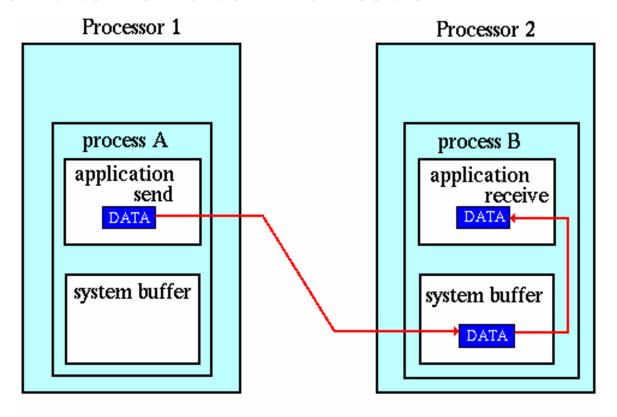
- Unique integer identifier for every process.
- Assigned by the system during initialization.
- Ranks are contiguous & begin at zero.
- Used to specify the source and destination of messages.
- Often used to control program execution (if rank=0 do this / if rank=1 do that).





MPI Point-to-Point Communication





Path of a message buffered at the receiving process



MPI Send and Receive: Syntax



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);

When MPI_Recv routine returns, the received message data have been copied into the buffer; and the tag, source, and actual count of data received are available via the status argument



MPI Send and Receive: Blocking



```
strcpy(Message, "Hello India");
Destination = 0; source= 1; BUFFER_SIZE = 32;
MPI_Send (Message, BUFFER_SIZE, MPI_CHAR, Destination, tag,MPI_COMM_WORLD);
```

MPI_Recv(Message, BUFFER_SIZE, MPI_CHAR, source, tag,MPI_COMM_WORLD, &status);

Arguments of MPI_send & Receive:

- Message: Address where the data starts.
- BUFFER_SIZE: Number of elements (items) of data in the message.
- MPI_CHAR: Datatype of the message passed / received.
- Destination/source: Rank of Receiving or Sending processes
- tag: Integer to distinguish messages
- MPI_COMM_WORLD: Communicator, status: contains status



Performance Analysis of MPI Programs



- Why Performance Analysis of MPI Applications
 - To get the benefit of parallelization
 - Tuning the Parallel algorithm
 - Tuning the application
- Communication Vs Computation Time
- Function Profiling



Challenges Involved in Debugging Parallel Applications



- Complexity increases with the multiplicity of processes
- Processes may be running on different machines.
- Co-coordinating the communication between processes.
- Processes may be operating on different data sets.



Debugging Parallel Applications



- Through Command Line Interface
 - . GDB
 - Valgrind
- Through Graphical User Interface (GUI)
 - TotalView debugger
 - Valgrind



Collective Communication - Overview



- Involves the sending and receiving of data among processes
- All processes need to participate in the communication.
- Usage of Point-to-point communication routines
- Customized communicator
- No message tags used



Collective Communications – Characteristics



- Communications are locally blocking
- Some routines use a root process to originate or receive all data
- Synchronization is not guaranteed (implementation dependent)
- Data amounts must exactly match
- Different types
 - ** One-to-All
 - ** All-to-One
 - ** All-to-All



Collective Communications – Patterns



- Synchronization (Ex: Barrier synchronization)
- Data movement (Ex: Broadcast, Scatter, Gather)
- Collective computation (Ex: SUM, MAX, MIN, etc)



MPI Collective Communication - Calls



- Barrier synchronization
- Broadcast from one member to all other members
- Gather data from an array spread across processors into one array
- Scatter data from one member to all members
- All-to-all exchange of data
- Global reduction (e.g., sum, min of "common" data elements)
- Scan across all members of a communicator



Data Movement - Calls



- Broadcast
- Gather
- Scatter
- Allgather
- Alltoall



MPI-2 Overview



- Extensions to the message-passing model
 - ** Parallel I/O
 - ** One-sided operations
 - ** Dynamic process management
- Making MPI more robust and convenient
 - ** C++ and Fortran 90 bindings
 - ** External interfaces, handlers
 - ** Extended collective operations
 - ** Language interoperability
 - ** MPI interaction with threads



MPI-3 Overview



- Major update to the MPI standard.
- Includes the extension of collective operations to include Non-blocking versions
- Extensions to the one-sided operations, and a new Fortran 2008 binding.
- Deprecated C++

Thank You!!