Message Passing Interface (MPI)

Author: Blaise Barney, Lawrence Livermore National Laboratory

UCRL-MI-133316

Table of Contents

Abstract

The Message Passing Interface Standard (MPI) is a message passing library standard based on the consensus of the MPI Forum, which has over 40 participating organizations, including vendors, researchers, software library developers, and users. The goal of the Message Passing Interface is to establish a portable, efficient, and flexible standard for message passing that will be widely used for writing message passing programs. As such, MPI is the first standardized, vendor independent, message passing library. The advantages of developing message passing software using MPI closely match the design goals of portability, efficiency, and flexibility. MPI is not an IEEE or ISO standard, but has in fact, become the "industry standard" for writing message passing programs on HPC platforms.

The goal of this tutorial is to teach those unfamiliar with MPI how to develop and run parallel programs according to the MPI standard. The primary topics that are presented focus on those which are the most useful for new MPI programmers. The tutorial begins with an introduction, background, and basic information for getting started with MPI. This is followed by a detailed look at the MPI routines that are most useful for new MPI programmers, including MPI Environment Management, Point-to-Point Communications, and Collective Communications routines. Numerous examples in both C and Fortran are provided, as well as a lab exercise.

The tutorial materials also include more advanced topics such as Derived Data Types, Group and Communicator Management Routines, and Virtual Topologies. However, these are not actually presented during the lecture, but are meant to serve as "further reading" for those who are interested.

Level/Prerequisites: This tutorial is one of the eight tutorials in the 4+ day "Using LLNL's Supercomputers" workshop. It is ideal for those who are new to parallel programming with MPI. A basic understanding of parallel programming in C or Fortran is required. For those who are unfamiliar with Parallel Programming in general, the material covered in EC3500: Introduction To Parallel Computing would be helpful.

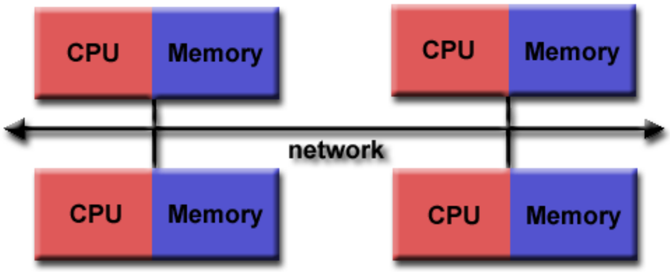
What is MPI?

An Interface Specification:

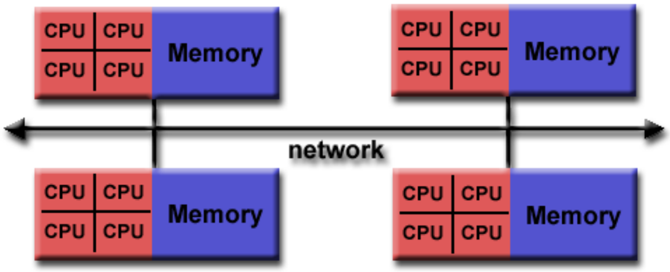
- **M P I = Message Passing Interface**
- MPI is a specification for the developers and users of message passing libraries. By itself, it is NOT a library - but rather the specification of what such a library should be.
- MPI primarily addresses the message-passing parallel programming model: data is moved from the address space of one process to that of another process through cooperative operations on each process.
- Simply stated, the goal of the Message Passing Interface is to provide a widely used standard for writing message passing programs. The interface attempts to be:
  - practical
  - portable
  - efficient
  - flexible
- The MPI standard has gone through a number of revisions, with the most recent version being MPI-3.
- Interface specifications have been defined for C and Fortran90 language bindings:
  - C++ bindings from MPI-1 are removed in MPI-3
  - MPI-3 also provides support for Fortran 2003 and 2008 features
- Actual MPI library implementations differ in which version and features of the MPI standard they support. Developers/users will need to be aware of this.

Programming Model:

- Originally, MPI was designed for distributed memory architectures, which were becoming increasingly popular at that time (1980s - early 1990s).



- As architecture trends changed, shared memory SMPs were combined over networks creating hybrid distributed memory / shared memory systems.
- MPI implementors adapted their libraries to handle both types of underlying memory architectures seamlessly. They also adapted/developed ways of handling different interconnects and protocols.



- Today, MPI runs on virtually any hardware platform:

    - Distributed Memory
    - Shared Memory
    - Hybrid

- The programming model clearly remains a distributed memory model however, regardless of the underlying physical architecture of the machine.

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

Reasons for Using MPI:

- **Standardization** - MPI is the only message passing library which can be considered a standard. It is supported on virtually all HPC platforms. Practically, it has replaced all previous message passing libraries.

- **Portability** - There is little or no need to modify your source code when you port your application to a different platform that supports (and is compliant with) the MPI standard.

- **Performance Opportunities** - Vendor implementations should be able to exploit native hardware features to optimize performance.

- **Functionality** - There are over 440 routines defined in MPI-3, which includes the majority of those in MPI-2 and MPI-1.

- **Availability** - A variety of implementations are available, both vendor and public domain.

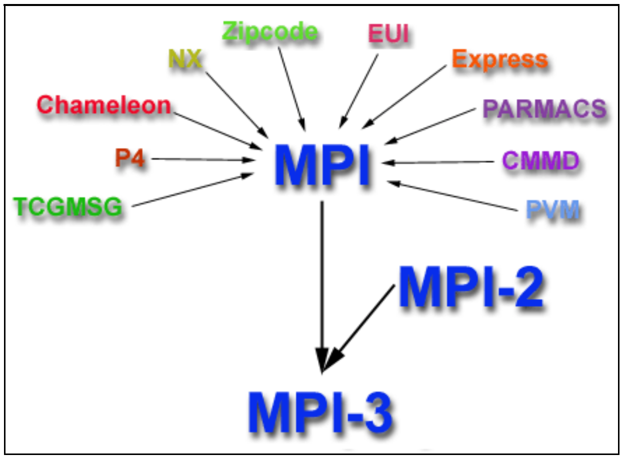
History and Evolution: (for those interested)

- MPI has resulted from the efforts of numerous individuals and groups that began in 1992. Some history:

- **1980s - early 1990s:** Distributed memory, parallel computing develops, as do a number of incompatible software tools for writing such programs - usually with tradeoffs between portability, performance, functionality and price. Recognition of the need for a standard arose.

- **Apr 1992:** Workshop on Standards for Message Passing in a Distributed Memory Environment, sponsored by the Center for Research on Parallel Computing, Williamsburg, Virginia. The basic features essential to a standard message passing interface were discussed, and a working group established to continue the standardization process. Preliminary draft proposal developed subsequently.

- **Nov 1992:** Working group meets in Minneapolis. MPI draft proposal (MPI1) from ORNL presented. Group adopts procedures and organization to form the MPI Forum. It eventually comprised of about 175 individuals from 40 organizations including parallel computer vendors, software writers, academia and application scientists.



- **Nov 1993:** Supercomputing 93 conference - draft MPI standard presented.

- **May 1994:** Final version of MPI-1.0 released

- MPI-1.0 was followed by versions MPI-1.1 (Jun 1995), MPI-1.2 (Jul 1997) and MPI-1.3 (May 2008).

- MPI-2 picked up where the first MPI specification left off, and addressed topics which went far beyond the MPI-1 specification. Was finalized in 1996.

- MPI-2.1 (Sep 2008), and MPI-2.2 (Sep 2009) followed

- **Sep 2012:** The MPI-3.0 standard was approved.

Documentation:

- Documentation for all versions of the MPI standard is available at: http://www.mpi-forum.org/docs/.

LLNL MPI Implementations and Compilers

Although the MPI programming interface has been standardized, actual library implementations will differ in which version and features of the standard they support. The way MPI programs are compiled and run on different platforms will also vary.

A summary of LC's MPI environment is provided here, along with links to additional detailed information.

MVAPICH

▶ General Info:

- MVAPICH MPI from Ohio State University is the default MPI library on all of LC's Linux clusters.

- As of June 2014, LC's default version is MVAPICH 1.2
  - MPI-1 implementation that includes support for MPI-I/O, but not for MPI one-sided communication.
  - Based on MPICH-1.2.7 MPI library from Argonne National Laboratory
  - Not thread-safe. All MPI calls should be made by the master thread in a multi-threaded MPI program.
  - See /usr/local/docs/mpi.mvapich.basics for LC usage details.

- MVAPICH2 is also available on LC Linux clusters
  - MPI-2 implementation based on MPICH2 MPI library from Argonne National Laboratory
  - Not currently the default - requires the "use" command to load the selected dotkit - see https://computing.llnl.gov/?set=jobs&page=dotkit for details.
  - Thread-safe
  - See /usr/local/docs/mpi.mvapich2.basics for LC usage details.
  - MVAPICH2 versions 1.9 and later implement MPI-3 according to the developer's documentation.

- A code compiled with MVAPICH on one LC Linux cluster should run on any LC Linux cluster.
  - Clusters with an interconnect - message passing is done in shared memory on-node and over the switch inter-node
  - Clusters without an interconnect - message passing is done in shared memory

- More information:
  - /usr/local/docs on LC's clusters:
    - `mpi.basics`
    - `mpi.mvapich.basics`
    - `mpi.mvapich2.basics`
  - MVAPICH 1.2 User Guide available HERE
  - MVAPICH2 1.7 User Guide available HERE
  - MVAPICH home page: mvapich.cse.ohio-state.edu/
  - MPICH1 home page: www.mcs.anl.gov/research/projects/mpi/mpich1-old/.
  - MPICH2 home page: www.mcs.anl.gov/research/projects/mpich2/.

▶ MPI Build Scripts:

- MPI compiler wrapper scripts are used to compile MPI programs - these should all be in your default $PATH unless you have changed it. These scripts mimic the familiar MPICH scripts in their functionality, meaning, they automatically include the appropriate MPI include files and link to the necessary MPI libraries and pass switches to the underlying compiler.

- Available scripts are listed below:

Language	Script Name	Underlying Compiler
C	`mpicc`	gcc
	`mpigcc`	gcc
	`mpiicc`	icc
	`mpipgcc`	pgcc
C++	`mpiCC`	g++

	mpig++	g++
	mpiicpc	icpc
	mpipgCC	pgCC
Fortran	**mpif77**	g77
	mpigfortran	gfortran
	mpiifort	ifort
	mpipgf77	pgf77
	mpipgf90	pgf90

- For additional information:
  - See the man page (if it exists)
  - Issue the script name with the `-help` option (almost useless)
  - View the script yourself directly

- By default, the scripts point to the default version of their underlying compiler and the default MPI library.
  - If you need to build with a different compiler version, you can use use LC's dotkit tool to query what's available and then load it. The MPI build script will then point to that. For example:

    ```
    use -l          (to list available compilers)
    use ic-13.1.163  (use the package of interest)
    ```

  - If you need to build with a different version of the MPI library, see /usr/local/docs/linux.basics for advice.

Running MVAPICH MPI Jobs:

- MPI executables are launched using the SLURM srun command with the appropriate options. For example, to launch an 8-process MPI job split across two different nodes in the `pdebug` pool:

  ```
  srun -N2 -n8 -ppdebug a.out
  ```

- The srun command is discussed in detail in the Running Jobs section of the Linux Clusters Overview tutorial.

Open MPI

General Information:

- Open MPI is a thread-safe, open source MPI-2 implementation that is developed and maintained by a consortium of academic, research, and industry partners.

- Open MPI is available on most LC Linux clusters. You'll need to load the desired dotkit package using the use command. For example:

  ```
  use -l                (list available packages)
  use openmpi-gnu-1.4.3  (use the package of interest)
  ```

- This ensures that LC's MPI wrapper scripts point to the desired version of Open MPI.

- Compiler commands are the same as shown above for MVAPICH.

- Launching an Open MPI job is done differently than with MVAPICH MPI - the mpiexec command is required.

- Detailed usage information for LC clusters can be found in the /usr/local/docs/mpi.openmpi.basics file.

- More info about Open MPI in general: www.open-mpi.org

IBM BG/Q Clusters:

- The IBM MPI library is the only supported library on these platforms.

- This is an IBM implementation based on MPICH2. Includes MPI-2 functionality minus Dynamic Processes.

- Thread-safe
- C, C++, Fortran77/90/95 are supported
- Compiling and running MPI programs, see the BG/Q Tutorial: computing.llnl.gov/tutorials/bgq/

Level of Thread Support

- MPI libraries vary in their level of thread support:
    - `MPI_THREAD_SINGLE` - Level 0: Only one thread will execute.
    - `MPI_THREAD_FUNNELED` - Level 1: The process may be multi-threaded, but only the main thread will make MPI calls - all MPI calls are funneled to the main thread.
    - `MPI_THREAD_SERIALIZED` - Level 2: The process may be multi-threaded, and multiple threads may make MPI calls, but only one at a time. That is, calls are not made concurrently from two distinct threads as all MPI calls are serialized.
    - `MPI_THREAD_MULTIPLE` - Level 3: Multiple threads may call MPI with no restrictions.
- Consult the `MPI_Init_thread()` man page for details.
- A simple C language example for determining thread level support is shown below.

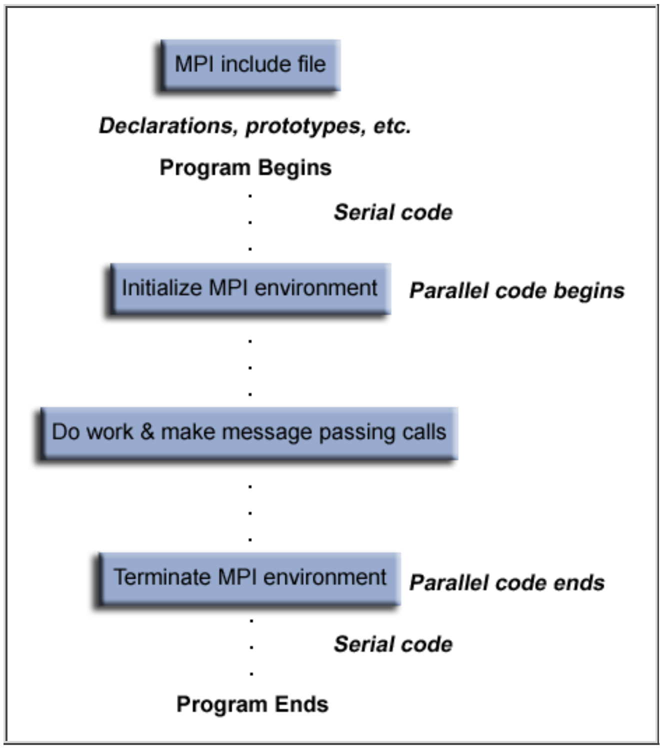
```
#include "mpi.h"
#include <stdio.h>

int main( int argc, char *argv[] )
{
    int provided, claimed;

/*** Select one of the following
    MPI_Init_thread( 0, 0, MPI_THREAD_SINGLE, &provided );
    MPI_Init_thread( 0, 0, MPI_THREAD_FUNNELED, &provided );
    MPI_Init_thread( 0, 0, MPI_THREAD_SERIALIZED, &provided );
    MPI_Init_thread( 0, 0, MPI_THREAD_MULTIPLE, &provided );
***/

    MPI_Init_thread(0, 0, MPI_THREAD_MULTIPLE, &provided );
    MPI_Query_thread( &claimed );
        printf( "Query thread level= %d  Init_thread level= %d\n", claimed, provided );

    MPI_Finalize();
}
```

Sample output:

```
Query thread level= 3  Init_thread level= 3
```

Getting Started

General MPI Program Structure:


MPI include file
Declarations, prototypes, etc.
Program Begins
Serial code
Initialize MPI environment
Parallel code begins
Do work & make message passing calls
Terminate MPI environment
Parallel code ends
Serial code
Program Ends

- Header File:
  - Required for all programs that make MPI library calls.

C include file	Fortran include file
`#include "mpi.h"`	`include 'mpif.h'`

  - With MPI-3 Fortran, the `USE mpi_f08` module is preferred over using the include file shown above.
- Format of MPI Calls:
  - C names are case sensitive; Fortran names are not.
  - Programs must not declare variables or functions with names beginning with the prefix MPI_ or PMPI_ (profiling interface).

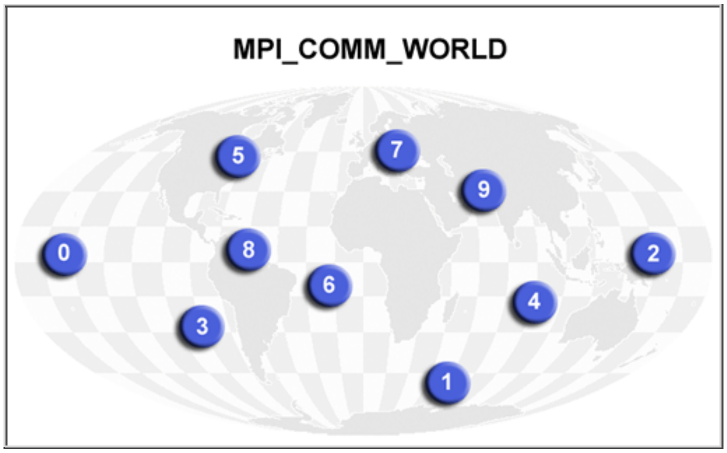
C Binding	
Format:	`rc = MPI_Xxxxx(parameter, ... )`
Example:	`rc = MPI_Bsend(&buf,count,type,dest,tag,comm)`
Error code:	Returned as "rc". MPI_SUCCESS if successful
Fortran Binding	

Format:	`CALL MPI_XXXXX(parameter,..., ierr)`
	`call mpi_xxxxx(parameter,..., ierr)`

Example:	`CALL MPI_BSEND(buf,count,type,dest,tag,comm,ierr)`
Error code:	Returned as "ierr" parameter. MPI_SUCCESS if successful

- Communicators and Groups:
  - MPI uses objects called communicators and groups to define which collection of processes may communicate with each other.

- Most MPI routines require you to specify a communicator as an argument.
- Communicators and groups will be covered in more detail later. For now, simply use **MPI_COMM_WORLD** whenever a communicator is required - it is the predefined communicator that includes all of your MPI processes.



Rank:

- Within a communicator, every process has its own unique, integer identifier assigned by the system when the process initializes. A rank is sometimes also called a "task ID". Ranks are contiguous and begin at zero.
- Used by the programmer to specify the source and destination of messages. Often used conditionally by the application to control program execution (if rank=0 do this / if rank=1 do that).

Error Handling:

- Most MPI routines include a return/error code parameter, as described in the "Format of MPI Calls" section above.
- However, according to the MPI standard, the default behavior of an MPI call is to abort if there is an error. This means you will probably not be able to capture a return/error code other than MPI_SUCCESS (zero).
- The standard does provide a means to override this default error handler. A discussion on how to do this is available HERE. You can also consult the error handling section of the relevant MPI Standard documentation located at http://www.mpi-forum.org/docs/.
- The types of errors displayed to the user are implementation dependent.

Environment Management Routines

This group of routines is used for interrogating and setting the MPI execution environment, and covers an assortment of purposes, such as initializing and terminating the MPI environment, querying a rank's identity, querying the MPI library's version, etc. Most of the commonly used ones are described below.

MPI_Init

Initializes the MPI execution environment. This function must be called in every MPI program, must be called before any other MPI functions and must be called only once in an MPI program. For C programs, MPI_Init may be used to pass the command line arguments to all processes, although this is not required by the standard and is implementation dependent.

```
MPI_Init (&argc,&argv)
MPI_INIT (ierr)
```

MPI_Comm_size

Returns the total number of MPI processes in the specified communicator, such as MPI_COMM_WORLD. If the communicator is MPI_COMM_WORLD, then it represents the number of MPI tasks available to your application.

```
MPI_Comm_size (comm,&size)
MPI_COMM_SIZE (comm,size,ierr)
```

MPI_Comm_rank

Returns the rank of the calling MPI process within the specified communicator. Initially, each process will be assigned a unique integer rank between 0 and number of tasks - 1 within the communicator MPI_COMM_WORLD. This rank is often referred to as a task ID. If a process becomes associated with other communicators, it will have a unique rank within each of these as well.

```
MPI_Comm_rank (comm,&rank)
MPI_COMM_RANK (comm,rank,ierr)
```

MPI_Abort

Terminates all MPI processes associated with the communicator. In most MPI implementations it terminates ALL processes regardless of the communicator specified.

```
MPI_Abort (comm,errorcode)
MPI_ABORT (comm,errorcode,ierr)
```

MPI_Get_processor_name

Returns the processor name. Also returns the length of the name. The buffer for "name" must be at least MPI_MAX_PROCESSOR_NAME characters in size. What is returned into "name" is implementation dependent - may not be the same as the output of the "hostname" or "host" shell commands.

```
MPI_Get_processor_name (&name,&resultlength)
MPI_GET_PROCESSOR_NAME (name,resultlength,ierr)
```

MPI_Get_version

Returns the version and subversion of the MPI standard that's implemented by the library.

```
MPI_Get_version (&version,&subversion)
MPI_GET_VERSION (version,subversion,ierr)
```

MPI_Initialized

Indicates whether MPI_Init has been called - returns flag as either logical true (1) or false(0). MPI requires that MPI_Init be called once and only once by each process. This may pose a problem for modules that want to use MPI and are prepared to call MPI_Init if necessary. MPI_Initialized solves this problem.

```
MPI_Initialized (&flag)
MPI_INITIALIZED (flag,ierr)
```

MPI_Wtime

Returns an elapsed wall clock time in seconds (double precision) on the calling processor.

```
MPI_Wtime ()
MPI_WTIME ()
```

MPI_Wtick

Returns the resolution in seconds (double precision) of MPI_Wtime.

```
MPI_Wtick ()
MPI_WTICK ()
```

MPI_Finalize

Terminates the MPI execution environment. This function should be the last MPI routine called in every MPI program - no other MPI routines may be called after it.

```
MPI_Finalize ()
MPI_FINALIZE (ierr)
```

Examples: Environment Management Routines

C Language - Environment Management Routines Example

```
#include "mpi.h"
#include <stdio.h>

int main(int argc, char *argv[]) {
int  numtasks, rank, len, rc;
char hostname[MPI_MAX_PROCESSOR_NAME];

rc = MPI_Init(&argc,&argv);
if (rc != MPI_SUCCESS) {
  printf ("Error starting MPI program. Terminating.\n");
  MPI_Abort(MPI_COMM_WORLD, rc);
  }

MPI_Comm_size(MPI_COMM_WORLD,&numtasks);
MPI_Comm_rank(MPI_COMM_WORLD,&rank);
MPI_Get_processor_name(hostname, &len);
printf ("Number of tasks= %d My rank= %d Running on %s\n", numtasks,rank,hostname);

/*******  do some work *******/

MPI_Finalize();
}
```

Fortran - Environment Management Routines Example

```
   program simple
   include 'mpif.h'

   integer numtasks, rank, len, ierr
   character(MPI_MAX_PROCESSOR_NAME) hostname

   call MPI_INIT(ierr)
   if (ierr .ne. MPI_SUCCESS) then
      print *,'Error starting MPI program. Terminating.'
      call MPI_ABORT(MPI_COMM_WORLD, rc, ierr)
   end if

   call MPI_COMM_RANK(MPI_COMM_WORLD, rank, ierr)
   call MPI_COMM_SIZE(MPI_COMM_WORLD, numtasks, ierr)
   call MPI_GET_PROCESSOR_NAME(hostname, len, ierr)
   print *, 'Number of tasks=',numtasks,' My rank=',rank,
  &         ' Running on=',hostname

C ****** do some work ******

   call MPI_FINALIZE(ierr)

   end
```

MPI Exercise 1

Getting Started

Overview:

- **Login to an LC cluster using your workshop username and OTP token**
- **Familiarize yourself with LC's MPI environment**
- **Write a simple "Hello World" MPI program using several MPI Environment**

Management routines
- **Successfully compile your program**
- **Successfully run your program - several different ways**
- **Familiarize yourself with LC's MPI documentation sources**

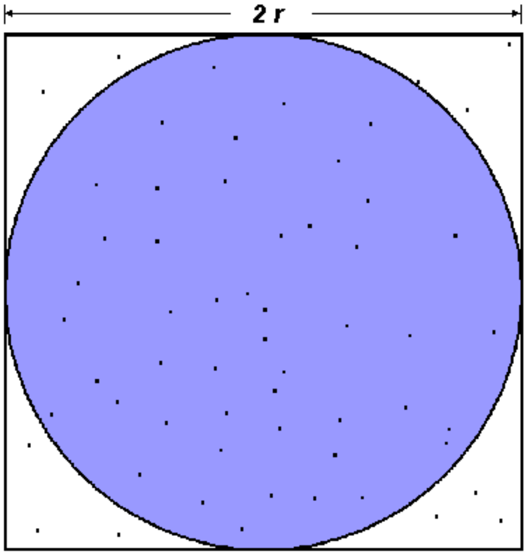
GO TO THE EXERCISE HERE

Point to Point Communication Routines

General Concepts

First, a Simple Example:

- The value of PI can be calculated in a number of ways. Consider the following method of approximating PI
  1. Inscribe a circle in a square
  2. Randomly generate points in the square
  3. Determine the number of points in the square that are also in the circle
  4. Let r be the number of points in the circle divided by the number of points in the square
  5. PI ~ 4 r
  6. Note that the more points generated, the better the approximation



$A_S = (2r)^2 = 4r^2$

$A_C = \pi r^2$

$\pi = 4 \times \frac{A_C}{A_S}$

- Serial pseudo code for this procedure:

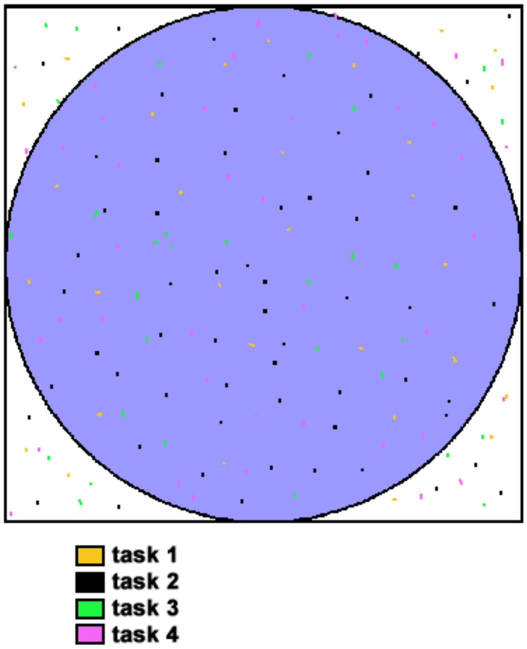
```
npoints = 10000
circle_count = 0

do j = 1,npoints
  generate 2 random numbers between 0 and 1
  xcoordinate = random1
  ycoordinate = random2
  if (xcoordinate, ycoordinate) inside circle
  then circle_count = circle_count + 1
end do

PI = 4.0*circle_count/npoints
```

- Leads to an "embarassingly parallel" solution:
  - Break the loop iterations into chunks that can be executed by different tasks simultaneously.
  - Each task executes its portion of the loop a number of times.
  - Each task can do its work without requiring any information from the other tasks (there are no data dependencies).
  - Master task recieves results from other tasks **using send/receive point-to-point operations**.

- Pseudo code solution: **red** highlights changes for parallelism.

```
npoints = 10000
circle_count = 0

p = number of tasks
num = npoints/p

find out if I am MASTER or WORKER

do j = 1,num
  generate 2 random numbers between 0 and 1
  xcoordinate = random1
  ycoordinate = random2
  if (xcoordinate, ycoordinate) inside circle
  then circle_count = circle_count + 1
end do

if I am MASTER
  receive from WORKERS their circle_counts
  compute PI (use MASTER and WORKER calculations)
else if I am WORKER
  send to MASTER circle_count
endif
```

Example MPI Program in C: mpi_pi_reduce.c
Example MPI Program in Fortran: mpi_pi_reduce.f



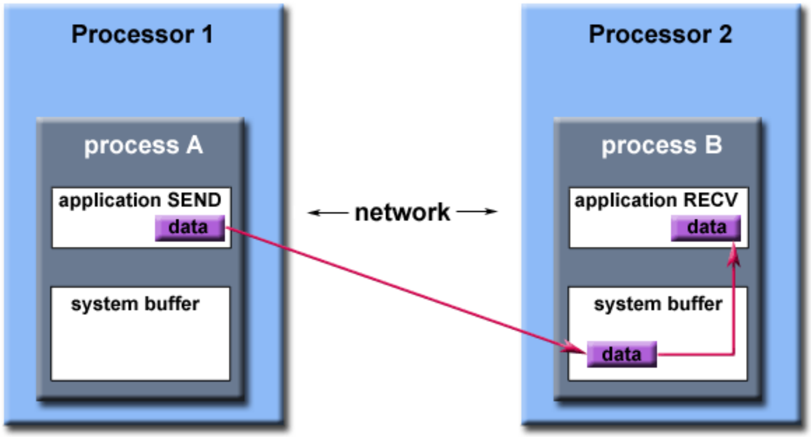
- **Key Concept:** Divide work between available tasks which communicate data via point-to-point message passing calls.

Types of Point-to-Point Operations:

- MPI point-to-point operations typically involve message passing between two, and only two, different MPI tasks. One task is performing a send operation and the other task is performing a matching receive operation.
- There are different types of send and receive routines used for different purposes. For example:
  - Synchronous send
  - Blocking send / blocking receive
  - Non-blocking send / non-blocking receive
  - Buffered send
  - Combined send/receive
  - "Ready" send
- Any type of send routine can be paired with any type of receive routine.
- MPI also provides several routines associated with send - receive operations, such as those used to wait for a message's arrival or probe to find out if a message has arrived.

Buffering:

- In a perfect world, every send operation would be perfectly synchronized with its matching receive. This is rarely the case. Somehow or other, the MPI implementation must be able to deal with storing data when the two tasks are out of sync.
- Consider the following two cases:
  - A send operation occurs 5 seconds before the receive is ready - where is the message while the receive is pending?
  - Multiple sends arrive at the same receiving task which can only accept one send at a time - what happens to the messages that are "backing up"?
- The MPI implementation (not the MPI standard) decides what happens to data in these types of cases. Typically, a **system buffer** area is reserved to hold data in transit. For example:



Path of a message buffered at the receiving process

- System buffer space is:
  - Opaque to the programmer and managed entirely by the MPI library
  - A finite resource that can be easy to exhaust
  - Often mysterious and not well documented
  - Able to exist on the sending side, the receiving side, or both
  - Something that may improve program performance because it allows send - receive operations to be asynchronous.

- User managed address space (i.e. your program variables) is called the **application buffer**. MPI also provides for a user managed send buffer.

Blocking vs. Non-blocking:

- Most of the MPI point-to-point routines can be used in either blocking or non-blocking mode.

- Blocking:
  - A blocking send routine will only "return" after it is safe to modify the application buffer (your send data) for reuse. Safe means that modifications will not affect the data intended for the receive task. Safe does not imply that the data was actually received - it may very well be sitting in a system buffer.
  - A blocking send can be synchronous which means there is handshaking occurring with the receive task to confirm a safe send.
  - A blocking send can be asynchronous if a system buffer is used to hold the data for eventual delivery to the receive.
  - A blocking receive only "returns" after the data has arrived and is ready for use by the program.

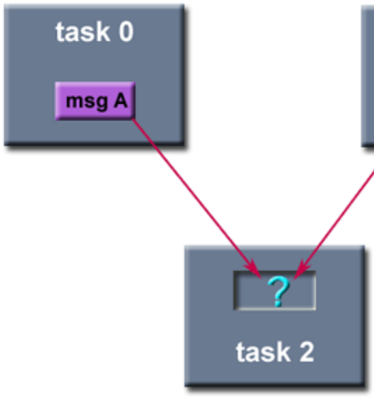
- Non-blocking:
  - Non-blocking send and receive routines behave similarly - they will return almost immediately. They do not wait for any communication events to complete, such as message copying from user memory to system buffer space or the actual arrival of message.
  - Non-blocking operations simply "request" the MPI library to perform the operation when it is able. The user can not predict when that will happen.
  - It is unsafe to modify the application buffer (your variable space) until you know for a fact the requested non-blocking operation was actually performed by the library. There are "wait" routines used to do this.
  - Non-blocking communications are primarily used to overlap computation with communication and exploit possible performance gains.

Order and Fairness:

- Order:
  - MPI guarantees that messages will not overtake each other.
  - If a sender sends two messages (Message 1 and Message 2) in succession to the same destination, and both match the same receive, the receive operation will receive Message 1 before Message 2.
  - If a receiver posts two receives (Receive 1 and Receive 2), in succession, and both are looking for the same message, Receive 1 will receive the message before Receive 2.

  - Order rules do not apply if there are multiple threads participating in the communication operations.

- Fairness:
  - MPI does not guarantee fairness - it's up to the programmer to prevent "operation starvation".
  - Example: task 0 sends a message to task 2. However, task 1 sends a competing message that matches task 2's receive. Only one of the sends will complete.



Point to Point Communication Routines

MPI Message Passing Routine Arguments

MPI point-to-point communication routines generally have an argument list that takes one of the following formats:

Blocking sends	`MPI_Send(buffer,count,type,dest,tag,comm)`
Non-blocking sends	`MPI_Isend(buffer,count,type,dest,tag,comm,request)`
Blocking receive	`MPI_Recv(buffer,count,type,source,tag,comm,status)`
Non-blocking receive	`MPI_Irecv(buffer,count,type,source,tag,comm,request)`

Buffer

Program (application) address space that references the data that is to be sent or received. In most cases, this is simply the variable name that is be sent/received. For C programs, this argument is passed by reference and usually must be prepended with an ampersand: `&var1`

Data Count

Indicates the number of data elements of a particular type to be sent.

Data Type

For reasons of portability, MPI predefines its elementary data types. The table below lists those required by the standard.

C Data Types		**Fortran Data Types**	
`MPI_CHAR`	signed char	`MPI_CHARACTER`	character(1)
`MPI_WCHAR`	wchar_t - wide character		
`MPI_SHORT`	signed short int		

`MPI_INT`	signed int	`MPI_INTEGER`
		`MPI_INTEGER1`
		`MPI_INTEGER2`
		`MPI_INTEGER4`
			integer
			integer*1
			integer*2

			integer*4
MPI_LONG	signed long int		
MPI_LONG_LONG_INT MPI_LONG_LONG	signed long long int		
MPI_SIGNED_CHAR	signed char		
MPI_UNSIGNED_CHAR	unsigned char		
MPI_UNSIGNED_SHORT	unsigned short int		
MPI_UNSIGNED	unsigned int		
MPI_UNSIGNED_LONG	unsigned long int		
MPI_UNSIGNED_LONG_LONG	unsigned long long int		
MPI_FLOAT	float	MPI_REAL MPI_REAL2 MPI_REAL4 MPI_REAL8	real real*2 real*4 real*8
MPI_DOUBLE	double	MPI_DOUBLE_PRECISION	double precision
MPI_LONG_DOUBLE	long double		
MPI_C_COMPLEX MPI_C_FLOAT_COMPLEX	float _Complex	MPI_COMPLEX	complex
MPI_C_DOUBLE_COMPLEX	double _Complex	MPI_DOUBLE_COMPLEX	double complex
MPI_C_LONG_DOUBLE_COMPLEX	long double _Complex		
MPI_C_BOOL	_Bool	MPI_LOGICAL	logical
MPI_C_LONG_DOUBLE_COMPLEX	long double _Complex		
MPI_INT8_T MPI_INT16_T MPI_INT32_T MPI_INT64_T	int8_t int16_t int32_t int64_t		
MPI_UINT8_T MPI_UINT16_T MPI_UINT32_T MPI_UINT64_T	uint8_t uint16_t uint32_t uint64_t		
MPI_BYTE	8 binary digits	MPI_BYTE	8 binary digits
MPI_PACKED	data packed or unpacked with MPI_Pack()/ MPI_Unpack	MPI_PACKED	data packed or unpacked with MPI_Pack()/ MPI_Unpack

Notes:

- Programmers may also create their own data types (see Derived Data Types).
- MPI_BYTE and MPI_PACKED do not correspond to standard C or Fortran types.
- Types shown in **GRAY FONT** are recommended if possible.
- Some implementations may include additional elementary data types (MPI_LOGICAL2, MPI_COMPLEX32, etc.). Check the MPI header file.

Destination

An argument to send routines that indicates the process where a message should be delivered. Specified as the rank of the receiving process.

Source

An argument to receive routines that indicates the originating process of the message. Specified as the rank of the sending process. This may be set to the wild card MPI_ANY_SOURCE to receive a message from any task.

Tag

Arbitrary non-negative integer assigned by the programmer to uniquely identify a message. Send and receive operations should match message tags. For a receive operation, the wild card MPI_ANY_TAG can be used to receive any message regardless of its tag. The MPI standard guarantees that integers 0-32767 can be used as tags, but most implementations allow a much larger range than this.

Communicator

Indicates the communication context, or set of processes for which the source or destination fields are valid. Unless the programmer is explicitly creating new communicators, the predefined communicator MPI_COMM_WORLD is usually used.

Status

For a receive operation, indicates the source of the message and the tag of the message. In C, this argument is a pointer to a predefined structure MPI_Status (ex. stat.MPI_SOURCE stat.MPI_TAG). In Fortran, it is an integer array of size MPI_STATUS_SIZE (ex. stat(MPI_SOURCE) stat(MPI_TAG)). Additionally, the actual number of bytes received is obtainable from Status via the MPI_Get_count routine.

Request

Used by non-blocking send and receive operations. Since non-blocking operations may return before the requested system buffer space is obtained, the system issues a unique "request number". The programmer uses this system assigned "handle" later (in a WAIT type routine) to determine completion of the non-blocking operation. In C, this argument is a pointer to a predefined structure MPI_Request. In Fortran, it is an integer.

Point to Point Communication Routines

Blocking Message Passing Routines

The more commonly used MPI blocking message passing routines are described below.

MPI_Send

Basic blocking send operation. Routine returns only after the application buffer in the sending task is free for reuse. Note that this routine may be implemented differently on different systems. The MPI standard permits the use of a system buffer but does not require it. Some implementations may actually use a synchronous send (discussed below) to implement the basic blocking send.

```
MPI_Send (&buf,count,datatype,dest,tag,comm)
MPI_SEND (buf,count,datatype,dest,tag,comm,ierr)
```

MPI_Recv

Receive a message and block until the requested data is available in the application buffer in the receiving task.

```
MPI_Recv (&buf,count,datatype,source,tag,comm,&status)
MPI_RECV (buf,count,datatype,source,tag,comm,status,ierr)
```

MPI_Ssend

Synchronous blocking send: Send a message and block until the application buffer in the sending task is free for reuse and the destination process has started to receive the message.

```
MPI_Ssend (&buf,count,datatype,dest,tag,comm)
MPI_SSEND (buf,count,datatype,dest,tag,comm,ierr)
```

MPI_Bsend

Buffered blocking send: permits the programmer to allocate the required amount of buffer space into which data can be copied until it is delivered. Insulates against the problems associated with insufficient system buffer space. Routine returns after the data has been copied from application buffer space to the allocated send buffer. Must be used with the MPI_Buffer_attach routine.

```
MPI_Bsend (&buf,count,datatype,dest,tag,comm)
MPI_BSEND (buf,count,datatype,dest,tag,comm,ierr)
```

MPI_Buffer_attach
MPI_Buffer_detach

Used by programmer to allocate/deallocate message buffer space to be used by the MPI_Bsend routine. The size argument is specified in actual data bytes - not a count of data elements. Only one buffer can be attached to a process at a time.

```
MPI_Buffer_attach (&buffer,size)
MPI_Buffer_detach (&buffer,size)
MPI_BUFFER_ATTACH (buffer,size,ierr)
MPI_BUFFER_DETACH (buffer,size,ierr)
```

MPI_Rsend

Blocking ready send. Should only be used if the programmer is certain that the matching receive has already been posted.

```
MPI_Rsend (&buf,count,datatype,dest,tag,comm)
MPI_RSEND (buf,count,datatype,dest,tag,comm,ierr)
```

MPI_Sendrecv

Send a message and post a receive before blocking. Will block until the sending application buffer is free for reuse and until the receiving application buffer contains the received message.

```
MPI_Sendrecv (&sendbuf,sendcount,sendtype,dest,sendtag,
...... &recvbuf,recvcount,recvtype,source,recvtag,
...... comm,&status)
MPI_SENDRECV (sendbuf,sendcount,sendtype,dest,sendtag,
...... recvbuf,recvcount,recvtype,source,recvtag,
...... comm,status,ierr)
```

MPI_Wait
MPI_Waitany
MPI_Waitall
MPI_Waitsome

MPI_Wait blocks until a specified non-blocking send or receive operation has completed. For multiple non-blocking operations, the programmer can specify any, all or some completions.

```
MPI_Wait (&request,&status)
MPI_Waitany (count,&array_of_requests,&index,&status)
MPI_Waitall (count,&array_of_requests,&array_of_statuses)
MPI_Waitsome (incount,&array_of_requests,&outcount,
...... &array_of_offsets, &array_of_statuses)
MPI_WAIT (request,status,ierr)
MPI_WAITANY (count,array_of_requests,index,status,ierr)
MPI_WAITALL (count,array_of_requests,array_of_statuses,
...... ierr)
MPI_WAITSOME (incount,array_of_requests,outcount,
...... array_of_offsets, array_of_statuses,ierr)
```

MPI_Probe

Performs a blocking test for a message. The "wildcards" MPI_ANY_SOURCE and MPI_ANY_TAG may be used to test for a message from any source or with any tag. For the C routine, the actual source and tag will be returned in the status structure as status.MPI_SOURCE and status.MPI_TAG. For the Fortran routine, they will be returned in the integer array status(MPI_SOURCE) and status(MPI_TAG).

```
MPI_Probe (source,tag,comm,&status)
MPI_PROBE (source,tag,comm,status,ierr)
```

Examples: Blocking Message Passing Routines

Task 0 pings task 1 and awaits return ping

C Language - Blocking Message Passing Routines Example

```
#include "mpi.h"
#include <stdio.h>

main(int argc, char *argv[])  {
int numtasks, rank, dest, source, rc, count, tag=1;
char inmsg, outmsg='x';
MPI_Status Stat;

MPI_Init(&argc,&argv);
MPI_Comm_size(MPI_COMM_WORLD, &numtasks);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);

if (rank == 0) {
  dest = 1;
  source = 1;
  rc = MPI_Send(&outmsg, 1, MPI_CHAR, dest, tag, MPI_COMM_WORLD);
  rc = MPI_Recv(&inmsg, 1, MPI_CHAR, source, tag, MPI_COMM_WORLD, &Stat);
  }

else if (rank == 1) {
  dest = 0;
  source = 0;
  rc = MPI_Recv(&inmsg, 1, MPI_CHAR, source, tag, MPI_COMM_WORLD, &Stat);
  rc = MPI_Send(&outmsg, 1, MPI_CHAR, dest, tag, MPI_COMM_WORLD);
  }

rc = MPI_Get_count(&Stat, MPI_CHAR, &count);
printf("Task %d: Received %d char(s) from task %d with tag %d \n",
       rank, count, Stat.MPI_SOURCE, Stat.MPI_TAG);


MPI_Finalize();
}
```

Fortran - Blocking Message Passing Routines Example

```
   program ping
   include 'mpif.h'

   integer numtasks, rank, dest, source, count, tag, ierr
   integer stat(MPI_STATUS_SIZE)
   character inmsg, outmsg
   outmsg = 'x'
   tag = 1

   call MPI_INIT(ierr)
   call MPI_COMM_RANK(MPI_COMM_WORLD, rank, ierr)
   call MPI_COMM_SIZE(MPI_COMM_WORLD, numtasks, ierr)

   if (rank .eq. 0) then
      dest = 1
      source = 1
      call MPI_SEND(outmsg, 1, MPI_CHARACTER, dest, tag,
 &            MPI_COMM_WORLD, ierr)
      call MPI_RECV(inmsg, 1, MPI_CHARACTER, source, tag,
 &            MPI_COMM_WORLD, stat, ierr)

   else if (rank .eq. 1) then
      dest = 0
      source = 0
      call MPI_RECV(inmsg, 1, MPI_CHARACTER, source, tag,
 &       MPI_COMM_WORLD, stat, err)
      call MPI_SEND(outmsg, 1, MPI_CHARACTER, dest, tag,
 &       MPI_COMM_WORLD, err)
   endif

   call MPI_GET_COUNT(stat, MPI_CHARACTER, count, ierr)
   print *, 'Task ',rank,': Received', count, 'char(s) from task',
  &         stat(MPI_SOURCE), 'with tag',stat(MPI_TAG)
```

```
   call MPI_FINALIZE(ierr)

   end
```

Point to Point Communication Routines

Non-Blocking Message Passing Routines

The more commonly used MPI non-blocking message passing routines are described below.

MPI_Isend

Identifies an area in memory to serve as a send buffer. Processing continues immediately without waiting for the message to be copied out from the application buffer. A communication request handle is returned for handling the pending message status. The program should not modify the application buffer until subsequent calls to MPI_Wait or MPI_Test indicate that the non-blocking send has completed.

```
MPI_Isend (&buf,count,datatype,dest,tag,comm,&request)
MPI_ISEND (buf,count,datatype,dest,tag,comm,request,ierr)
```

MPI_Irecv

Identifies an area in memory to serve as a receive buffer. Processing continues immediately without actually waiting for the message to be received and copied into the the application buffer. A communication request handle is returned for handling the pending message status. The program must use calls to MPI_Wait or MPI_Test to determine when the non-blocking receive operation completes and the requested message is available in the application buffer.

```
MPI_Irecv (&buf,count,datatype,source,tag,comm,&request)
MPI_IRECV (buf,count,datatype,source,tag,comm,request,ierr)
```

MPI_Issend

Non-blocking synchronous send. Similar to MPI_Isend(), except MPI_Wait() or MPI_Test() indicates when the destination process has received the message.

```
MPI_Issend (&buf,count,datatype,dest,tag,comm,&request)
MPI_ISSEND (buf,count,datatype,dest,tag,comm,request,ierr)
```

MPI_Ibsend

Non-blocking buffered send. Similar to MPI_Bsend() except MPI_Wait() or MPI_Test() indicates when the destination process has received the message. Must be used with the MPI_Buffer_attach routine.

```
MPI_Ibsend (&buf,count,datatype,dest,tag,comm,&request)
MPI_IBSEND (buf,count,datatype,dest,tag,comm,request,ierr)
```

MPI_Irsend

Non-blocking ready send. Similar to MPI_Rsend() except MPI_Wait() or MPI_Test() indicates when the destination process has received the message. Should only be used if the programmer is certain that the matching receive has already been posted.

```
MPI_Irsend (&buf,count,datatype,dest,tag,comm,&request)
MPI_IRSEND (buf,count,datatype,dest,tag,comm,request,ierr)
```

MPI_Test
MPI_Testany
MPI_Testall
MPI_Testsome

MPI_Test checks the status of a specified non-blocking send or receive operation. The "flag" parameter is returned logical true (1) if the operation has completed, and logical false (0) if not. For multiple non-blocking operations, the programmer can specify any, all or some completions.

```
MPI_Test (&request,&flag,&status)
MPI_Testany (count,&array_of_requests,&index,&flag,&status)
MPI_Testall (count,&array_of_requests,&flag,&array_of_statuses)
MPI_Testsome (incount,&array_of_requests,&outcount,
...... &array_of_offsets, &array_of_statuses)
MPI_TEST (request,flag,status,ierr)
MPI_TESTANY (count,array_of_requests,index,flag,status,ierr)
MPI_TESTALL (count,array_of_requests,flag,array_of_statuses,ierr)
MPI_TESTSOME (incount,array_of_requests,outcount,
...... array_of_offsets, array_of_statuses,ierr)
```

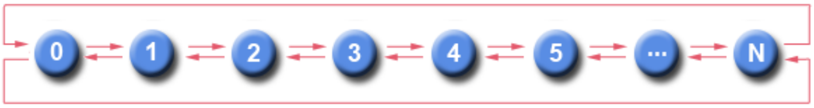
MPI_Iprobe

Performs a non-blocking test for a message. The "wildcards" MPI_ANY_SOURCE and MPI_ANY_TAG may be used to test for a message from any source or with any tag. The integer "flag" parameter is returned logical true (1) if a message has arrived, and logical false (0) if not. For the C routine, the actual source and tag will be returned in the status structure as status.MPI_SOURCE and status.MPI_TAG. For the Fortran routine, they will be returned in the integer array status(MPI_SOURCE) and status(MPI_TAG).

```
MPI_Iprobe (source,tag,comm,&flag,&status)
MPI_IPROBE (source,tag,comm,flag,status,ierr)
```

Examples: Non-Blocking Message Passing Routines

Nearest neighbor exchange in a ring topology



C Language - Non-Blocking Message Passing Routines Example

```
#include "mpi.h"
#include <stdio.h>

main(int argc, char *argv[])  {
int numtasks, rank, next, prev, buf[2], tag1=1, tag2=2;
MPI_Request reqs[4];
MPI_Status stats[4];

MPI_Init(&argc,&argv);
MPI_Comm_size(MPI_COMM_WORLD, &numtasks);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);

prev = rank-1;
next = rank+1;
if (rank == 0)  prev = numtasks - 1;
if (rank == (numtasks - 1))  next = 0;

MPI_Irecv(&buf[0], 1, MPI_INT, prev, tag1, MPI_COMM_WORLD, &reqs[0]);
MPI_Irecv(&buf[1], 1, MPI_INT, next, tag2, MPI_COMM_WORLD, &reqs[1]);

MPI_Isend(&rank, 1, MPI_INT, prev, tag2, MPI_COMM_WORLD, &reqs[2]);
MPI_Isend(&rank, 1, MPI_INT, next, tag1, MPI_COMM_WORLD, &reqs[3]);

      {  do some work  }

MPI_Waitall(4, reqs, stats);

MPI_Finalize();
}
```

Fortran - Non-Blocking Message Passing Routines Example

```
   program ringtopo
   include 'mpif.h'

   integer numtasks, rank, next, prev, buf(2), tag1, tag2, ierr
   integer stats(MPI_STATUS_SIZE,4), reqs(4)
   tag1 = 1
   tag2 = 2

   call MPI_INIT(ierr)
   call MPI_COMM_RANK(MPI_COMM_WORLD, rank, ierr)
   call MPI_COMM_SIZE(MPI_COMM_WORLD, numtasks, ierr)

   prev = rank - 1
   next = rank + 1
   if (rank .eq. 0) then
      prev = numtasks - 1
   endif
   if (rank .eq. numtasks - 1) then
      next = 0
   endif

   call MPI_IRECV(buf(1), 1, MPI_INTEGER, prev, tag1,
 &     MPI_COMM_WORLD, reqs(1), ierr)
   call MPI_IRECV(buf(2), 1, MPI_INTEGER, next, tag2,
 &     MPI_COMM_WORLD, reqs(2), ierr)

   call MPI_ISEND(rank, 1, MPI_INTEGER, prev, tag2,
 &     MPI_COMM_WORLD, reqs(3), ierr)
   call MPI_ISEND(rank, 1, MPI_INTEGER, next, tag1,
 &     MPI_COMM_WORLD, reqs(4), ierr)

C        do some work

   call MPI_WAITALL(4, reqs, stats, ierr);

   call MPI_FINALIZE(ierr)

   end
```

MPI Exercise 2

Point-to-Point Message Sending

Overview:

- **Login to the LC workshop cluster, if you are not already logged in**
- **Using your "Hello World" MPI program from Exercise 1, add MPI blocking point-to-point routines to send and receive messages**
- **Successfully compile your program**
- **Successfully run your program - several different ways**
- **Try the same thing with nonblocking send/receive routines**

GO TO THE EXERCISE HERE

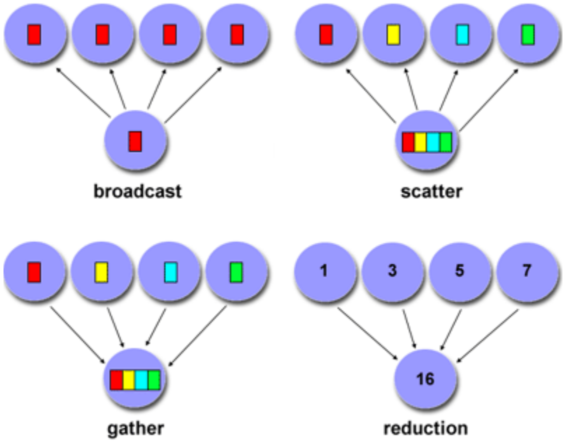
Collective Communication Routines

Scope:

- Collective communication routines must involve **all** processes within the scope of a communicator.
  - All processes are by default, members in the communicator MPI_COMM_WORLD.
  - Additional communicators can be defined by the programmer. See the Group and Communicator Management Routines section for details.
- Unexpected behavior, including program failure, can occur if even one task in the communicator doesn't participate.
- It is the programmer's responsibility to ensure that all processes within a communicator participate in any collective operations.

Types of Collective Operations:

- **Synchronization** - processes wait until all members of the group have reached the synchronization point.
- **Data Movement** - broadcast, scatter/gather, all to all.
- **Collective Computation** (reductions) - one member of the group collects data from the other members and performs an operation (min, max, add, multiply, etc.) on that data.



Programming Considerations and Restrictions:

- With MPI-3, collective operations can be blocking or non-blocking. Only blocking operations are covered in this tutorial.
- Collective communication routines do not take message tag arguments.
- Collective operations within subsets of processes are accomplished by first partitioning the subsets into new groups and then attaching the new groups to new communicators (discussed in the Group and Communicator Management Routines section).
- Can only be used with MPI predefined datatypes - not with MPI Derived Data Types.
- MPI-2 extended most collective operations to allow data movement between intercommunicators (not covered here).

Collective Communication Routines

MPI_Barrier

Synchronization operation. 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. Then all tasks are free to proceed.

```
MPI_Barrier (comm)
MPI_BARRIER (comm,ierr)
```

MPI_Bcast

Data movement operation. Broadcasts (sends) a message from the process with rank "root" to all other processes in the group.

Diagram Here

```
MPI_Bcast (&buffer,count,datatype,root,comm)
MPI_BCAST (buffer,count,datatype,root,comm,ierr)
```

MPI_Scatter

Data movement operation. Distributes distinct messages from a single source task to each task in the group.

Diagram Here

```
MPI_Scatter (&sendbuf,sendcnt,sendtype,&recvbuf,
...... recvcnt,recvtype,root,comm)
MPI_SCATTER (sendbuf,sendcnt,sendtype,recvbuf,
...... recvcnt,recvtype,root,comm,ierr)
```

MPI_Gather

Data movement operation. Gathers distinct messages from each task in the group to a single destination task. This routine is the reverse operation of MPI_Scatter.

Diagram Here

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

MPI_Allgather

Data movement operation. Concatenation of data to all tasks in a group. Each task in the group, in effect, performs a one-to-all broadcasting operation within the group.

Diagram Here

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

MPI_Reduce

Collective computation operation. Applies a reduction operation on all tasks in the group and places the result in one task.

Diagram Here

```
MPI_Reduce (&sendbuf,&recvbuf,count,datatype,op,root,comm)
MPI_REDUCE (sendbuf,recvbuf,count,datatype,op,root,comm,ierr)
```

The predefined MPI reduction operations appear below. Users can also define their own reduction functions by using the MPI_Op_create routine.

MPI Reduction Operation		C Data Types	Fortran Data Type
`MPI_MAX`	maximum	integer, float	integer, real, complex
`MPI_MIN`	minimum	integer, float	integer, real, complex
`MPI_SUM`	sum	integer, float	integer, real, complex
`MPI_PROD`	product	integer, float	integer, real, complex
`MPI_LAND`	logical AND	integer	logical
`MPI_BAND`	bit-wise AND	integer, MPI_BYTE	integer, MPI_BYTE
`MPI_LOR`	logical OR	integer	logical
`MPI_BOR`	bit-wise OR	integer, MPI_BYTE	integer, MPI_BYTE
`MPI_LXOR`	logical XOR	integer	logical
`MPI_BXOR`	bit-wise XOR	integer, MPI_BYTE	integer, MPI_BYTE
`MPI_MAXLOC`	max value and location	float, double and long double	real, complex,double precision
`MPI_MINLOC`	min value and location	float, double and long double	real, complex, double precision

MPI_Allreduce

Collective computation operation + data movement. Applies a reduction operation and places the result in all tasks in the group. This is equivalent to an MPI_Reduce followed by an MPI_Bcast.

Diagram Here

```
MPI_Allreduce (&sendbuf,&recvbuf,count,datatype,op,comm)
MPI_ALLREDUCE (sendbuf,recvbuf,count,datatype,op,comm,ierr)
```

MPI_Reduce_scatter

Collective computation operation + data movement. First does an element-wise reduction on a vector across all tasks in the group. Next, the result vector is split into disjoint segments and distributed across the tasks. This is equivalent to an MPI_Reduce followed by an MPI_Scatter operation.

Diagram Here

```
MPI_Reduce_scatter (&sendbuf,&recvbuf,recvcount,datatype,
...... op,comm)
MPI_REDUCE_SCATTER (sendbuf,recvbuf,recvcount,datatype,
...... op,comm,ierr)
```

MPI_Alltoall

Data movement operation. Each task in a group performs a scatter operation, sending a distinct message to all the tasks in the group in order by index.

Diagram Here

```
MPI_Alltoall (&sendbuf,sendcount,sendtype,&recvbuf,
...... recvcnt,recvtype,comm)
MPI_ALLTOALL (sendbuf,sendcount,sendtype,recvbuf,
...... recvcnt,recvtype,comm,ierr)
```

MPI_Scan

Performs a scan operation with respect to a reduction operation across a task group.

Diagram Here

```
MPI_Scan (&sendbuf,&recvbuf,count,datatype,op,comm)
MPI_SCAN (sendbuf,recvbuf,count,datatype,op,comm,ierr)
```

Examples: Collective Communications

Perform a scatter operation on the rows of an array

C Language - Collective Communications Example

```
#include "mpi.h"
#include <stdio.h>
#define SIZE 4

main(int argc, char *argv[])  {
int numtasks, rank, sendcount, recvcount, source;
float sendbuf[SIZE][SIZE] = {
  {1.0, 2.0, 3.0, 4.0},
  {5.0, 6.0, 7.0, 8.0},
  {9.0, 10.0, 11.0, 12.0},
  {13.0, 14.0, 15.0, 16.0}  };
float recvbuf[SIZE];

MPI_Init(&argc,&argv);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_size(MPI_COMM_WORLD, &numtasks);

if (numtasks == SIZE) {
  source = 1;
  sendcount = SIZE;
  recvcount = SIZE;
  MPI_Scatter(sendbuf,sendcount,MPI_FLOAT,recvbuf,recvcount,
             MPI_FLOAT,source,MPI_COMM_WORLD);
  printf("rank= %d  Results: %f %f %f %f\n",rank,recvbuf[0],
         recvbuf[1],recvbuf[2],recvbuf[3]);
  }
else
  printf("Must specify %d processors. Terminating.\n",SIZE);

MPI_Finalize();
}
```

Fortran - Collective Communications Example

```
   program scatter
   include 'mpif.h'

   integer SIZE
   parameter(SIZE=4)
   integer numtasks, rank, sendcount, recvcount, source, ierr
   real*4 sendbuf(SIZE,SIZE), recvbuf(SIZE)

C  Fortran stores this array in column major order, so the
C  scatter will actually scatter columns, not rows.
   data sendbuf /1.0, 2.0, 3.0, 4.0,
 &           5.0, 6.0, 7.0, 8.0,
 &           9.0, 10.0, 11.0, 12.0,
 &           13.0, 14.0, 15.0, 16.0 /

   call MPI_INIT(ierr)
   call MPI_COMM_RANK(MPI_COMM_WORLD, rank, ierr)
   call MPI_COMM_SIZE(MPI_COMM_WORLD, numtasks, ierr)

   if (numtasks .eq. SIZE) then
      source = 1
      sendcount = SIZE
      recvcount = SIZE
      call MPI_SCATTER(sendbuf, sendcount, MPI_REAL, recvbuf,
 &   recvcount, MPI_REAL, source, MPI_COMM_WORLD, ierr)
      print *, 'rank= ',rank,' Results: ',recvbuf
   else
      print *, 'Must specify',SIZE,' processors.  Terminating.'
   endif

   call MPI_FINALIZE(ierr)

   end
```

Sample program output:

```
rank= 0  Results: 1.000000 2.000000 3.000000 4.000000
rank= 1  Results: 5.000000 6.000000 7.000000 8.000000
rank= 2  Results: 9.000000 10.000000 11.000000 12.000000
rank= 3  Results: 13.000000 14.000000 15.000000 16.000000
```

Derived Data Types

- As previously mentioned, MPI predefines its primitive data types:

C Data Types		Fortran Data Types
MPI_CHAR	MPI_C_COMPLEX	MPI_CHARACTER
MPI_WCHAR	MPI_C_FLOAT_COMPLEX	MPI_INTEGER
MPI_SHORT	MPI_C_DOUBLE_COMPLEX	MPI_INTEGER1
MPI_INT	MPI_C_LONG_DOUBLE_COMPLEX	MPI_INTEGER2
MPI_LONG	MPI_C_BOOL	MPI_INTEGER4
MPI_LONG_LONG_INT	MPI_LOGICAL	MPI_REAL
MPI_LONG_LONG	MPI_C_LONG_DOUBLE_COMPLEX	MPI_REAL2

MPI_SIGNED_CHAR MPI_UNSIGNED_CHAR MPI_UNSIGNED_SHORT MPI_UNSIGNED_LONG MPI_UNSIGNED MPI_FLOAT MPI_DOUBLE MPI_LONG_DOUBLE	MPI_INT8_T MPI_INT16_T MPI_INT32_T MPI_INT64_T MPI_UINT8_T MPI_UINT16_T MPI_UINT32_T MPI_UINT64_T MPI_BYTE MPI_PACKED	MPI_REAL4 MPI_REAL8 MPI_DOUBLE_PRECISION MPI_COMPLEX MPI_DOUBLE_COMPLEX MPI_LOGICAL MPI_BYTE MPI_PACKED

- MPI also provides facilities for you to define your own data structures based upon sequences of the MPI primitive data types. Such user defined structures are called derived data types.
- Primitive data types are contiguous. Derived data types allow you to specify non-contiguous data in a convenient manner and to treat it as though it was contiguous.
- MPI provides several methods for constructing derived data types:
  - Contiguous
  - Vector
  - Indexed
  - Struct

Derived Data Type Routines

MPI_Type_contiguous

The simplest constructor. Produces a new data type by making count copies of an existing data type.

```
MPI_Type_contiguous (count,oldtype,&newtype)
MPI_TYPE_CONTIGUOUS (count,oldtype,newtype,ierr)
```

MPI_Type_vector
MPI_Type_hvector

Similar to contiguous, but allows for regular gaps (stride) in the displacements. MPI_Type_hvector is identical to MPI_Type_vector except that stride is specified in bytes.

```
MPI_Type_vector (count,blocklength,stride,oldtype,&newtype)
MPI_TYPE_VECTOR (count,blocklength,stride,oldtype,newtype,ierr)
```

MPI_Type_indexed
MPI_Type_hindexed

An array of displacements of the input data type is provided as the map for the new data type. MPI_Type_hindexed is identical to MPI_Type_indexed except that offsets are specified in bytes.

```
MPI_Type_indexed (count,blocklens[],offsets[],old_type,&newtype)
MPI_TYPE_INDEXED (count,blocklens(),offsets(),old_type,newtype,ierr)
```

MPI_Type_struct

The new data type is formed according to completely defined map of the component data types.

```
MPI_Type_struct (count,blocklens[],offsets[],old_types,&newtype)
MPI_TYPE_STRUCT (count,blocklens(),offsets(),old_types,newtype,ierr)
```

MPI_Type_extent

Returns the size in bytes of the specified data type. Useful for the MPI subroutines that require specification of offsets in bytes.

```
MPI_Type_extent (datatype,&extent)
MPI_TYPE_EXTENT (datatype,extent,ierr)
```

MPI_Type_commit

Commits new datatype to the system. Required for all user constructed (derived) datatypes.

```
MPI_Type_commit (&datatype)
MPI_TYPE_COMMIT (datatype,ierr)
```

MPI_Type_free

Deallocates the specified datatype object. Use of this routine is especially important to prevent memory exhaustion if many datatype objects are created, as in a loop.

```
MPI_Type_free (&datatype)
MPI_TYPE_FREE (datatype,ierr)
```

Examples: Contiguous Derived Data Type

Create a data type representing a row of an array and distribute a different row to all processes.

Diagram Here

C Language - Contiguous Derived Data Type Example

```
#include "mpi.h"
#include <stdio.h>
#define SIZE 4

main(int argc, char *argv[])  {
int numtasks, rank, source=0, dest, tag=1, i;
float a[SIZE][SIZE] =
  {1.0, 2.0, 3.0, 4.0,
   5.0, 6.0, 7.0, 8.0,
   9.0, 10.0, 11.0, 12.0,
   13.0, 14.0, 15.0, 16.0};
float b[SIZE];

MPI_Status stat;
MPI_Datatype rowtype;

MPI_Init(&argc,&argv);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_size(MPI_COMM_WORLD, &numtasks);

MPI_Type_contiguous(SIZE, MPI_FLOAT, &rowtype);
MPI_Type_commit(&rowtype);

if (numtasks == SIZE) {
  if (rank == 0) {
     for (i=0; i<numtasks; i++)
       MPI_Send(&a[i][0], 1, rowtype, i, tag, MPI_COMM_WORLD);
     }

  MPI_Recv(b, SIZE, MPI_FLOAT, source, tag, MPI_COMM_WORLD, &stat);
  printf("rank= %d  b= %3.1f %3.1f %3.1f %3.1f\n",
         rank,b[0],b[1],b[2],b[3]);
  }
else
  printf("Must specify %d processors. Terminating.\n",SIZE);

MPI_Type_free(&rowtype);
MPI_Finalize();
}
```

Fortran - Contiguous Derived Data Type Example

```
   program contiguous
   include 'mpif.h'

   integer SIZE
   parameter(SIZE=4)
   integer numtasks, rank, source, dest, tag, i,  ierr
   real*4 a(0:SIZE-1,0:SIZE-1), b(0:SIZE-1)
   integer stat(MPI_STATUS_SIZE), columntype

C  Fortran stores this array in column major order
```

```
   data a  /1.0, 2.0, 3.0, 4.0,
  &         5.0, 6.0, 7.0, 8.0,
  &         9.0, 10.0, 11.0, 12.0,
  &         13.0, 14.0, 15.0, 16.0 /

   call MPI_INIT(ierr)
   call MPI_COMM_RANK(MPI_COMM_WORLD, rank, ierr)
   call MPI_COMM_SIZE(MPI_COMM_WORLD, numtasks, ierr)

   call MPI_TYPE_CONTIGUOUS(SIZE, MPI_REAL, columntype, ierr)
   call MPI_TYPE_COMMIT(columntype, ierr)

   tag = 1
   if (numtasks .eq. SIZE) then
      if (rank .eq. 0) then
         do 10 i=0, numtasks-1
         call MPI_SEND(a(0,i), 1, columntype, i, tag,
  &                     MPI_COMM_WORLD,ierr)
 10      continue
      endif

      source = 0
      call MPI_RECV(b, SIZE, MPI_REAL, source, tag,
  &                 MPI_COMM_WORLD, stat, ierr)
         print *, 'rank= ',rank,' b= ',b

   else
      print *, 'Must specify',SIZE,' processors.  Terminating.'
   endif

   call MPI_TYPE_FREE(columntype, ierr)
   call MPI_FINALIZE(ierr)

   end
```

Sample program output:

```
rank= 0  b= 1.0 2.0 3.0 4.0
rank= 1  b= 5.0 6.0 7.0 8.0
rank= 2  b= 9.0 10.0 11.0 12.0
rank= 3  b= 13.0 14.0 15.0 16.0
```

Examples: Vector Derived Data Type

Create a data type representing a column of an array and distribute different columns to all processes.

Diagram Here

C Language - Vector Derived Data Type Example

```
#include "mpi.h"
#include <stdio.h>
#define SIZE 4

main(int argc, char *argv[])  {
int numtasks, rank, source=0, dest, tag=1, i;
float a[SIZE][SIZE] =
  {1.0, 2.0, 3.0, 4.0,
   5.0, 6.0, 7.0, 8.0,
   9.0, 10.0, 11.0, 12.0,
  13.0, 14.0, 15.0, 16.0};
float b[SIZE];

MPI_Status stat;
MPI_Datatype columntype;

MPI_Init(&argc,&argv);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_size(MPI_COMM_WORLD, &numtasks);
MPI_Type_vector(SIZE, 1, SIZE, MPI_FLOAT, &columntype);
MPI_Type_commit(&columntype);

if (numtasks == SIZE) {
  if (rank == 0) {
     for (i=0; i<numtasks; i++)
       MPI_Send(&a[0][i], 1, columntype, i, tag, MPI_COMM_WORLD);
        }

  MPI_Recv(b, SIZE, MPI_FLOAT, source, tag, MPI_COMM_WORLD, &stat);
  printf("rank= %d  b= %3.1f %3.1f %3.1f %3.1f\n",
        rank,b[0],b[1],b[2],b[3]);
  }
else
  printf("Must specify %d processors. Terminating.\n",SIZE);

MPI_Type_free(&columntype);
MPI_Finalize();
}
```

Fortran - Vector Derived Data Type Example

```
   program vector
   include 'mpif.h'

   integer SIZE
   parameter(SIZE=4)
   integer numtasks, rank, source, dest, tag, i,  ierr
   real*4 a(0:SIZE-1,0:SIZE-1), b(0:SIZE-1)
   integer stat(MPI_STATUS_SIZE), rowtype

C  Fortran stores this array in column major order
   data a  /1.0, 2.0, 3.0, 4.0,
  &         5.0, 6.0, 7.0, 8.0,
  &         9.0, 10.0, 11.0, 12.0,
  &         13.0, 14.0, 15.0, 16.0 /

   call MPI_INIT(ierr)
   call MPI_COMM_RANK(MPI_COMM_WORLD, rank, ierr)
   call MPI_COMM_SIZE(MPI_COMM_WORLD, numtasks, ierr)

   call MPI_TYPE_VECTOR(SIZE, 1, SIZE, MPI_REAL, rowtype, ierr)
   call MPI_TYPE_COMMIT(rowtype, ierr)

   tag = 1
   if (numtasks .eq. SIZE) then
      if (rank .eq. 0) then
         do 10 i=0, numtasks-1
         call MPI_SEND(a(i,0), 1, rowtype, i, tag,
  &                    MPI_COMM_WORLD, ierr)
 10      continue
      endif

      source = 0
      call MPI_RECV(b, SIZE, MPI_REAL, source, tag,
  &                MPI_COMM_WORLD, stat, ierr)
      print *, 'rank= ',rank,' b= ',b

   else
      print *, 'Must specify',SIZE,' processors.  Terminating.'
   endif

   call MPI_TYPE_FREE(rowtype, ierr)
   call MPI_FINALIZE(ierr)

   end
```

Sample program output:

```
rank= 0  b= 1.0 5.0 9.0 13.0
rank= 1  b= 2.0 6.0 10.0 14.0
rank= 2  b= 3.0 7.0 11.0 15.0
```

```
rank= 3  b= 4.0 8.0 12.0 16.0
```

Examples: Indexed Derived Data Type

Create a datatype by extracting variable portions of an array and distribute to all tasks.

Diagram Here

C Language - Indexed Derived Data Type Example

```
#include "mpi.h"
#include <stdio.h>
#define NELEMENTS 6

main(int argc, char *argv[])  {
int numtasks, rank, source=0, dest, tag=1, i;
int blocklengths[2], displacements[2];
float a[16] =
  {1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0,
   9.0, 10.0, 11.0, 12.0, 13.0, 14.0, 15.0, 16.0};
float b[NELEMENTS];

MPI_Status stat;
MPI_Datatype indextype;

MPI_Init(&argc,&argv);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_size(MPI_COMM_WORLD, &numtasks);

blocklengths[0] = 4;
blocklengths[1] = 2;
displacements[0] = 5;
displacements[1] = 12;

MPI_Type_indexed(2, blocklengths, displacements, MPI_FLOAT, &indextype);
MPI_Type_commit(&indextype);

if (rank == 0) {
  for (i=0; i<numtasks; i++)
     MPI_Send(a, 1, indextype, i, tag, MPI_COMM_WORLD);
  }

MPI_Recv(b, NELEMENTS, MPI_FLOAT, source, tag, MPI_COMM_WORLD, &stat);
printf("rank= %d  b= %3.1f %3.1f %3.1f %3.1f %3.1f %3.1f\n",
     rank,b[0],b[1],b[2],b[3],b[4],b[5]);

MPI_Type_free(&indextype);
MPI_Finalize();
}
```

Fortran - Indexed Derived Data Type Example

```
   program indexed
   include 'mpif.h'

   integer NELEMENTS
   parameter(NELEMENTS=6)
   integer numtasks, rank, source, dest, tag, i,  ierr
   integer blocklengths(0:1), displacements(0:1)
   real*4 a(0:15), b(0:NELEMENTS-1)
   integer stat(MPI_STATUS_SIZE), indextype

   data a  /1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0,
  &         9.0, 10.0, 11.0, 12.0, 13.0, 14.0, 15.0, 16.0 /

   call MPI_INIT(ierr)
   call MPI_COMM_RANK(MPI_COMM_WORLD, rank, ierr)
   call MPI_COMM_SIZE(MPI_COMM_WORLD, numtasks, ierr)

   blocklengths(0) = 4
   blocklengths(1) = 2
   displacements(0) = 5
   displacements(1) = 12

   call MPI_TYPE_INDEXED(2, blocklengths, displacements, MPI_REAL,
  &                      indextype, ierr)
   call MPI_TYPE_COMMIT(indextype, ierr)

   tag = 1
   if (rank .eq. 0) then
      do 10 i=0, numtasks-1
      call MPI_SEND(a, 1, indextype, i, tag, MPI_COMM_WORLD, ierr)
 10   continue
   endif

   source = 0
   call MPI_RECV(b, NELEMENTS, MPI_REAL, source, tag, MPI_COMM_WORLD,
  &              stat, ierr)
   print *, 'rank= ',rank,' b= ',b

   call MPI_TYPE_FREE(indextype, ierr)
   call MPI_FINALIZE(ierr)

   end
```

Sample program output:

```
rank= 0  b= 6.0 7.0 8.0 9.0 13.0 14.0
rank= 1  b= 6.0 7.0 8.0 9.0 13.0 14.0
rank= 2  b= 6.0 7.0 8.0 9.0 13.0 14.0
rank= 3  b= 6.0 7.0 8.0 9.0 13.0 14.0
```

Examples: Struct Derived Data Type

Create a data type that represents a particle and distribute an array of such particles to all processes.

Diagram Here

C Language - Struct Derived Data Type Example

```
#include "mpi.h"
#include <stdio.h>
#define NELEM 25

main(int argc, char *argv[])  {
int numtasks, rank, source=0, dest, tag=1, i;

typedef struct {
  float x, y, z;
  float velocity;
  int  n, type;
  }          Particle;
Particle     p[NELEM], particles[NELEM];
MPI_Datatype particletype, oldtypes[2];
int          blockcounts[2];

/* MPI_Aint type used to be consistent with syntax of */
/* MPI_Type_extent routine */
MPI_Aint    offsets[2], extent;

MPI_Status stat;

MPI_Init(&argc,&argv);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_size(MPI_COMM_WORLD, &numtasks);

/* Setup description of the 4 MPI_FLOAT fields x, y, z, velocity */
offsets[0] = 0;
oldtypes[0] = MPI_FLOAT;
blockcounts[0] = 4;
/* Setup description of the 2 MPI_INT fields n, type */
/* Need to first figure offset by getting size of MPI_FLOAT */
MPI_Type_extent(MPI_FLOAT, &extent);
offsets[1] = 4 * extent;
oldtypes[1] = MPI_INT;
blockcounts[1] = 2;

/* Now define structured type and commit it */
MPI_Type_struct(2, blockcounts, offsets, oldtypes, &particletype);
MPI_Type_commit(&particletype);

/* Initialize the particle array and then send it to each task */
if (rank == 0) {
  for (i=0; i<NELEM; i++) {
     particles[i].x = i * 1.0;
     particles[i].y = i * -1.0;
     particles[i].z = i * 1.0;
     particles[i].velocity = 0.25;
     particles[i].n = i;
     particles[i].type = i % 2;
     }
  for (i=0; i<numtasks; i++)
     MPI_Send(particles, NELEM, particletype, i, tag, MPI_COMM_WORLD);
  }

MPI_Recv(p, NELEM, particletype, source, tag, MPI_COMM_WORLD, &stat);

/* Print a sample of what was received */
printf("rank= %d   %3.2f %3.2f %3.2f %3.2f %d %d\n", rank,p[3].x,
     p[3].y,p[3].z,p[3].velocity,p[3].n,p[3].type);

MPI_Type_free(&particletype);
MPI_Finalize();
}
```

Fortran - Struct Derived Data Type Example

```
   program struct
   include 'mpif.h'

   integer NELEM
   parameter(NELEM=25)
   integer numtasks, rank, source, dest, tag, i,  ierr
   integer stat(MPI_STATUS_SIZE)

   type Particle
   sequence
   real*4 x, y, z, velocity
   integer n, type
   end type Particle

   type (Particle) p(NELEM), particles(NELEM)
   integer particletype, oldtypes(0:1), blockcounts(0:1),
  &        offsets(0:1), extent

   call MPI_INIT(ierr)
   call MPI_COMM_RANK(MPI_COMM_WORLD, rank, ierr)
   call MPI_COMM_SIZE(MPI_COMM_WORLD, numtasks, ierr)

C  Setup description of the 4 MPI_REAL fields x, y, z, velocity
   offsets(0) = 0
   oldtypes(0) = MPI_REAL
   blockcounts(0) = 4

C  Setup description of the 2 MPI_INTEGER fields n, type
C  Need to first figure offset by getting size of MPI_REAL
   call MPI_TYPE_EXTENT(MPI_REAL, extent, ierr)
   offsets(1) = 4 * extent
   oldtypes(1) = MPI_INTEGER
   blockcounts(1) = 2

C  Now define structured type and commit it
   call MPI_TYPE_STRUCT(2, blockcounts, offsets, oldtypes,
  &                     particletype, ierr)
   call MPI_TYPE_COMMIT(particletype, ierr)
```

```
C  Initialize the particle array and then send it to each task
   tag = 1
   if (rank .eq. 0) then
      do 10 i=0, NELEM-1
      particles(i) = Particle ( 1.0*i, -1.0*i, 1.0*i,
  &                    0.25, i, mod(i,2) )
 10   continue

      do 20 i=0, numtasks-1
      call MPI_SEND(particles, NELEM, particletype, i, tag,
  &                   MPI_COMM_WORLD, ierr)
 20   continue
   endif

   source = 0
   call MPI_RECV(p, NELEM, particletype, source, tag,
  &                MPI_COMM_WORLD, stat, ierr)

   print *, 'rank= ',rank,' p(3)= ',p(3)
   call MPI_TYPE_FREE(particletype, ierr)
   call MPI_FINALIZE(ierr)
   end
```

Sample program output:

```
rank= 0   3.00 -3.00 3.00 0.25 3 1
rank= 2   3.00 -3.00 3.00 0.25 3 1
rank= 1   3.00 -3.00 3.00 0.25 3 1
rank= 3   3.00 -3.00 3.00 0.25 3 1
```

Group and Communicator Management Routines

Groups vs. Communicators:

- A group is an ordered set of processes. Each process in a group is associated with a unique integer rank. Rank values start at zero and go to N-1, where N is the number of processes in the group. In MPI, a group is represented within system memory as an object. It is accessible to the programmer only by a "handle". A group is always associated with a communicator object.

- A communicator encompasses a group of processes that may communicate with each other. All MPI messages must specify a communicator. In the simplest sense, the communicator is an extra "tag" that must be included with MPI calls. Like groups, communicators are represented within system memory as objects and are accessible to the programmer only by "handles". For example, the handle for the communicator that comprises all tasks is MPI_COMM_WORLD.

- From the programmer's perspective, a group and a communicator are one. The group routines are primarily used to specify which processes should be used to construct a communicator.

Primary Purposes of Group and Communicator Objects:

1. Allow you to organize tasks, based upon function, into task groups.

2. Enable Collective Communications operations across a subset of related tasks.

3. Provide basis for implementing user defined virtual topologies

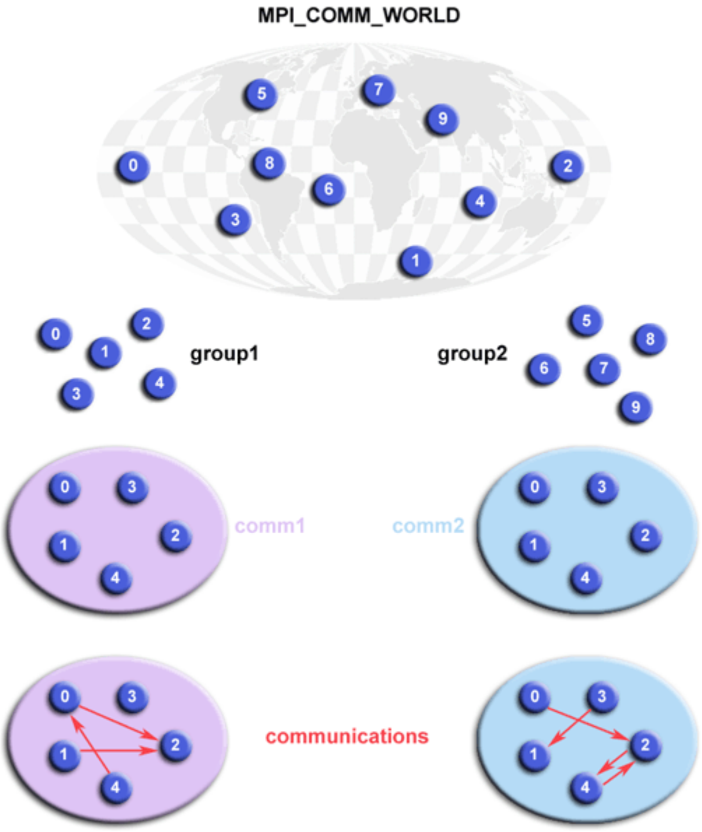
4. Provide for safe communications

Programming Considerations and Restrictions:

- Groups/communicators are dynamic - they can be created and destroyed during program execution.

- Processes may be in more than one group/communicator. They will have a unique rank within each group/communicator.

- MPI provides over 40 routines related to groups, communicators, and virtual topologies.
- Typical usage:
  1. Extract handle of global group from MPI_COMM_WORLD using MPI_Comm_group
  2. Form new group as a subset of global group using MPI_Group_incl
  3. Create new communicator for new group using MPI_Comm_create
  4. Determine new rank in new communicator using MPI_Comm_rank
  5. Conduct communications using any MPI message passing routine
  6. When finished, free up new communicator and group (optional) using MPI_Comm_free and MPI_Group_free



Group and Communicator Management Routines

Create two different process groups for separate collective communications exchange. Requires creating new communicators also.

C Language - Group and Communicator Routines Example

```
#include "mpi.h"
#include <stdio.h>
#define NPROCS 8

main(int argc, char *argv[])  {
int        rank, new_rank, sendbuf, recvbuf, numtasks,
           ranks1[4]={0,1,2,3}, ranks2[4]={4,5,6,7};
MPI_Group  orig_group, new_group;
MPI_Comm   new_comm;

MPI_Init(&argc,&argv);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_size(MPI_COMM_WORLD, &numtasks);

if (numtasks != NPROCS) {
  printf("Must specify MP_PROCS= %d. Terminating.\n",NPROCS);
  MPI_Finalize();
  exit(0);
  }

sendbuf = rank;

/* Extract the original group handle */
MPI_Comm_group(MPI_COMM_WORLD, &orig_group);

/* Divide tasks into two distinct groups based upon rank */
if (rank < NPROCS/2) {
  MPI_Group_incl(orig_group, NPROCS/2, ranks1, &new_group);
  }
else {
  MPI_Group_incl(orig_group, NPROCS/2, ranks2, &new_group);
  }

/* Create new new communicator and then perform collective communications */
MPI_Comm_create(MPI_COMM_WORLD, new_group, &new_comm);
MPI_Allreduce(&sendbuf, &recvbuf, 1, MPI_INT, MPI_SUM, new_comm);

MPI_Group_rank (new_group, &new_rank);
printf("rank= %d newrank= %d recvbuf= %d\n",rank,new_rank,recvbuf);

MPI_Finalize();
}
```

Fortran - Group and Communicator Routines Example

```
   program group
   include 'mpif.h'

   integer NPROCS
   parameter(NPROCS=8)
   integer rank, new_rank, sendbuf, recvbuf, numtasks
   integer ranks1(4), ranks2(4), ierr
   integer orig_group, new_group, new_comm
   data ranks1 /0, 1, 2, 3/, ranks2 /4, 5, 6, 7/

   call MPI_INIT(ierr)
   call MPI_COMM_RANK(MPI_COMM_WORLD, rank, ierr)
   call MPI_COMM_SIZE(MPI_COMM_WORLD, numtasks, ierr)

   if (numtasks .ne. NPROCS) then
     print *, 'Must specify NPROCS= ',NPROCS,' Terminating.'
     call MPI_FINALIZE(ierr)
     stop
   endif

   sendbuf = rank

C  Extract the original group handle
   call MPI_COMM_GROUP(MPI_COMM_WORLD, orig_group, ierr)

C  Divide tasks into two distinct groups based upon rank
   if (rank .lt. NPROCS/2) then
      call MPI_GROUP_INCL(orig_group, NPROCS/2, ranks1,
 &                 new_group, ierr)
   else
      call MPI_GROUP_INCL(orig_group, NPROCS/2, ranks2,
 &                 new_group, ierr)
   endif

   call MPI_COMM_CREATE(MPI_COMM_WORLD, new_group,
 &                 new_comm, ierr)
   call MPI_ALLREDUCE(sendbuf, recvbuf, 1, MPI_INTEGER,
 &                 MPI_SUM, new_comm, ierr)

   call MPI_GROUP_RANK(new_group, new_rank, ierr)
   print *, 'rank= ',rank,' newrank= ',new_rank,' recvbuf= ',
 &     recvbuf

   call MPI_FINALIZE(ierr)
   end
```

Sample program output:

```
rank= 7 newrank= 3 recvbuf= 22
rank= 0 newrank= 0 recvbuf= 6
rank= 1 newrank= 1 recvbuf= 6
rank= 2 newrank= 2 recvbuf= 6
rank= 6 newrank= 2 recvbuf= 22
rank= 3 newrank= 3 recvbuf= 6
rank= 4 newrank= 0 recvbuf= 22
rank= 5 newrank= 1 recvbuf= 22
```

Virtual Topologies

What Are They?

- In terms of MPI, a virtual topology describes a mapping/ordering of MPI processes into a geometric "shape".
- The two main types of topologies supported by MPI are Cartesian (grid) and Graph.
- MPI topologies are virtual - there may be no relation between the physical structure of the parallel machine and the process topology.
- Virtual topologies are built upon MPI communicators and groups.
- Must be "programmed" by the application developer.

Why Use Them?

- Convenience
  - Virtual topologies may be useful for applications with specific communication patterns - patterns that match an MPI topology structure.
  - For example, a Cartesian topology might prove convenient for an application that requires 4-way nearest neighbor communications for grid based data.
- Communication Efficiency
  - Some hardware architectures may impose penalties for communications between successively distant "nodes".
  - A particular implementation may optimize process mapping based upon the physical characteristics of a given parallel machine.
  - The mapping of processes into an MPI virtual topology is dependent upon the MPI implementation, and may be totally ignored.

Example:

A simplified mapping of processes into a Cartesian virtual topology appears below:

0 (0,0)	1 (0,1)	2 (0,2)	3 (0,3)
4 (1,0)	5 (1,1)	6 (1,2)	7 (1,3)
8 (2,0)	9 (2,1)	10 (2,2)	11 (2,3)
12 (3,0)	13 (3,1)	14 (3,2)	15 (3,3)

Virtual Topology Routines

Create a 4 x 4 Cartesian topology from 16 processors and have each process exchange its rank with four neighbors.

C Language - Cartesian Virtual Topology Example

```
#include "mpi.h"
#include <stdio.h>
#define SIZE 16
#define UP    0
#define DOWN  1
#define LEFT  2
#define RIGHT 3

main(int argc, char *argv[])  {
int numtasks, rank, source, dest, outbuf, i, tag=1,
   inbuf[4]={MPI_PROC_NULL,MPI_PROC_NULL,MPI_PROC_NULL,MPI_PROC_NULL,},
   nbrs[4], dims[2]={4,4},
   periods[2]={0,0}, reorder=0, coords[2];

MPI_Request reqs[8];
MPI_Status stats[8];
MPI_Comm cartcomm;

MPI_Init(&argc,&argv);
MPI_Comm_size(MPI_COMM_WORLD, &numtasks);

if (numtasks == SIZE) {
  MPI_Cart_create(MPI_COMM_WORLD, 2, dims, periods, reorder, &cartcomm);
  MPI_Comm_rank(cartcomm, &rank);
  MPI_Cart_coords(cartcomm, rank, 2, coords);
  MPI_Cart_shift(cartcomm, 0, 1, &nbrs[UP], &nbrs[DOWN]);
  MPI_Cart_shift(cartcomm, 1, 1, &nbrs[LEFT], &nbrs[RIGHT]);

  printf("rank= %d coords= %d %d  neighbors(u,d,l,r)= %d %d %d %d\n",
         rank,coords[0],coords[1],nbrs[UP],nbrs[DOWN],nbrs[LEFT],
         nbrs[RIGHT]);

  outbuf = rank;

  for (i=0; i<4; i++) {
     dest = nbrs[i];
     source = nbrs[i];
     MPI_Isend(&outbuf, 1, MPI_INT, dest, tag,
               MPI_COMM_WORLD, &reqs[i]);
     MPI_Irecv(&inbuf[i], 1, MPI_INT, source, tag,
               MPI_COMM_WORLD, &reqs[i+4]);
     }

  MPI_Waitall(8, reqs, stats);

  printf("rank= %d                  inbuf(u,d,l,r)= %d %d %d %d\n",
         rank,inbuf[UP],inbuf[DOWN],inbuf[LEFT],inbuf[RIGHT]);  }
else
  printf("Must specify %d processors. Terminating.\n",SIZE);

MPI_Finalize();
}
```

Fortran - Cartesian Virtual Topology Example

```
   program cartesian
   include 'mpif.h'

   integer SIZE, UP, DOWN, LEFT, RIGHT
   parameter(SIZE=16)
   parameter(UP=1)
   parameter(DOWN=2)
   parameter(LEFT=3)
   parameter(RIGHT=4)
   integer numtasks, rank, source, dest, outbuf, i, tag, ierr,
  &        inbuf(4), nbrs(4), dims(2), coords(2),
  &        stats(MPI_STATUS_SIZE, 8), reqs(8), cartcomm,
  &        periods(2), reorder
   data inbuf /MPI_PROC_NULL,MPI_PROC_NULL,MPI_PROC_NULL,
  &     MPI_PROC_NULL/,  dims /4,4/, tag /1/,
  &     periods /0,0/, reorder /0/

   call MPI_INIT(ierr)
   call MPI_COMM_SIZE(MPI_COMM_WORLD, numtasks, ierr)

   if (numtasks .eq. SIZE) then
      call MPI_CART_CREATE(MPI_COMM_WORLD, 2, dims, periods, reorder,
  &                        cartcomm, ierr)
      call MPI_COMM_RANK(cartcomm, rank, ierr)
      call MPI_CART_COORDS(cartcomm, rank, 2, coords, ierr)
      call MPI_CART_SHIFT(cartcomm, 0, 1, nbrs(UP), nbrs(DOWN), ierr)
      call MPI_CART_SHIFT(cartcomm, 1, 1, nbrs(LEFT), nbrs(RIGHT),
  &                       ierr)

      write(*,20) rank,coords(1),coords(2),nbrs(UP),nbrs(DOWN),
  &               nbrs(LEFT),nbrs(RIGHT)

      outbuf = rank
      do i=1,4
         dest = nbrs(i)
         source = nbrs(i)
         call MPI_ISEND(outbuf, 1, MPI_INTEGER, dest, tag,
  &                     MPI_COMM_WORLD, reqs(i), ierr)
         call MPI_IRECV(inbuf(i), 1, MPI_INTEGER, source, tag,
  &                     MPI_COMM_WORLD, reqs(i+4), ierr)
      enddo

      call MPI_WAITALL(8, reqs, stats, ierr)

      write(*,30) rank,inbuf

   else
     print *, 'Must specify',SIZE,' processors.  Terminating.'
   endif
   call MPI_FINALIZE(ierr)

20 format('rank= ',I3,' coords= ',I2,I2,
  &       ' neighbors(u,d,l,r)= ',I3,I3,I3,I3 )
30 format('rank= ',I3,'                 ',
  &       ' inbuf(u,d,l,r)= ',I3,I3,I3,I3 )

   end
```

Sample program output: (partial)

```
rank=   0 coords=  0 0 neighbors(u,d,l,r)=  -1  4 -1  1
rank=   0                  inbuf(u,d,l,r)=  -1  4 -1  1
rank=   8 coords=  2 0 neighbors(u,d,l,r)=   4 12 -1  9
rank=   8                  inbuf(u,d,l,r)=   4 12 -1  9
rank=   1 coords=  0 1 neighbors(u,d,l,r)=  -1  5  0  2
rank=   1                  inbuf(u,d,l,r)=  -1  5  0  2
rank=  13 coords=  3 1 neighbors(u,d,l,r)=   9 -1 12 14
rank=  13                  inbuf(u,d,l,r)=   9 -1 12 14
...
...
rank=   3 coords=  0 3 neighbors(u,d,l,r)=  -1  7  2 -1
rank=   3                  inbuf(u,d,l,r)=  -1  7  2 -1
rank=  11 coords=  2 3 neighbors(u,d,l,r)=   7 15 10 -1
rank=  11                  inbuf(u,d,l,r)=   7 15 10 -1
rank=  10 coords=  2 2 neighbors(u,d,l,r)=   6 14  9 11
rank=  10                  inbuf(u,d,l,r)=   6 14  9 11
rank=   9 coords=  2 1 neighbors(u,d,l,r)=   5 13  8 10
rank=   9                  inbuf(u,d,l,r)=   5 13  8 10
```

A Brief Word on MPI-2 and MPI-3

▶ MPI-2:

- Intentionally, the MPI-1 specification did not address several "difficult" issues. For reasons of expediency, these issues were deferred to a second specification, called MPI-2 in 1997.
- MPI-2 was a major revision to MPI-1 adding new functionality and corrections.
- Key areas of new functionality in MPI-2:
    - **Dynamic Processes** - extensions that remove the static process model of MPI. Provides routines to create new processes after job startup.
    - **One-Sided Communications** - provides routines for one directional communications. Include shared memory operations (put/get) and remote accumulate operations.
    - **Extended Collective Operations** - allows for the application of collective operations to inter-communicators
    - **External Interfaces** - defines routines that allow developers to layer on top of MPI, such as for debuggers and profilers.
    - **Additional Language Bindings** - describes C++ bindings and discusses Fortran-90 issues.
    - **Parallel I/O** - describes MPI support for parallel I/O.

▶ MPI-3:

- The MPI-3 standard was adopted in 2012, and contains significant extensions to MPI-1 and MPI-2 functionality including:
    - **Nonblocking Collective Operations** - permits tasks in a collective to perform operations without blocking, possibly offering performance improvements.
    - **New One-sided Communication Operations** - to better handle different memory models.
    - **Neighborhood Collectives** - Extends the distributed graph and Cartesian process topologies with additional communication power.
    - **Fortran 2008 Bindings** - expanded from Fortran90 bindings
    - **MPIT Tool Interface** - This new tool interface allows the MPI implementation to expose certain internal variables, counters, and other states to the user (most likely performance tools).
    - **Matched Probe** - Fixes an old bug in MPI-2 where one could not probe for messages in a multi-threaded environment.

▶ More Information on MPI-2 and MPI-3:

- MPI Standard documents: http://www.mpi-forum.org/docs/

MPI Exercise 3

Your Choice

Overview:

- **Login to the LC workshop cluster, if you are not already logged in**
- **Following the Exercise 3 instructions will take you through all sorts of MPI programs - pick any/all that are of interest.**
- **The intention is review the codes and see what's happening - not just compile and run.**
- **Several codes provide serial examples for a comparison with the parallel MPI versions.**
- **Check out the "bug" programs.**

GO TO THE EXERCISE HERE

This completes the tutorial.

Evaluation Form

Please complete the online evaluation form - unless you are doing the exercise, in which case please complete it at the end of the exercises.

Where would you like to go now?

- Exercise 3
- Agenda
- Back to the top

References and More Information

- Author: Blaise Barney, Livermore Computing.
- MPI Standard documents:
  http://www.mpi-forum.org/docs/
- "Using MPI", Gropp, Lusk and Skjellum. MIT Press, 1994.
- MPI Tutorials:
  www.mcs.anl.gov/research/projects/mpi/tutorial
- Livermore Computing specific information:
  - Linux Clusters Overview tutorial
    computing.llnl.gov/tutorials/linux_clusters
  - Using the Dawn BG/P System tutorial
    computing.llnl.gov/tutorials/bgp
  - Using the Sequoia/Vulcan BG/Q Systems tutorial
    computing.llnl.gov/tutorials/bgq
- "A User's Guide to MPI", Peter S. Pacheco. Department of Mathematics, University of San Francisco.

Appendix A: MPI-1 Routine Index

- These man pages were derived from the MVAPICH 0.9 implementation of MPI and may differ from the man pages of other implementations.
- Not all MPI routines are shown
- The complete MPI-3 standard (2012) defines over 440 routines.

Environment Management Routines

MPI_Abort	MPI_Errhandler_create	MPI_Errhandler_free	MPI_Errhandler_get
MPI_Errhandler_set	MPI_Error_class	MPI_Error_string	MPI_Finalize
MPI_Get_processor_name	MPI_Get_version	MPI_Init	MPI_Initialized
MPI_Wtick	MPI_Wtime		
Point-to-Point Communication Routines			
MPI_Bsend	MPI_Bsend_init	MPI_Buffer_attach	MPI_Buffer_detach
MPI_Cancel	MPI_Get_count	MPI_Get_elements	MPI_Ibsend
MPI_Iprobe	MPI_Irecv	MPI_Irsend	MPI_Isend
MPI_Issend	MPI_Probe	MPI_Recv	MPI_Recv_init
MPI_Request_free	MPI_Rsend	MPI_Rsend_init	MPI_Send
MPI_Send_init	MPI_Sendrecv	MPI_Sendrecv_replace	MPI_Ssend
MPI_Ssend_init	MPI_Start	MPI_Startall	MPI_Test
MPI_Test_cancelled	MPI_Testall	MPI_Testany	MPI_Testsome
MPI_Wait	MPI_Waitall	MPI_Waitany	MPI_Waitsome
Collective Communication Routines			
MPI_Allgather	MPI_Allgatherv	MPI_Allreduce	MPI_Alltoall
MPI_Alltoallv	MPI_Barrier	MPI_Bcast	MPI_Gather
MPI_Gatherv	MPI_Op_create	MPI_Op_free	MPI_Reduce
MPI_Reduce_scatter	MPI_Scan	MPI_Scatter	MPI_Scatterv
Process Group Routines			
MPI_Group_compare	MPI_Group_difference	MPI_Group_excl	MPI_Group_free
MPI_Group_incl	MPI_Group_intersection	MPI_Group_range_excl	MPI_Group_range_incl
MPI_Group_rank	MPI_Group_size	MPI_Group_translate_ranks	MPI_Group_union
Communicators Routines			
MPI_Comm_compare	MPI_Comm_create	MPI_Comm_dup	MPI_Comm_free
MPI_Comm_group	MPI_Comm_rank	MPI_Comm_remote_group	MPI_Comm_remote_size
MPI_Comm_size	MPI_Comm_split	MPI_Comm_test_inter	MPI_Intercomm_create
MPI_Intercomm_merge			
Derived Types Routines			
MPI_Type_commit	MPI_Type_contiguous	MPI_Type_extent	MPI_Type_free
MPI_Type_hindexed	MPI_Type_hvector	MPI_Type_indexed	MPI_Type_lb
MPI_Type_size	MPI_Type_struct	MPI_Type_ub	MPI_Type_vector
Virtual Topology Routines			
MPI_Cart_coords	MPI_Cart_create	MPI_Cart_get	MPI_Cart_map
MPI_Cart_rank	MPI_Cart_shift	MPI_Cart_sub	MPI_Cartdim_get
MPI_Dims_create	MPI_Graph_create	MPI_Graph_get	MPI_Graph_map
MPI_Graph_neighbors	MPI_Graph_neighbors_count	MPI_Graphdims_get	MPI_Topo_test
Miscellaneous Routines			
MPI_Address	MPI_Attr_delete	MPI_Attr_get	MPI_Attr_put
MPI_Keyval_create	MPI_Keyval_free	MPI_Pack	MPI_Pack_size
MPI_Pcontrol	MPI_Unpack		

https://computing.llnl.gov/tutorials/mpi/
Last Modified: 12/15/2014 12:28:35 blaiseb@llnl.gov

UCRL-MI-133316