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

Memory - Node-2

Message Passing Interface

Interconnect

Memory - Node-1

Memory

Node-3

Memory - Node-4

Memory

Block 1

Block 2

Block 3

Block 4
Explicit Parallelization with MPI (traditional way)

1. Working Sequential Application
2. Identify Concurrency in the Sequential Application
   - Select a Data and Task Distribution Scheme
   - Insert MPI APIs
   - Reengineering
3. Parallel Application
   - Manual Optimization
   - Compiler-based Optimization
   - Reengineering
General Structure of MPI Programs

Process 0 (myProgram.c)

- MPI include file
- Declarations, prototypes, etc.
- Program Begins
- Initialize MPI environment
- Do work & make message passing calls
- Terminate MPI environment
- Program Ends

Serial code

Parallel code begins

Parallel code ends

Serial code

Process 1 (myProgram.c)

- MPI include file
- Declarations, prototypes, etc.
- Program Begins
- Initialize MPI environment
- Do work & make message passing calls
- Terminate MPI environment
- Program Ends

Adapted from: https://computing.llnl.gov/tutorials/mpi/
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: &\texttt{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

- 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**)

<table>
<thead>
<tr>
<th>C</th>
<th>Fortran</th>
</tr>
</thead>
<tbody>
<tr>
<td>#include &quot;mpi.h&quot;</td>
<td>include 'mpif.h'</td>
</tr>
<tr>
<td>MPI_Xxx(. . .);</td>
<td>CALL MPI_XXX(. . ., ierr)</td>
</tr>
<tr>
<td></td>
<td>Call mpi_ddd(. . ., ierr)</td>
</tr>
<tr>
<td>MPI_Init(NULL, NULL)</td>
<td>MPI_INIT(ierr)</td>
</tr>
<tr>
<td>MPI_Init(&amp;argc, &amp;argv)</td>
<td></td>
</tr>
<tr>
<td>MPI_Finalize()</td>
<td>MPI_FINALIZE(ierr)</td>
</tr>
</tbody>
</table>
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

```c
#include <stdio.h>

int main(){

    printf("Wonderful Class!\n");

    return(0);

}
```

Compiling:
```
login3$ icc -o example1 example1.c
```

Running:
```
login3$ ./example1

Wonderful Class!
```
#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

```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`

```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
```

<table>
<thead>
<tr>
<th>Compiler</th>
<th>Program</th>
<th>File Extension</th>
</tr>
</thead>
<tbody>
<tr>
<td>mpicc</td>
<td>C</td>
<td>.c</td>
</tr>
</tbody>
</table>
| 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

```bash
#!/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
#SBATCH -A xxxxx # Mention your account name (xxxxx)

set -x # Echo commands

ibrun ./mpiExample1 # Run the MPI executable
```

Note: **ibrun** is a wrapper for **mpirun/mpiexec** that is exclusive to TACC resources
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!
Wonderful Class!
Wonderful Class!
Wonderful Class!
Wonderful Class!
Wonderful Class!
Wonderful Class!
Wonderful Class!
Wonderful Class!
Wonderful Class!
...
TACC: Shutting down parallel environment.
TACC: Cleaning up after job: 2339942
TACC: Done.
Using Communicator: mpiExample2.c

1. #include <stdio.h>
2. #include "mpi.h"

3. int main(int argc, char* argv[]){

4.    int rank, size; ← Extend the variable declaration section

5.    MPI_Init(&argc, &argv); ← Note argc and argv

6.    MPI_Comm_rank(MPI_COMM_WORLD, &rank); ← Finding process rank

7.    MPI_Comm_size(MPI_COMM_WORLD, &size); ← Finding number of processes

8.    printf("Hello MPI World from process \%d!", rank);

9.    MPI_Finalize();

10.   return 0;
11. }

Extend the variable declaration section
FINDING PROCESS RANK
FINDING NUMBER OF PROCESSES
USING RANK
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

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  – Examples

• Summary
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)

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>buf</td>
<td>Initial address of the send buffer</td>
</tr>
<tr>
<td>count</td>
<td>Number of items to send</td>
</tr>
<tr>
<td>dType</td>
<td>MPI data type of items to send</td>
</tr>
<tr>
<td>dest</td>
<td>MPI rank or task that would receive the data</td>
</tr>
<tr>
<td>tag</td>
<td>Message ID</td>
</tr>
<tr>
<td>comm</td>
<td>MPI communicator where the exchange occurs</td>
</tr>
</tbody>
</table>

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)

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>buf</td>
<td>Initial address of receive buffer</td>
</tr>
<tr>
<td>count</td>
<td>Number of items to receive</td>
</tr>
<tr>
<td>dType</td>
<td>MPI data type of items to receive</td>
</tr>
<tr>
<td>source</td>
<td>MPI rank of task sending the data</td>
</tr>
<tr>
<td>tag</td>
<td>Message ID</td>
</tr>
<tr>
<td>comm</td>
<td>MPI communicator where the exchange occurs</td>
</tr>
<tr>
<td>status</td>
<td>Returns information on the message received, indicates the source of message and tag of the message</td>
</tr>
</tbody>
</table>
Point-to-Point Communication
(blocking send and receive in code)

```c
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);
}
```
Point-to-Point Communication
(this code will deadlock)

```c
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)

```c
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 send | MPI_Isend(  
<table>
<thead>
<tr>
<th></th>
<th>buffer,count,type,dest,tag,comm,request)</th>
</tr>
</thead>
</table>
| 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

  ```c
  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
  \[
  \text{MPI\_Bcast}( & \text{buffer}, \text{count}, \text{datatype}, \text{root}, \text{comm})
  \]

- **MPI_Scatter** distributes distinct messages from a single source task to each task in the group
  \[
  \text{MPI\_Scatter}( & \text{sendbuf}, \text{sendcnt}, \text{sendtype}, \\
  & \text{recvbuf}, \text{recvcnt}, \text{recvtype}, \text{root}, \text{comm})
  \]
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

  \[
  \text{MPI\_Gather}(&\text{sendbuf, sendcnt, sendtype,} \\
  \text{&recvbuf, recvcount, recvtype, root, comm})
  \]

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

  \[
  \text{MPI\_Allgather}(&\text{sendbuf, sendcount,} \\
  \text{sendtype, &recvbuf, recvcount, recvtype, comm})
  \]
Collective Communication (collective computation)

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

\[
\text{MPI\_Reduce} (&\text{sendbuf}, &\text{recvbuf}, \text{count}, \text{datatype}, \text{mpi\_red\_operation}, \text{root}, \text{comm})
\]

<table>
<thead>
<tr>
<th>MPI Reduction Operation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>MPI_MAX</td>
<td>maximum</td>
</tr>
<tr>
<td>MPI_MIN</td>
<td>minimum</td>
</tr>
<tr>
<td>MPI_SUM</td>
<td>sum</td>
</tr>
<tr>
<td>MPI_PROD</td>
<td>product</td>
</tr>
</tbody>
</table>
Collective Communication
(collective computation)

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

\[
\text{MPI\_Allreduce} \left( \&\text{sendbuf}, \&\text{recvbuf}, \text{count}, \text{datatype}, \text{mpi\_red\_operation}, \text{comm} \right)
\]

• Many more functions that the audience might want to explore on their own, example, MPI\_Reduce\_scatter, MPI\_All\_to\_all, MPI\_Scatterv, MPI\_Gatherv, ...
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Sequential Program with a For-Loop: example4.c

1. #include <stdio.h>
2. int main(int argc, char *argv[]){

3.     int i, sum, upToVal;
4.     upToVal = 10000;
5.     sum = 0;
6. 
7.     for(i=1; i<= upToVal; i++){
8.         sum = sum +i;
9.     }

10.    printf("\nSum is %d\n", sum);

11.    return 0;

12. }

TACC
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++){
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>
2. #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);
10.  MPI_Comm_size(MPI_COMM_WORLD,&size);
11.  MPI_Comm_rank(MPI_COMM_WORLD,&rank);
12.  root=0;
13.  count=4;
if(rank == root){
    for(i=0; i<count; i++){
        buffer[i]=i;
    }
}

MPI_Bcast(buffer,count,MPI_INT,root,MPI_COMM_WORLD);

printf("Rank is: %d, Value at buffer[%d] is: %d \n", rank, count-1, buffer[count-1]);

printf("\n");

MPI_Finalize();

return 0;
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

<table>
<thead>
<tr>
<th>C</th>
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</tr>
</thead>
<tbody>
<tr>
<td>MPI_Init (&amp;argc,&amp;argv)</td>
<td>MPI_INIT (ierr)</td>
</tr>
<tr>
<td>MPI_Comm_size (comm,&amp;size)</td>
<td>MPI_COMM_SIZE (comm,size,ierr)</td>
</tr>
<tr>
<td>MPI_Comm_rank (comm,&amp;rank)</td>
<td>MPI_COMM_RANK (comm,rank,ierr)</td>
</tr>
<tr>
<td>MPI_Finalize ()</td>
<td>MPI_FINALIZE (ierr)</td>
</tr>
<tr>
<td>MPI_Send(&amp;buf,count,datatype,...)</td>
<td>MPI_SEND (buf,count,datatype,...)</td>
</tr>
<tr>
<td>MPI_Recv(&amp;buf,count,datatype,...)</td>
<td>MPI_RECV(&amp;buf,count,datatype,...)</td>
</tr>
<tr>
<td>MPI_Wtime()</td>
<td>MPI_WTIME()</td>
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</table>
### MPI Routines Needed for Doing Exercises in the Lab

<table>
<thead>
<tr>
<th>C</th>
<th>Fortran</th>
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<tr>
<td><code>MPI_Wtime()</code></td>
<td><code>MPI_WTIME()</code></td>
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<tr>
<td><code>MPI_Bcast(&amp;buffer, count, datatype, root, comm)</code></td>
<td><code>MPI_BCAST(buffer, count, datatype, root, comm, ierr)</code></td>
</tr>
<tr>
<td><code>MPI_Reduce (&amp;sendbuf,&amp;recvbuf, count, datatype, mpi_red_operation, root, comm)</code></td>
<td><code>MPI_Reduce (sendbuf,recvbuf, count, datatype, mpi_red_operation, root, comm, ierr)</code></td>
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<tr>
<td><code>MPI_Allreduce (&amp;sendbuf, &amp;recvbuf, count, datatype, mpi_red_operation, comm)</code></td>
<td><code>MPI_Allreduce (sendbuf, recvbuf, count, datatype, mpi_red_operation, comm, ierr)</code></td>
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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,
                    recvbuf, count, MPI_REAL, 1, recvtag,
                    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,req2,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,req2,ierr)
ENDIF
CALL MPI_WAIT(req1, wait_status, ierr)
CALL MPI_WAIT(req2, wait_status, ierr)
Thanks!

Questions?