Introduction to MPI

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Course Objectives & Assumptions

Objectives

- Teach basics of MPI-Programming
- Share information related to running MPI programs on Stampede

Assumptions

- The audience has the basic understanding of C or Fortran programming
- The audience has access to MPI installation either locally or remotely





Content Overview

- Basic concepts related to MPI
- Environment Management MPI routines
- Compiling and running MPI programs
- Types of communication
 - Point-to-Point communication routines
 - Collective communication routines
- Examples
- Summary





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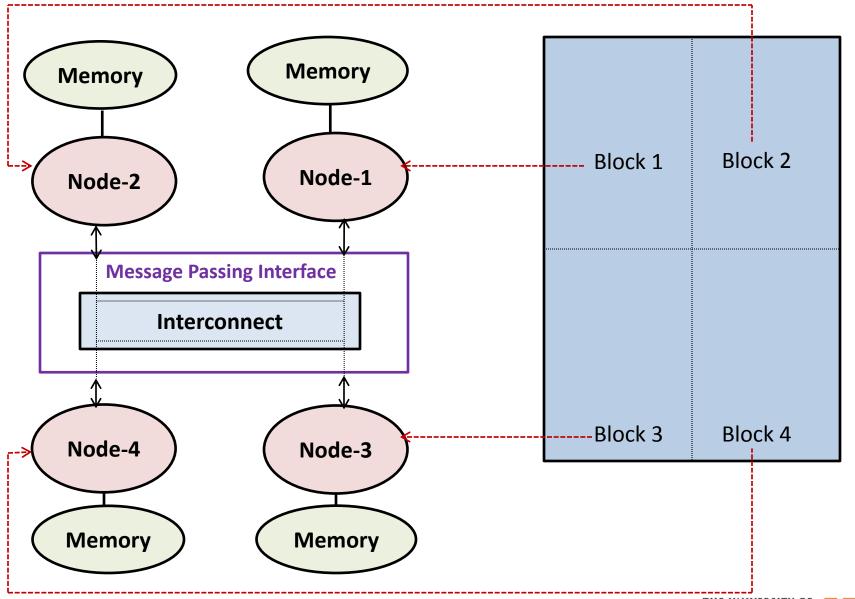
Message Passing Interface (MPI)

- MPI is a specification for message passing library that is standardized by MPI Forum
- Multiple vendor-specific implementations: MPICH, OpenMPI
- MPI implementations are used for programming systems with distributed memory
 - Each process has a different address space
 - Processes need to communicate with each other
 - Synchronization
 - Data Exchange
 - Can also be used for shared memory and hybrid architectures
- MPI specifications have been defined for C, C++ and Fortran programs





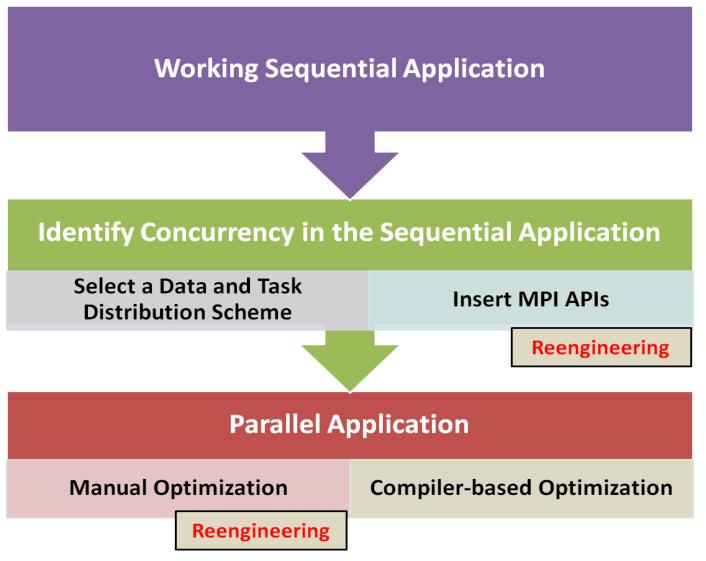
Divide & Conquer







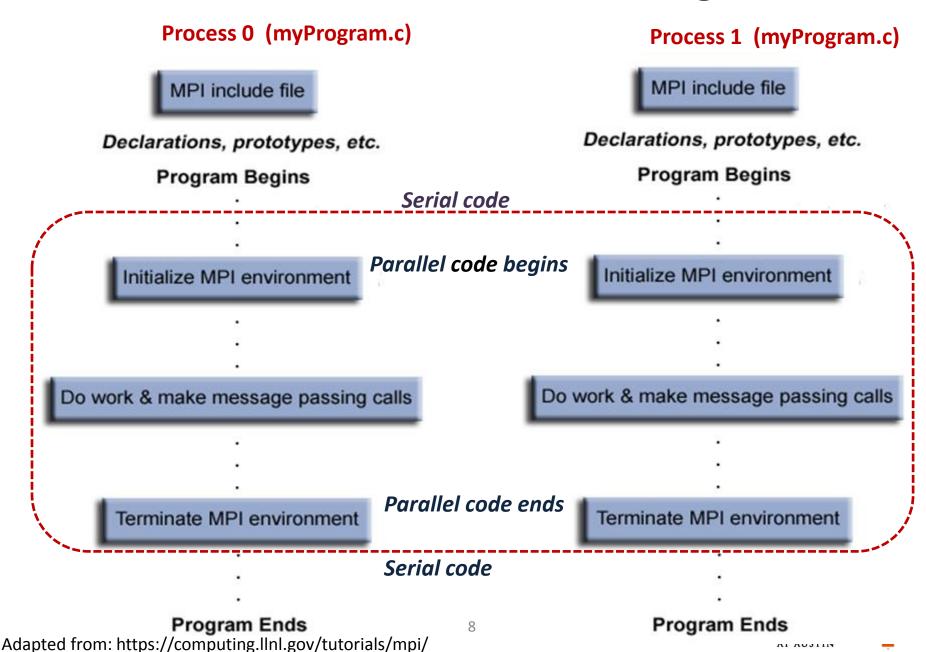
Explicit Parallelization with MPI (traditional way)







General Structure of MPI Programs



Arguments for MPI Routine (buffer, data count, data type, destination)

- Buffer: the name of a variable (including arrays and structures) that is to be sent/received. For C programs, this argument is passed by reference and usually must be prepended with an ampersand: &var1
- Data Count: number of data elements to be sent or received
- Data Type: could be elementary data type or derived
- Destination: the process where a message is to be delivered





Arguments for MPI Routine (source, tag, status, request)

- **Source:** indicates the process from which the message originated
- Tag: non-negative integer value to uniquely identify a message
- Status: for a receive operation, indicates the source and tag of a message
- **Request:** a unique "request number" issued by the system that can be used to check if a particular category of operation has completed or not (more on this later)





Concept of Communicators and Groups

MPI_COMM_WORLD

- Communicators and groups are objects that are used to define which collection of processes may communicate with each other
- Most MPI routines require a communicator as an argument
- MPI_COMM_WORLD is the predefined communicator that includes all MPI processes
- Multiple communicators and groups can be defined

Source: https://computing.llnl.gov/tutorials/mpi/





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Every MPI Program...

- Includes the MPI header file (mpi.h)
- Has a routine to initialize the MPI environment (MPI Init)
- Has a routine to terminate the MPI environment (MPI_Finalize)

С	Fortran
#include "mpi.h"	include 'mpif.h'
MPI_Xxx();	CALL MPI_XXX(, ierr)
	Call mpi_xxx(, ierr)
MPI_Init(NULL, NULL)	MPI_INIT(ierr)
MPI_Init(&argc, &argv)	
MPI_Finalize()	MPI_FINALIZE(ierr)





Environment Management Routines (1)

- MPI_Init initializes the MPI execution environment, must be called before any other MPI routine is called, and is invoked only once in an MPI program
- MPI_Finalize terminates the MPI execution environment and must be called in the last
- MPI_Comm_size determines the number of processes (size) in a communicator (comm)
 - C: MPI_Comm_size (comm,&size)
 - Fortran: MPI_COMM_SIZE (comm, size, ierr)

Note: If comm is MPI_COMM_WORLD, then size is total number of processes in the program.





Environment Management Routines (2)

- MPI_Comm_rank determines the number of processes within a communicator, ranges from 0 to N-1
 - -C: MPI Comm rank (comm, &rank)
 - Fortran: MPI_COMM_RANK (comm,rank,ierr)
- MPI_Wtime is a timer routine that returns elapsed wall clock time in seconds
 - -C: MPI Wtime()
 - Fortran: MPI WTIME()





Notes for Fortran Programmers

- Except MPI_WTIME and MPI_WTICK, all MPI routines in Fortran
 have an additional argument ierr at the end of the argument list.
- ierr is an integer and has the same meaning as the return value of the routine in C.
- In Fortran, MPI routines are subroutines, and are invoked with the call statement – see examples beginning at slide # 62.
- All MPI objects (e.g., MPI_Datatype, MPI_Comm) are of type INTEGER in Fortran.





Serial Program: example1.c

```
#include <stdio.h>
int main(){
 printf("Wonderful Class!\n");
                Compiling:
  return(0);
                login3$ icc -o example1 example1.c
                Running:
                login3$ ./example1
                Wonderful Class!
```





Serial to Parallel: example1.c to mpiExample1.c

```
#include <stdio.h>
#include "mpi.h" <--- Include the header file "mpi.h"
int main(){
 printf("Wonderful Class!\n");
  return(0);
```





Serial to Parallel: example1.c to mpiExample1.c

```
#include <stdio.h>
#include "mpi.h" Include the header file "mpi.h"
int main(){
 MPI Init(NULL, NULL); Start up MPI
 printf("Wonderful Class!\n");
 return(0);
```

Notice the NULL value being passed to MPI_Init. We will come back to this later.





Serial to Parallel: example1.c to mpiExample1.c

```
#include <stdio.h>
#include "mpi.h" Include the header file "mpi.h"
int main(){
 MPI Init (NULL, NULL); Start up MPI
 printf("Wonderful Class!\n");
 MPI Finalize(); Shut down MPI
 return(0);
```





Passing NULL to MPI_Init

 In MPI-1.1, an implementation is allowed to require that the arguments argc and argv that are passed to main, be also passed to MPI Init

 In MPI-2, conforming implementations are required to allow applications to pass NULL for both the argc and argv arguments of main





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Compiling mpiExample1.c on Stampede

- Only MPI-2 is available (MVAPICH2 and Intel MPI)
- Intel compiler available as a default option
- The GCC compiler module is also available but Intel is recommended
- Note: only 64-bit versions of the MPI libraries have been built on Stampede





Compiling mpiExample1.c on Stampede

Compiling the example program

login1\$ mpicc -o mpiExample1 mpiExample1.c

Compiler	Program	File Extension
mpicc	С	.c
mpicxx	C++	Intel: .C/c/cc/cpp/cxx/c++ PGI: .C/c/cc/cpp/cxx/
mpif90	F77/F90	.f, .for, .ftn, .f90, .f95, .fpp





Running mpiExample1.c

- To run your application on TACC resources
 - Please consult the userguide and write a job script (myJob.sh)
 http://www.tacc.utexas.edu/user-services/user-guides/stampede-user-guide
 - Submit the job to the SLURM queue
 login1\$ sbatch myJob.sh
 - Remember that Stampede has 16 cores per node. Also note that the words "tasks" and "MPI processes" mean the same thing this lecture.





Job Script for Stampede: myJob.sh

```
#!/bin/bash
#SBATCH -J myMPI
                               # Job Name
#SBATCH -o myMPI.o%j
                               # Name of the output file
#SBATCH -n 32
                               # Requests 16 tasks/node, 32 cores total
#SBATCH -p normal
                               # Queue name normal
#SBATCH -t 01:30:00
                               # Run time (hh:mm:ss) - 1.5 hours
                               # Mention your account name (xxxxx)
#SBATCH -A xxxxx
                               # Echo commands
set -x
ibrun ./mpiExample1
                               # Run the MPI executable
```

Note: ibrun is a wrapper for mpirun/mpiexec that is exclusive to TACC resources





Output from mpiExample1.c

```
login3$ cat myMPI.o2339942
TACC: Starting up job 2339942
TACC: Setting up parallel environment for MVAPICH ssh-based mpirun.
TACC: Setup complete. Running job script.
TACC: starting parallel tasks...
Wonderful Class!
TACC: Shutting down parallel environment.
TACC: Cleaning up after job: 2339942
TACC: Done.
```

Using Communicator: mpiExample2.c

```
#include <stdio.h>
2. #include "mpi.h"
3. int main(int argc, char* argv[]){
  int rank, size; section
                         Extend the variable declaration
5. MPI_Init(&argc, &argv); Note argc and argv
  MPI_Comm_rank(MPI_COMM_WORLD, &rank); Finding process
6.
    MPI_Comm_size(MPI COMM WORLD, &size); Finding number
7.
                                     of processes
8.
    printf("Hello MPI World from process %d!", rank);
9. MPI Finalize();
                                           Using rank
10. return 0;
11.}
                          28
```

Output from mpiExample2.c

TACC: Setup complete. Running job script.

TACC: starting parallel tasks...

Hello MPI World from process 5!

Hello MPI World from process 1!

Hello MPI World from process 0!

Hello MPI World from process 6!

Hello MPI World from process 7!

Hello MPI World from process 2!

Hello MPI World from process 3!

Hello MPI World from process 4!

TACC: Shutting down parallel environment.

TACC: Shutdown complete. Exiting.

TACC: Cleaning up after job: 2340827

TACC: Done





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Modes of Communication

- Point-to-Point
 - Synchronous (only send)
 - Blocking (send and receive)
 - Non-blocking (send and receive)
 - Buffered (only send)
 - Combined (send/receive together)
 - "Ready" (send)
- Collective

Review: http://www.mcs.anl.gov/research/projects/mpi/sendmode.html





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Point-to-Point Communication

- Involve message passing between two different MPI processes
- One process performs a send operation and the other task performs a matching receive operation
- There should be a matching receive routine for every send routine
 - If a send is not paired with a matching receive then the code will have a deadlock





Point-to-Point Communication (blocking versus non-blocking)

Blocking:

- A blocking receive only "returns" after the data has arrived and is ready for use by the program
- A blocking send routine returns after it is safe to modify the application buffer for reuse

Non-blocking:

- Non-blocking send and receive routines will return almost immediately
- It is unsafe to modify the application buffer until you know for a fact that the requested non-blocking operation was actually performed





Point-to-Point Communication (blocking send in C)

MPI_Send(void *buf, int count, MPI_Datatype dType, int dest, int tag, MPI Comm comm)

Argument	Description
buf	Initial address of the send buffer
count	Number of items to send
dType	MPI data type of items to send
dest	MPI rank or task that would receive the data
tag	Message ID
comm	MPI communicator where the exchange occurs

Some elementary data types: MPI_CHAR , MPI_SHORT , MPI_INT, MPI_LONG, MPI_FLOAT , MPI_DOUBLE , ...





Point-to-Point Communication (blocking receive)

```
MPI_Recv(void *buf, int count, MPI_Datatype
   dType, int source, int tag, MPI_Comm comm,
   MPI Status *status)
```

Argument	Description
buf	Initial address of receive buffer
count	Number of items to receive
dType	MPI data type of items to receive
source	MPI rank of task sending the data
tag	Message ID
comm	MPI communicator where the exchange occurs
status	Returns information on the message received, indicates the source of message and tag of the message

Point-to-Point Communication (blocking send and receive in code)

```
if (rank == 0) {
  dest = 1;
  source = 1;
 MPI Send(&outmsg, 1, MPI CHAR, dest, tag,
                                           MPI COMM WORLD);
 MPI Recv(&inmsg, 1, MPI CHAR, source, tag,
                                    MPI COMM WORLD, &Stat);
}else if (rank == 1) {
 dest = 0;
  source = 0;
 MPI Recv(&inmsg, 1, MPI CHAR, source, tag,
                                    MPI COMM WORLD, &Stat);
 MPI Send(&outmsg, 1, MPI CHAR, dest, tag,
                                           MPI COMM WORLD);
                             37
```

Point-to-Point Communication (this code will deadlock)

```
if (rank == 0) {
  dest = 1;
  source = 1;
 MPI Recv(&inmsg, 1, MPI CHAR, source, tag,
                                   MPI COMM WORLD, &Stat);
 MPI Send(&outmsg, 1, MPI CHAR, dest, tag,
                                           MPI COMM WORLD);
}else if (rank == 1) {
  dest = 0;
  source = 0;
 MPI Recv(&inmsg, 1, MPI CHAR, source, tag,
                                    MPI COMM WORLD, &Stat);
 MPI Send(&outmsg, 1, MPI CHAR, dest, tag,
                                           MPI COMM WORLD);
```





Point-to-Point Communication (blocking but combined send & receive)

- Send and Receive stages use the same communicator but have distinct tags
- Useful for communication patterns where each node both sends and receives messages (two-way communication)

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

- Send arguments
- Receive arguments
- Common to both send and receive





Point-to-Point Communication (non-blocking send & receive)

Non blocking cond	<pre>MPI_Isend(buffer,count,type,dest,tag,comm,request)</pre>
Non-blocking receive	MPI_Irecv(buffer,count,type,source,tag,comm,request)

- MPI_Request objects are used by non-blocking send & receive calls
 - In C, this argument is a pointer to a predefined structure named
 MPI Request
 - The programmer uses this system assigned "handle" later (in a WAIT type routine) to determine completion of the non-blocking operation





Point-to-Point Communication (MPI_Wait)

• MPI Wait is a blocking routine

```
MPI Wait (&request, &status)
```

- It blocks until a specified non-blocking send or receive operation has completed
- Check MPI Waitany, MPI Waitall
- Also check MPI Test





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Collective Communication

- Defined as communication between > 2 processes
 - One-to-many, many-to-one, many-to-many
- All processes within the communicator group call the same collective communication function with matching arguments
- Collective communication routines are blocking
- The size of data sent must exactly match the size of data received





Collective Communication (synchronization)

- MPI Barrier creates a barrier synchronization in a group
 - Each task, when reaching the MPI_Barrier call, blocks until all tasks in the group reach the same MPI_Barrier call

MPI Barrier (comm)





Collective Communication (data movement)

 MPI_Bcast broadcasts (sends) a message from the process designated as "root" to all other processes in the group
 MPI_Bcast (&buffer, count, datatype, root, comm)

 MPI_Scatter distributes distinct messages from a single source task to each task in the group





Collective Communication (data movement)

 MPI_Gather is reverse of MPI_Scatter and gathers distinct messages from each task in the group to a single destination task

```
MPI_Gather(&sendbuf, sendcnt, sendtype,
&recvbuf, recvcount, recvtype, root, comm)
```

 MPI_Allgather gathers data from all tasks in a group and distributes to all tasks

```
MPI_Allgather(&sendbuf, sendcount,
sendtype,&recvbuf, recvcount,recvtype,comm)
```





Collective Communication (collective computation)

 MPI_Reduce applies a reduction operation on all tasks in a group and places the result in one task

MPI_Reduce (&sendbuf,&recvbuf, count,
 datatype, mpi red operation, root, comm)

MPI Reduction Operation	Description
MPI_MAX	maximum
MPI_MIN	minimum
MPI_SUM	sum
MPI_PROD	product





Collective Communication (collective computation)

 MPI_Allreduce applies a reduction operation on all tasks in a group and passes the result to all tasks

```
MPI_Allreduce (&sendbuf,&recvbuf, count,
   datatype, mpi_red_operation, comm)
```

 Many more functions that the audience might want to explore on their own, example, MPI_Reduce_scatter,
 MPI All to all, MPI Scattery, MPI Gathery, ...





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Sequential Program with a For-Loop:

example4.c

```
1.
     #include <stdio.h>
2.
     int main(int argc,char *argv[]){
        int i, sum, upToVal;
3.
4.
        upToVal = 10000;
5.
        sum = 0;
6.
7.
         for (i=1; i<= upToVal; i++) {</pre>
8.
              sum = sum + i;
9.
10.
        printf("\nSum is %d\n", sum);
11.
        return 0;
12. }
```





```
For-Loop & MPI Reduce: mpiExample4.c (1)
1. #include <stdio.h>
2. #include "mpi.h"
3.
   int main(int argc,char *argv[]){
4.
      int i, sum, sumTotal, upToVal;
5.
      int start, end, size, rank;
6.
    upToVal = 10000;
7.
     MPI Init(&argc, &argv);
8.
      MPI Comm size(MPI COMM WORLD, &size);
9.
      MPI Comm rank(MPI COMM WORLD, &rank);
10.
      start = rank*(upToVal/size) + 1;
11.
      if (rank==(size-1)) {
12.
           end = upToVal;
13. }else{
14.
           end = start + (upToVal/size)-1;
15.
```

For-Loop & MPI_Reduce: mpiExample4.c (2)

```
16. sum = 0;
17. sumTotal=0;
18. for(i=start; i<= end; i++) {</pre>
19.
       sum = sum + i;
20.
21. MPI Reduce (&sum, &sumTotal, 1, MPI INT, MPI SUM, 0,
                                        MPI COMM WORLD );
22. printf("\nRank: %d, sum: %d, sumTotal: %d\n", rank,
                                          sum, sumTotal);
23. MPI Finalize();
24. return 0;
25.}
```





Output from mpiExample4.c

Rank: 6, sum: 10156875, sumTotal: 0

Rank: 4, sum: 7031875, sumTotal: 0

Rank: 7, sum: 11719375, sumTotal: 0

Rank: 5, sum: 8594375, sumTotal: 0

Rank: 3, sum: 5469375, sumTotal: 0

Rank: 2, sum: 3906875, sumTotal: 0

Rank: 1, sum: 2344375, sumTotal: 0

Rank: 0, sum: 781875, sumTotal: 50005000





MPI_Bcast Example: mpiExample7.c (1)

```
1. #include <stdio.h>
  #include <mpi.h>
3.
   int main(int argc, char *argv[]){
4.
       int i,rank,size;
5.
       int root, count;
6.
       int buffer[4];
7.
       MPI Status status;
8.
       MPI Request request;
9.
       MPI Init(&argc, &argv);
       MPI Comm size(MPI COMM WORLD,&size);
10.
11.
       MPI Comm rank(MPI COMM WORLD, &rank);
12.
       root=0;
13.
       count=4;
```





MPI_Bcast Example: mpiExample7.c (2)

```
14. if (rank == root) {
15.
         for(i=0; i<count; i++){</pre>
16.
           buffer[i]=i;
17.
18.
     MPI Bcast(buffer,count,MPI_INT,root,MPI_COMM_WORLD);
19.
20. printf("Rank is: %d, Value at buffer[%d] is: %d \n",
                        rank, count-1, buffer[count-1]);
21. printf("\n");
22. MPI Finalize();
23. return 0;
24.}
```





Output from mpiExample7.c

TACC: starting parallel tasks...

Rank is: 0, Value at buffer[4] is: 4

Rank is: 1, Value at buffer[4] is: 4

Rank is: 2, Value at buffer[4] is: 4

Rank is: 3, Value at buffer[4] is: 4

Rank is: 6, Value at buffer[4] is: 4

Rank is: 4, Value at buffer[4] is: 4

Rank is: 7, Value at buffer[4] is: 4

Rank is: 5, Value at buffer[4] is: 4

TACC: Shutting down parallel environment.

Note: Do not expect the output to be printed in any particular order. You might see jumbled up output.





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Summary of Key MPI Routines

С	Fortran
MPI_Init (&argc,&argv)	MPI_INIT (ierr)
MPI_Comm_size (comm, &size)	<pre>MPI_COMM_SIZE (comm, size, ierr)</pre>
MPI_Comm_rank (comm, &rank)	<pre>MPI_COMM_RANK (comm, rank, ierr)</pre>
MPI_Finalize ()	MPI_FINALIZE (ierr)
<pre>MPI_Send(&buf,count,datatype,)</pre>	<pre>MPI_SEND (buf,count,datatype,)</pre>
<pre>MPI_Recv(&buf,count,datatype,)</pre>	<pre>MPI_RECV(&buf,count,datatype,)</pre>
MPI_Wtime()	MPI_WTIME()





MPI Routines Needed for Doing Exercises in the Lab

C	Fortran
MPI_Wtime()	MPI_WTIME()
<pre>MPI_Bcast(&buffer, count, datatype, root, comm)</pre>	<pre>MPI_BCAST(buffer, count, datatype, root, comm, ierr)</pre>
<pre>MPI_Reduce (&sendbuf,&recvbuf, count, datatype, mpi_red_operation, root, comm)</pre>	<pre>MPI_Reduce (sendbuf,recvbuf, count, datatype, mpi_red_operation, root, comm, ierr)</pre>
<pre>MPI_Allreduce (&sendbuf, &recvbuf, count, datatype, mpi_red_operation, comm)</pre>	<pre>MPI_Allreduce (sendbuf, recvbuf, count, datatype, mpi_red_operation, comm, ierr)</pre>





Words of Caution!

- Not all applications can be parallelized
 - Analyze and understand the data dependencies in your application
- Not all parallelization result in speed-up (parallel slowdown)
 - Too much communication could be an overkill!

Note:

Total Execution Time = Computation Time + Communication Time + I/O time





References

https://computing.llnl.gov/tutorials/mpi/

http://www.mpi-forum.org

http://www.cs.usfca.edu/~peter/ppmpi/

http://www.mcs.anl.gov/research/projects/mpi/usingmpi/

http://geco.mines.edu/workshop/class2/examples/mpi/index.html





For Fortran Users





Sample MPI code (F90)

```
program samplempi
     use mpi
     [other includes]
     integer :: ierr, np, rank
     [other declarations]
     call mpi_init(ierr)
     call mpi_comm_size(MPI_COMM_WORLD, np, ierr)
     call mpi_comm_rank(MPI_COMM_WORLD, rank, ierr)
     [actual work goes here]
     call mpi_finalize(ierr)
end program
```





Send/Recv Pairs in Code

Blocking Send & Blocking Recv

```
IF (rank==0) THEN

CALL MPI_SEND(sendbuf,count,MPI_REAL,1,tag,MPI_COMM_WORLD,ierr)

ELSEIF (rank==1) THEN

CALL MPI_RECV(recvbuf,count,MPI_REAL,0,tag,MPI_COMM_WORLD,status,ierr)

ENDIF
```

Non-blocking Send & Blocking Recv

```
IF (rank==0) THEN

CALL MPI_ISEND(sendbuf,count,MPI_REAL,1,tag,MPI_COMM_WORLD,req,ierr)

ELSEIF (rank==1) THEN

CALL MPI_RECV(recvbuf,count,MPI_REAL,0,tag,MPI_COMM_WORLD,status,ierr)

ENDIF

CALL MPI_WAIT(req, wait_status)
```





Deadlock Example

```
! The following code contains a deadlock... can you spot it?
IF (rank==0) THEN
   CALL MPI_RECV(recvbuf,count,MPI_REAL,1,tag,MPI_COMM_WORLD,status,ierr)
   CALL MPI SEND(sendbuf,count,MPI REAL,1,tag,MPI COMM WORLD,ierr)
ELSEIF (rank==1) THEN
   CALL MPI RECV(recvbuf,count,MPI REAL,0,tag,MPI COMM WORLD,status,ierr)
   CALL MPI SEND(sendbuf,count,MPI REAL,0,tag,MPI COMM WORLD,ierr)
ENDIF
! Solution
IF (rank==0) THEN
   CALL MPI_SEND(sendbuf,count,MPI_REAL,1,tag,MPI_COMM_WORLD,ierr)
   CALL MPI RECV(recvbuf,count,MPI REAL,1,tag,MPI COMM WORLD,status,ierr)
ELSEIF (rank==1) THEN
   CALL MPI_RECV(recvbuf,count,MPI_REAL,0,tag,MPI_COMM_WORLD,status,ierr)
   CALL MPI SEND(sendbuf,count,MPI REAL,0,tag,MPI COMM WORLD,ierr)
ENDIF
```





Alternative Deadlock Solutions

```
! Solution using sendrecv
IF (rank==0) THEN
   CALL MPI SENDRECV(sendbuf, count, MPI REAL, 1, sendtag,
           recybuf, count, MPI REAL, 1, recytag,
           MPI_COMM_WORLD, status, ierr)
ELSEIF (rank==1) THEN
   CALL MPI_SENDRECV(sendbuf, count, MPI_REAL, 0, sendtag,
           recvbuf, count, MPI_REAL, 0, recvtag,
           MPI COMM WORLD, status, ierr)
ENDIF
! Another possible solution (using all non-blocking calls)
IF (rank==0) THEN
   CALL MPI_ISEND(sendbuf,count,MPI_REAL,1,tag,MPI_COMM_WORLD,req1,ierr)
   CALL MPI_IRECV(recvbuf,count,MPI_REAL,0,tag,MPI_COMM_WORLD,reg2,ierr)
ELSEIF (rank==1) THEN
   CALL MPI_ISEND(sendbuf,count,MPI_REAL,0,tag,MPI_COMM_WORLD,req1,ierr)
   CALL MPI_IRECV(recvbuf,count,MPI_REAL,1,tag,MPI_COMM_WORLD,reg2,ierr)
ENDIF
CALL MPI WAIT(reg1, wait status, ierr)
CALL MPI WAIT(reg2, wait status, ierr)
```





Thanks!

Questions?



