Introduction to Parallel Programming with MPI
Outline

• Introduction

• Message Passing Interface (MPI)

• Point to Point Communications

• Collective Communications

• Derived Datatypes

• Resources for Users
Outline: Introduction

- What is Parallel Computing?
- Why go parallel?
- Types of Parallelism - Two Extremes.
- Parallel Computer Architectures
- Parallel “Architectures”
- Parallel Programming Models
What is Parallel Computing?

- *Parallel computing* - the use of multiple computers, processors or cores working together on a common task.
  - Each processor works on a section of the problem
  - Processors are allowed to exchange information (data in local memory) with other processors

Grid of Problem to be solved

```
  CPU #1 works on this area of the problem  exchange  CPU #2 works on this area of the problem
  CPU #3 works on this area of the problem  exchange  CPU #4 works on this area of the problem
```

Why go parallel?

- Limits of single CPU computing
  - Available memory
  - Performance
- Parallel computing allows:
  - Solve problems that don’t fit on a single CPU
  - Solve problems that can’t be solved in a reasonable time
- We can run…
  - Larger problems
  - Faster
  - More cases
Types of Parallelism - Two Extremes.

- Data parallel
  - Each processor performs the same task on different data
  - Example - grid problems
- Task parallel
  - Each processor performs a different task
  - Example - signal processing
- Most real applications fall somewhere on the continuum between these two extremes and involve more than one type of problem mapping
Parallel Computer Architectures

- SIMD - Single Instruction/Multiple Data
- MIMD - Multiple Instructions/Multiple Data

Control Mechanism:

Memory Model:
Parallel “Architectures”

- SPMD - Single Process/Multiple Data, or Single Program/Multiple Data
- MPMD - Multiple Process/Multiple Data, or Multiple Program/Multiple Data
Parallel Programming Models

- There are several parallel programming models in common use:
  - Shared Memory
  - Threads
  - Message Passing
  - Data Parallel
  - Hybrid
  - Other...

- Parallel programming models exist as an abstraction above hardware and memory architectures.

- In hybrid model any two or more parallel programming models are combined.

- Jaguar is an example of a common hybrid model which is the combination of the message passing model (MPI) with the shared memory model (OpenMP) which is also a combination of threads model.

- This document discusses the message passing (MPI) parallel programming model.
Outline: Message Passing Interface (MPI)

- What is MPI?
- MPI in Summary
- First MPI Program: Hello World!
- Four Major Benefits of MPI
- MPI Message Components
- Typical Message Passing Communication Components
- Message Passing Programming Concept
- Essentials of MPI Programs
- MPI Function Format
- MPI Communicators and Groups
- MPI Environment Management Routines
- MPI Process Identifiers
- MPI_COMM_WORLD communicator
- MPI_COMM_WORLD example
- Example: “Hello From …”
What is MPI?

• From a programming perspective, message passing implementations commonly comprise a library of subroutines that are imbedded in a source code. The programmer is responsible for determining all the parallelism.

• Historically, a variety of message passing libraries have been available since the 1980s. These implementations differed substantially from each other making it difficult for programmers to develop portable applications.

• In 1992, the MPI Forum, which had over 40 participating organizations, including vendors, researchers, software library developers, and users was formed with the primary goal of establishing a portable, efficient, and flexible standard specification for message passing implementations.

• As a result of this forum Part 1 of the Message Passing Interface (MPI) was released in 1994. Part 2 (MPI-2) was released in 1996.

• MPI is now the "de facto" industry standard for message passing implementations, replacing virtually all other implementations used for production work.
MPI in Summary

• MPI is dominant parallel programming approach in the USA.
• By itself, MPI is NOT a library - but rather the specification of what such a library should be.
• MPI is not an IEEE or ISO standard, but has in fact, become the "industry standard" for message passing implementations.
• As such, MPI is the first standardized vendor independent, message passing specification.
  – the syntax of MPI is standardized!
  – the functional behavior of MPI calls is standardized!
• Popular implementations: MPICH, OpenMPI (not to be confused with openMP), LAM, Cray MPT…
• MPI specifications (as well as MPICH implementation) are available on the web at http://www.mcs.anl.gov/research/projects/mpi/index.htm
First MPI Program: Hello World!

**C:**
```c
#include <stdio.h>
#include "mpi.h"

int main(int argc, char** argv) {
    MPI_Init(&argc, &argv);
    printf("Hello world \n");
    MPI_Finalize();
}
```

**Fortran:**
```fortran
program Hello_World
    include 'mpif.h'
    integer ierror
    call MPI_INIT(ierr)
    print *, 'Hello World'
    call MPI_FINALIZE(ierr)
end
```

**C++:**
```cpp
#include "mpi.h"
#include <iostream>

int main(int argc, char** argv) {
    MPI::Init(argc, argv);
    cout <<"Hello world \n";
    MPI::Finalize();
}
```
Four Major Benefits of MPI

Before the standard MPI specification appeared, message passing development was based on the tradeoffs between portability, performance and functionality.

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

**Portability** - Usually there is 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.

**Functionality** - Over 450 routines are defined in MPI-1 and MPI-2.

**Availability** - A variety of implementations are available on both vendor and public domains.
MPI Message Components

• Envelope:
  - sending processor (processor_id)
  - source location (group_id, tag)
  - receiving processor (processor_id)
  - destination location (group_id, tag)

• Data (letter):
  - data type (integer, float, complex, char...)
  - data length (buffer size, count, strides)
Typical Message Passing Communication Components

- Environment Identifiers
  \[ \text{processor}_id, \text{group}_id, \text{initialization} \]

- Point to Point Communications
  - blocking operations
  - non-blocking operations

- Collective Communications
  - barriers
  - broadcast
  - reduction operations
Message Passing Programming Concept

- Originally was used in distributed memory computing environment
- Can also be used in shared memory environment
- Since memory is local, any data stored in the memory of a remote processor must be explicitly requested by a programmer. In MPI implementations for systems which are collections of SM nodes the support for message passing on a node is included.
- Usually each processor executes the SAME program using partitioned data set (SPMD)
- Written in sequential language (FORTRAN, C, C++) plus MPI functions

```plaintext
Sum.exe (P0) :
myid =0, N=10
Data A, B(1:10)
  Do I=1,N
  AL(1:10)=A(myid*N+(1:10))
  BL(1:10)=B(myid*N+(1:10))
  CL=AL+BL
  SUM CL (MPI_Allreduce, C)
  Print global_sum C

Sum.exe (P1) :
myid =1, N=10
Data A, B(11:20)
  Do I=1,N
  AL(1:10)=A(myid*N+(1:10))
  BL(1:10)=B(myid*N+(1:10))
  CL=AL+BL
  SUM CL (MPI_Allreduce, C)
  Print global_sum C
```
Essentials of MPI Programs

Header files:

- **C:** `#include "mpi.h"

- **Fortran:** `include 'mpif.h'

- **C++:** `#include "mpi.h"

Initializing MPI:

- **C:** `int MPI_Init(int argc, char**argv)`

- **Fortran:** `call MPI_INIT(IERROR)`

- **C++:** `void MPI::Init(int& argc, char**& argv);`

Exiting MPI:

- **C:** `int MPI_Finalize(void)`

- **Fortran:** `call MPI_FINALIZE(IERROR)`

- **C++:** `void MPI::Finalize();`
MPI Function Format

MPI format:

C: \texttt{err = MPI\_Xxxx(parameter,...)}

Fortran: \texttt{call MPI\_XXXX(parameter,..., ierror)}

C++: \texttt{void MPI\::Xxxx(parameter,...)}

Errors:

C: Returned as \texttt{err. MPI\_SUCCESS} if successful

Fortran: Returned as \texttt{ierror parameter. MPI\_SUCCESS} if successful

C++ functions do not return error codes. If the default error handler has been set to \texttt{MPI\::ERRORS\_THROW\_EXCEPTIONS}, the C++ exception mechanism is used to signal an error by throwing an MPI::Exception object.

It should be noted that the default error handler (i.e., \texttt{MPI\::ERRORS\_ARE\_FATAL}) on a given type has not changed. User error handlers are also permitted. \texttt{MPI\::ERRORS\_RETURN} simply returns control to the calling function; there is no provision for the user to retrieve the error code.

User callback functions that return integer error codes should not throw exceptions; the returned error will be handled by the MPI implementation by invoking the appropriate error handler.
MPI Communicators and Groups

• MPI uses objects called *communicators* and *groups* to define which collection of processes may communicate with each other.

• All MPI communication calls require a *communicator argument* and MPI processes can only communicate if they share a communicator.

• Every communicator contains a *group of tasks* with a *system supplied identifier* (for message context) as an extra match field.

• The *base group* is the group that contains all processes, which are associated with the `MPI_COMM_WORLD` predefined communicator.

• Communicators are used to create independent “message universe”

• `MPI_Init` initializes all tasks with `MPI_COMM_WORLD`

• Communicators are particularly important for user supplied libraries
MPI Environment Management Routines

- MPI environment management routines are used for an assortment of purposes, such as initializing and terminating the MPI environment, querying the environment and identity, etc. Most of the commonly used ones are:

  MPI_Init
  MPI_Comm_size
  MPI_Comm_rank
  MPI_Abort
  MPI_Get_processor_name
  MPI_Initiated
  MPI_Wtime
  MPI_Wtick
  MPI_Finalize
MPI Process Identifiers

- **MPI_COMM_RANK**
  - Gets a process’s rank (ID) within a process group
  - C: `int MPI_Comm_rank(MPI_Comm comm, int *rank)`
  - Fortran: `call MPI_COMM_RANK(mpi_comm, rank, ierror)`
  - C++: `int MPI::Comm::Get_rank() const;`

- **MPI_COMM_SIZE**
  - Gets the number of processes within a process group
  - C: `int MPI_Comm_size(MPI_Comm comm, int *size)`
  - Fortran: `call MPI_COMM_SIZE(mpi_comm, size, ierror)`
  - C++: `int MPI::Comm::Get_size() const;`

- **MPI_Comm**: Communicator
MPI_COMM_WORLD communicator

- MPI_COMM_WORLD is the default communicator setup by MPI_Init()
- It contains all the processes
- For simplicity just use it wherever a communicator is required!
Every process has three communicating groups and a distinct rank associated to it.
Example: “Hello From …” – C

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

int main(int argc, char** argv)
{
    int my_PE_num, err;
    err = MPI_Init(&argc, &argv);
    if (err != MPI_SUCCESS) {
        printf ("Error initializing MPI.\n");
        MPI_Abort(MPI_COMM_WORLD, err);
    }
    MPI_Comm_rank(MPI_COMM_WORLD, &my_PE_num);
    printf("Hello from \%d. \n", my_PE_num);
    MPI_Finalize();
}

Example: “Hello From …” – Fortran

program Hello_From
include 'mpif.h'
integer my_PE_num, ierror, rc
call MPI_INIT(ierr)
if (ierror .ne. MPI_SUCCESS) then
   print *, 'Error initializing MPI.'
call MPI_ABORT(MPI_COMM_WORLD, rc, ierr)
end if

call MPI_COMM_RANK(MPI_COMM_WORLD, my_PE_num, ierr)
print *, 'Hello from', my_PE_num

end
Example: “Hello From …” – C++

#include "mpi.h"
#include <iostream>
int main(int argc, char** argv)
{
    int my_PE_num;
    MPI::Init(argc, argv);
    my_PE_num = MPI::COMM_WORLD.Get_rank();
    cout << "Hello from " << my_PE_num << endl;
    MPI::Finalize();
}
Outline: Point to Point Communications

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- Communication Modes: Non-Blocking Behavior
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Overview

- Point to point is sending a message from one process to another, i.e. source process sends message to destination process
- Communication takes place within a given communicator
- MPI defines four communication modes for blocking and non-blocking send:
  - synchronous mode ("safest")
  - ready mode (lowest system overhead)
  - buffered mode (decouples sender from receiver)
  - standard mode (compromise)
- The receive call does not specify communication mode - it is simply blocking and non-blocking
  - Blocking call stops the program until the message buffer is safe to use
  - Non-blocking call separates communication from computation
- Two messages sent from one process to another will arrive in same relative order as they are sent.
Buffering the Messages

• In a perfect world, every send operation would be perfectly synchronized with its matching receive. And there are cases when that may not be desirable. 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 two cases. Typically, a system buffer area is reserved to hold data in transit.
Buffering the Messages (2)

- System buffer space:
  - Memory in the processes
  - Opaque to the programmer and managed entirely by the MPI library
  - A finite resource that can be exhausted
  - May exist on a sending side, a receiving side, or both
  - May improve program performance because it allows send - receive operations to be asynchronous.

Path of a message buffered at the receiving process
Blocking Calls

- A blocking send or receive call suspends execution of user’s program until the message buffer being sent/received is safe to use.

- In case of a blocking send, this means the data to be sent have been copied out of the send buffer, but these data have not necessarily been received in the receiving task. The contents of the send buffer can be modified without affecting the message that was sent.

- The blocking receive implies that the data in the receive buffer are valid.
Blocking Send and Receive

- A blocking MPI call means that the program execution will be suspended until the message buffer is safe to use. The MPI standards specify that a blocking SEND or RECV does not return until the send buffer is safe to reuse (for MPI_SEND), or the receive buffer is ready to use (for MPI_RECV).
Non-Blocking Calls

• Non-blocking calls return immediately after initiating the communication.

• In order to reuse the send message buffer, the programmer must check for its status.

• The programmer can choose to block before the message buffer is used or test for the status of the message buffer.

• A blocking or non-blocking send can be paired to a blocking or non-blocking receive
Non-Blocking Send and Receive

- Separate Non-Blocking communication into three phases:
  - Initiate non-blocking communication.
  - Do some work (perhaps involving other communications?)
  - Wait for non-blocking communication to complete.

Non-Blocking Send Diagram:

<table>
<thead>
<tr>
<th>Send Process</th>
<th>User</th>
<th>MPI</th>
<th>User</th>
<th>MPI</th>
<th>User</th>
</tr>
</thead>
<tbody>
<tr>
<td>Start send</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>time</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>message</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Receive</td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Complete send</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(wait)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Non-Blocking Receive Diagram:

<table>
<thead>
<tr>
<th>Send Process</th>
<th>User</th>
<th>MPI</th>
<th>User</th>
</tr>
</thead>
<tbody>
<tr>
<td>Start send</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>time</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>message</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Receive</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Complete receive</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(wait)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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Order in MPI

- Order:
  - MPI guarantees that messages from same process 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 in MPI

- Fairness:
  - A parallel algorithm is *fair* if no process is effectively ignored
  - In the example below processes with low rank (like process zero) may be the only one whose messages are received.
  - MPI does not guarantee fairness - it's up to the programmer to prevent "operation starvation".
  - Another 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.

```c
if (rank == 0) {
    for (i=0; i<100*(size-1); i++) {
        MPI_Recv(buf, 1, MPI_INT, ANY_SOURCE, ANY_TAG, MPI_COMM_WORLD, &status);
        printf("Msg from %d with tag %d\n", status.MPI_SOURCE, status.MPI_TAG);
    }
} else {
    for (i=0; i<100; i++)
        MPI_Send( buf, 1, MPI_INT, 0, i, MPI_COMM_WORLD );
}
```
For a Communication to Succeed…

- Sender must specify a valid destination rank
- Receiver must specify a valid source rank
  - may use wildcard: \texttt{MPI\_ANY\_SOURCE}
- The communicator must be the same
- Tags must match
  - may use wildcard: \texttt{MPI\_ANY\_TAG}
- Message types must match
- Receiver’s buffer must be large enough
## MPI Basic Datatypes for C

<table>
<thead>
<tr>
<th>MPI Datatypes</th>
<th>C Datatypes</th>
</tr>
</thead>
<tbody>
<tr>
<td>MPI_CHAR</td>
<td>signed char</td>
</tr>
<tr>
<td>MPI_INT</td>
<td>signed int</td>
</tr>
<tr>
<td>MPI_LONG</td>
<td>signed long int</td>
</tr>
<tr>
<td>MPI_FLOAT</td>
<td>float</td>
</tr>
<tr>
<td>MPI_DOUBLE</td>
<td>double</td>
</tr>
<tr>
<td>MPI_LONG_DOUBLE</td>
<td>long double</td>
</tr>
<tr>
<td>MPI_BYTE</td>
<td>------</td>
</tr>
<tr>
<td>MPI_SHORT</td>
<td>signed short int</td>
</tr>
<tr>
<td>MPI_UNSIGNED_CHAR</td>
<td>unsigned char</td>
</tr>
<tr>
<td>MPI_UNSIGNED_SHORT</td>
<td>unsigned short int</td>
</tr>
<tr>
<td>MPI_UNSIGNED_LONG</td>
<td>unsigned long int</td>
</tr>
<tr>
<td>MPI_UNSIGNED</td>
<td>unsigned int</td>
</tr>
<tr>
<td>MPI_PACKED</td>
<td>------</td>
</tr>
</tbody>
</table>
## MPI Basic Datatypes for Fortran

<table>
<thead>
<tr>
<th>MPI Datatypes</th>
<th>Fortran Datatypes</th>
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<tbody>
<tr>
<td>MPI_INTEGER</td>
<td>integer</td>
</tr>
<tr>
<td>MPI_REAL</td>
<td>real</td>
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<tr>
<td>MPI_DOUBLE_PRECISION</td>
<td>double precision</td>
</tr>
<tr>
<td>MPI_COMPLEX</td>
<td>complex</td>
</tr>
<tr>
<td>MPI_DOUBLE_COMPLEX</td>
<td>double complex</td>
</tr>
<tr>
<td>MPI_LOGICAL</td>
<td>logical</td>
</tr>
<tr>
<td>MPI_CHARACTER</td>
<td>character(1)</td>
</tr>
<tr>
<td>MPI_BYTE</td>
<td>--------</td>
</tr>
<tr>
<td>MPI_PACKED</td>
<td>--------</td>
</tr>
</tbody>
</table>
## MPI Basic Datatypes for C++

<table>
<thead>
<tr>
<th>MPI Datatypes</th>
<th>C++ Datatypes</th>
</tr>
</thead>
<tbody>
<tr>
<td>MPI::CHAR</td>
<td>char</td>
</tr>
<tr>
<td>MPI::WCHAR</td>
<td>wchar_t</td>
</tr>
<tr>
<td>MPI::SHORT</td>
<td>signed short</td>
</tr>
<tr>
<td>MPI::INT</td>
<td>signed int</td>
</tr>
<tr>
<td>MPI::LONG</td>
<td>signed long</td>
</tr>
<tr>
<td>MPI::SIGNED_CHAR</td>
<td>signed char</td>
</tr>
<tr>
<td>MPI::UNSIGNED_CHAR</td>
<td>unsigned char</td>
</tr>
<tr>
<td>MPI::UNSIGNED_SHORT</td>
<td>unsigned short</td>
</tr>
<tr>
<td>MPI::UNSIGNED</td>
<td>unsigned int</td>
</tr>
<tr>
<td>MPI::UNSIGNED_LONG</td>
<td>unsigned long int</td>
</tr>
<tr>
<td>MPI::FLOAT</td>
<td>float</td>
</tr>
<tr>
<td>MPI::DOUBLE</td>
<td>double</td>
</tr>
<tr>
<td>MPI::LONG_DOUBLE</td>
<td>long double</td>
</tr>
<tr>
<td>MPI::BOOL</td>
<td>bool</td>
</tr>
<tr>
<td>MPI::COMPLEX</td>
<td>Complex&lt;float&gt;</td>
</tr>
<tr>
<td>MPI::DOUBLE_COMPLEX</td>
<td>Complex&lt;double&gt;</td>
</tr>
<tr>
<td>MPI::LONG_DOUBLE_COMPLEX</td>
<td>Complex&lt;long double&gt;</td>
</tr>
<tr>
<td>MPI::BYTE</td>
<td>------</td>
</tr>
<tr>
<td>MPI::PACKED</td>
<td>------</td>
</tr>
</tbody>
</table>
Communication Modes

- MPI has 8 different types of Send
- The non-blocking send has an extra argument of *request handle*

<table>
<thead>
<tr>
<th></th>
<th>Blocking</th>
<th>Non-Blocking</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Standard</strong></td>
<td>MPI_Send</td>
<td>MPI_Isend</td>
</tr>
<tr>
<td><strong>Synchronous</strong></td>
<td>MPI_Ssend</td>
<td>MPI_Issend</td>
</tr>
<tr>
<td><strong>Buffer</strong></td>
<td>MPI_Bsend</td>
<td>MPI_Ibsend</td>
</tr>
<tr>
<td><strong>Ready</strong></td>
<td>MPI_Rsend</td>
<td>MPI_Iresend</td>
</tr>
<tr>
<td></td>
<td>MPI_RECV</td>
<td>MPI_I_RECV</td>
</tr>
<tr>
<td></td>
<td>MPI_SEND_RECV</td>
<td></td>
</tr>
</tbody>
</table>
## Communication Modes: Blocking Behavior

<table>
<thead>
<tr>
<th>Mode</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Synchronous Send</td>
<td>MPI_SSEND Return when the message buffer can be safely reused. Can be started whether or not a matching receive was posted. However, the send will complete successfully only if a matching receive is posted.</td>
</tr>
<tr>
<td>Buffered Send</td>
<td>MPI_BSEND Return when message is copied to the system buffer</td>
</tr>
<tr>
<td>Ready Send</td>
<td>MPI_RSEND Complete if matching receive is already waiting</td>
</tr>
<tr>
<td>Standard Send</td>
<td>MPI_SEND Either synchronous or buffered, implemented by vendor to give good performance for most programs</td>
</tr>
</tbody>
</table>
Blocking Synchronous Send: \texttt{MPI\_SSEND}

- the sending task tells the receiver that a message is ready for it and waits for the receiver to acknowledge
- system overhead: buffer to network and vice versa
- synchronization overhead: handshake + waiting
- safest, most portable
Blocking Ready Send: MPI_RSEND

- requires a “ready to receive” notification, if not => error, exit
- sends message out over network
- minimize overhead
Blocking Buffered Send: `MPI_BSEND`

- Blocking buffer send - user-supply buffer on send node
- Buffer can be statically or dynamically allocated
- Send: data copy to buffer and return
- Receive: when notify, data are copied from buffer
Blocking Standard Send: \texttt{MPI\_Send}

- Implemented by vendors to give good performance for most programs.
- Simple and easy to use
- Either synchronous or buffered
- CRAY XT:
  - Based on MPICH2
  - Use a portals device for MPICH2
  - Support MPI2-RMA (one-sided)
  - Full MPI-IO support
  - No dynamic process management (NO Spawn process!!)
  - \texttt{man intro mpi} for more information
Syntax of Blocking Send

**C:**

```c
int MPI_Send(&buf, count, datatype, dest, tag, comm)
```

- **&buf:** pointer of object to be sent
- **count:** the number of items to be sent, e.g. 10
- **datatype:** the type of object to be sent, e.g. MPI_INT
- **dest:** destination of message (rank of receiver), e.g. 6
- **tag:** message tag, e.g. 78
- **comm:** communicator, e.g. MPI_COMM_WORLD

**Fortran:**

```fortran
call MPI_SEND(buf, count, datatype, dest, tag, comm, ierror)
```

**C++:**

```cpp
void MPI::Comm::Send(const void* buf, int count, const
                      MPI::Datatype& datatype, int dest, int tag) const
```
Syntax of Blocking Receive

C:
int MPI_Recv(&buf, count, datatype, source, tag, comm, &status)
    source: the node to receive from, e.g. 0
    &status: a structure which contains three fields, the source, tag, and error code of the incoming message.

Fortran:
call MPI_RECV(buf, count, datatype, source, tag, comm,
    status(MPI_STATUS_SIZE), ierror)
    status: an array of integers of size MPI_STATUS_SIZE

C++:
void MPI::Comm::Recv(void* buf, int count, const MPI::Datatype&
    datatype, int source, int tag, MPI::Status& status) const
Example: Passing a Message – Schematic

RANK ID

Core 0
Core 1
Core 2
... Core N

P0

message = Hello World

Send

B

Recv

P0

message = Hello World

P0

print

P1

message = Hello World

P1

print

Core 0
Core 1
Core 2
... Core N

helloworld

Core 1
Core 2
... Core N

Core 0
Core 1
Core 2
... Core N

helloworld

Message Passing Done (exit)
Example: Passing a Message – Hello World Again!

C Example

```c
#include <stdio.h>
#include "mpi.h"
int main(int argc, char ** argv)
{
    int my_PE_num, ntag = 100;
    char message[12] = "Hello, world";
    MPI_Status status;
    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &my_PE_num);

    if ( my_PE_num == 0 )
        MPI_Send(&message, 12, MPI_CHAR, 1, ntag, MPI_COMM_WORLD);
    else if ( my_PE_num == 1 ) {
        MPI_Recv(&message, 12, MPI_CHAR, 0, ntag, MPI_COMM_WORLD, &status);
        printf("Node \%d : \%s\n", my_PE_num, message);
    }
    MPI_Finalize();
}
```
Example: Passing a Message – Hello World Again!

Fortran Example

```fortran
program Hello_World
include 'mpif.h'
integer me, ierror, ntag, status(MPI_STATUS_SIZE)
character(12) message
call MPI_INIT(ierr)
call MPI_COMM_RANK(MPI_COMM_WORLD, me, ierr)
ntag = 100
if ( me .eq . 0) then
    message = 'Hello, World'
call MPI_Send(message, 12, MPI_CHARACTER, 1, ntag, 
                   MPI_COMM_WORLD, ierr)
else if ( me .eq . 1) then
    call MPI_Recv(message, 12, MPI_CHARACTER, 0, ntag, 
                   MPI_COMM_WORLD, status, ierr)
    print *, 'Node',me, ':', message
endif
call MPI_FINALIZE(ierr)
end
```
#include "mpi.h"
#include <iostream>
#include <string>
int main(int argc, char ** argv)
{
    int my_PE_num, ntag = 100;
    char message[13] = "Hello, world";
    MPI::Status status;
    MPI::Init(argc, argv);
    my_PE_num = MPI::COMM_WORLD.Get_rank();

    if ( my_PE_num == 0 )
        MPI::COMM_WORLD.Send(message,12,MPI::CHAR,1,ntag);
    else if ( my_PE_num == 1 ) {
        MPI::COMM_WORLD.Recv(message,12,MPI::CHAR,0,ntag, status);
        cout << "Node " << my_PE_num <<" : " << message << endl; }

    MPI::Finalize();
}
Example: Deadlock Situation

- You should be careful with your communications pattern to avoid getting into a deadlock. A *deadlock* is a situation that arises when a process cannot proceed because it is waiting on another process that is, in turn, waiting on the first process.

- **Deadlock**
  - All tasks are waiting for events that haven’t been initiated
  - common to SPMD program with blocking communication, e.g. every task sends, but none receives
  - insufficient system buffer space is available

- **Remedies**:
  - arrange one task to receive
  - *use MPI_Ssendrecv*
  - use non-blocking communication
Example: Deadlock – Fortran

c Improper use of blocking calls results in deadlock run on two nodes
c author: Roslyn Leibensperger, (CTC)

program deadlock
implicit none
include 'mpif.h'
integer MSGLEN, ITAG_A, ITAG_B
parameter (MSGLEN = 2048, ITAG_A = 100, ITAG_B = 200)
real rmsg1(MSGLEN) , rmsg2(MSGLEN)
integer irank, idest, isrc, istag, iretag,
istatus(MPI_STATUS_SIZE), ierr, I

call MPI_Init (ierr)
call MPI_Comm_rank( MPI_COMM_WORLD, irank, ierr)
do I = 1, MSGLEN
   rmsg1(I) = 100
   rmsg2(I) = -100
end do
Example: Deadlock – Fortran (Cont’d)

```fortran
if ( irank .eq. 0 ) then
    idest = 1
    isrc = 1
    istag = ITAG_A
    iretag = ITAG_B
else if ( irank .eq. 1 ) then
    idest = 0
    isrc = 0
    istag = ITAG_B
    iretag = ITAG_A
end if
print *, "Task ", irank, " has sent the message "
call MPI_Ssend (rmsg1, MSGLEN, MPI_REAL, idest, istag, MPI_COMM_WORLD, ierr)
call MPI_Recv (rmsg2, MSGLEN, MPI_REAL, isrc, iretag, MPI_COMM_WORLD, istatus, ierr)
print*, "Task", irank, " has received the message "
call MPI_Finalize (ierr)
end
```
Example: Deadlock – Fortran (fixed)

c Solution program showing the use of a non-blocking send to eliminate deadlock
c author: Roslyn Leibensperger (CTC)
program fixed
implicit none
include 'mpif.h'
interior MSGLEN, ITAG_A, ITAG_B
parameter (MSGLEN = 2048, ITAG_A = 100, ITAG_B = 200)
real rmsg1(MSGLEN), rmsg2(MSGLEN)
interior irank, dest, isrc, istag, iretag
integer ierr, I, request, istatus(MPI_STATUS_SIZE)
interior isstatus(MPI_STATUS_SIZE)
------------------//--------------------
print *, "Task", irank, "has started the send"
call MPI_Isend (rmsg1, MSGLEN, MPI_REAL, dest, istag,
MPI_COMM_WORLD, request, ierr)
call MPI_Recv (rmsg2, MSGLEN, MPI_REAL, isrc, iretag,
MPI_COMM_WORLD, istatus, ierr)
call MPI_Wait (request, isstatus, ierr)
print *, "Task ", irank, "has completed the send"
call MPI_Finalize (ierr) 
end
Example: Deadlock – C

```c
#include <stdio.h>
#include "mpi.h"
int main(int argc, char *argv[])
{
#define MSGLEN 2048
    int ITAG_A = 100, ITAG_B = 200;
    int irank, i, idest, isrc, istag, iretag;
    float rmsg1[MSGLEN];
    float rmsg2[MSGLEN];
    MPI_Status recv_status;

    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &irank);

    for (i = 1; i <= MSGLEN; i++)
    {
        rmsg1[i] = 100;
        rmsg2[i] = -100;
    }
```

Example: Deadlock – C (Cont’d)

```c
if ( irank == 0 )
{
    idest = 1;
    isrc = 1;
    istag = ITAG_A;
    iretag = ITAG_B;
}
else if ( irank == 1 )
{
    idest = 0;
    isrc = 0;
    istag = ITAG_B;
    iretag = ITAG_A;
}
printf("Task %d has sent the message\n", irank);
MPI_Ssend(&rmsg1, MSGLEN, MPI_FLOAT, idest, istag,
            MPI_COMM_WORLD);
MPI_Recv(&rmsg2, MSGLEN, MPI_FLOAT, isrc, iretag,
            MPI_COMM_WORLD, &recv_status);
printf("Task %d has received the message\n", irank);
MPI_Finalize();
```
Example: Deadlock – C (fixed)

//Solution program showing the use of a non-blocking send to eliminate deadlock
#include <stdio.h>
#include "mpi.h"
int main(int argc, char *argv[])
{
#define MSGLEN 2048
int ITAG_A = 100, ITAG_B = 200;
int irank, i, idest, isrc, istag, iretag;
float rmsg1[MSGLEN];
float rmsg2[MSGLEN];
MPI_Status irstatus, isstatus;
MPI_Request request;
------------------//--------------------
printf("Task %d has sent the message\n", irank);
MPI_Isend(&rmsg1, MSGLEN, MPI_FLOAT, idest, istag,
MPI_COMM_WORLD, &request);
MPI_Recv(&rmsg2, MSGLEN, MPI_FLOAT, isrc, iretag,
MPI_COMM_WORLD, &irstatus);
MPI_Wait(&request, &isstatus);
printf("Task %d has received the message\n", irank);
MPI_Finalize();
}
Example: Deadlock – C++

#include "mpi.h"
#include <iostream>

int main(int argc, char *argv[])
{
    #define MSGLEN 2048
    int ITAG_A = 100, ITAG_B = 200;
    int irank, i, idest, isrc, istag, iretag;
    float rmsg1[MSGLEN];
    float rmsg2[MSGLEN];
    MPI::Status recv_status;

    MPI::Init(argc, argv);
    irank = MPI::COMM_WORLD.Get_rank();

    for (i = 1; i <= MSGLEN; i++)
    {
        rmsg1[i] = 100;
        rmsg2[i] = -100;
    }
}
Example: Deadlock – C++ (Cont’d)

```c
if ( irank == 0 )
{
    idest = 1;
    isrc = 1;
    istag = ITAG_A;
    iretag = ITAG_B;
}
else if ( irank == 1 )
{
    idest = 0;
    isrc = 0;
    istag = ITAG_B;
    iretag = ITAG_A;
}

cout << "Task " << irank << " has sent the message" << endl;
MPI::COMM_WORLD.Ssend(rmsg1, MSGLEN, MPI::FLOAT, idest, istag);
MPI::COMM_WORLD.Recv(rmsg2, MSGLEN, MPI::FLOAT, isrc, iretag, recv_status);
cout << "Task " << irank << " has received the message" << endl;
MPI::Finalize();
```
Example: Deadlock – C++ (fixed)

```cpp
#include "mpi.h"
#include <iostream>

int main(int argc, char *argv[])
{
    #define MSGLEN 2048
    int ITAG_A = 100, ITAG_B = 200;
    int irank, i, idest, isrc, istag, iretag;
    float rmsg1[MSGLEN];
    float rmsg2[MSGLEN];
    MPI::Status irstatus, isstatus;
    MPI::Request request;
    cout << "Task " << irank << " has sent the message" << endl;
    request = MPI::COMM_WORLD.Isend(rmsg1, MSGLEN, MPI::FLOAT, idest, istag);
    MPI::COMM_WORLD.Recv(rmsg2, MSGLEN, MPI::FLOAT, isrc, iretag, irstatus);
    MPI_Wait(request, isstatus);
    cout << "Task " << irank << " has received the message" << endl;
    MPI::Finalize();
}
```
Communication Modes: Non-Blocking Behavior

• The non-blocking calls have the same syntax as the blocking calls with two exceptions:
  – Each call has an “I” immediately following the “_”
  – The last argument is a handle to an opaque request object that contains information about the message

• Non-blocking call returns immediately after initiating the communication

• The programmer can block or check for the status of the message buffer: MPI_Wait or MPI_Test.
Syntax of Non-Blocking Calls

Fortran:
- call MPI_Isend(buf, count, datatype, dest, tag, comm, handle, ierr)
- call MPI_Irecv(buff, count, datatype, src, tag, comm, handle, ierr)
- call MPI_Test(handle, flag, status, ierr)
- call MPI_Wait(handle, status, ierr)

C:
- MPI_Isend(&buf, count, datatype, dest, tag, comm, &handle)
- MPI_Irecv(&buff, count, datatype, src, tag, comm, &handle)
- MPI_Test(&handle, &flag, &status)
- MPI_Wait(&handle, &status)

C++:
- MPI::Request MPI::Comm::Isend(const void *buf, int count, const MPI::Datatype& datatype, int dest, int tag) const;
- MPI::Request MPI::Comm::Irecv(void *buf, int count, const MPI::Datatype& datatype, int source, int tag) const;
- bool MPI::Request::Test(MPI::Status& status);
- void MPI::Request::Wait(MPI::Status& status);
Sendrecv

- useful for executing a shift operation across a chain of processes
- system takes care of possible deadlock due to blocking calls

\[
\text{MPI\_Sendrecv(sbuf, scount, stype, dest, stag, rbuf, rcount, rtype, source, rtag, comm, status)}
\]

sbuf (rbuf): initial address of send (receive) buffer
scount (rcount): number of elements in send (receive) buffer
stype (rtype): type of elements in send (receive) buffer
stag (rtag): send (receive) tag
dest: rank of destination
source: rank of source
comm: communicator
status: status object
Testing Communications for Completion

- **MPI\_Wait**(request, status)
  - These routines block until the communication has completed. They are useful when the data from the communication buffer is about to be re-used

- **MPI\_Test**(request, flag, status)
  - This routine blocks until the communication specified by the handle *request* has completed. The *request* handle will have been returned by an earlier call to a non-blocking communication routine. The routine queries completion of the communication and the result (TRUE or FALSE) is returned in *flag*
Timer: MPI_Wtime

C: double MPI_Wtime(void)
Fortran: double precision MPI_Wtime()
C++: double MPI::Wtime();

- Time is measured in seconds.
- Time to perform a task is measured by consulting the timer before and after.
- Modify your program to measure its execution time and print it out.
Example: Ring (Blocking Communication) – Schematic

myrank=0
size=4
leftid=3
rightid=1
Val=3,2,1,0

myrank=1
size=4
leftid=0
rightid=2
Val=0,3,2,1

myrank=2
size=4
leftid=1
rightid=3
Val=1,0,3,2

myrank=3
size=4
leftid=2
rightid=0
Val=2,1,0,3
Example: Ring (Blocking Communication) – C

```c
#include <stdio.h>
#include "mpi.h"
int main(int argc, char *argv[]) {
    int myrank, nprocs, leftid, rightid, val, sum, tmp;
    MPI_Status recv_status;
    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
    MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
    if((leftid=(myrank-1)) < 0) leftid = nprocs -1;
    if((rightid=(myrank+1)) == nprocs) rightid = 0;
    val = myrank;
    sum = 0;
    do {
        MPI_Send(&val,1,MPI_INT,rightid,99, MPI_COMM_WORLD);
        MPI_Recv(&tmp,1, MPI_INT, leftid, 99, MPI_COMM_WORLD, &recv_status);
        val = tmp;
        sum += val;
    } while (val != myrank);
    printf("proc %d sum = %d \n", myrank, sum);
    MPI_Finalize();
}
```
Example: Ring (Blocking Communication) – Fortran

PROGRAM ring
IMPLICIT NONE
include "mpif.h"
INTEGER ierror, val, my_rank, nprocs, rightid, leftid, tmp, sum, request
INTEGER send_status(MPI_STATUS_SIZE), recv_status(MPI_STATUS_SIZE)
CALL MPI_INIT(ierr)
CALL MPI_COMM_RANK(MPI_COMM_WORLD, my_rank, ierr)
CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nprocs, ierr)
rightid = my_rank + 1
IF (rightid .EQ. nprocs) rightid = 0
leftid = my_rank - 1
IF (leftid .EQ. -1) leftid = nprocs-1
sum = 0
val = my_rank
100 CONTINUE
CALL MPI_SEND(val, 1, MPI_INTEGER, rightid, 99,
 $   MPI_COMM_WORLD, request, ierr)
CALL MPI_RECV(tmp, 1, MPI_INTEGER, leftid, 99,
 $   MPI_COMM_WORLD, recv_status, ierr)
sum = sum + tmp
val = tmp
IF(tmp .NE. my_rank) GOTO 100
PRINT *, 'Proc ', my_rank, ' Sum = ',sum
CALL MPI_FINALIZE(ierr)
STOP
END
Example: Ring (Non-blocking Communication) – Schematic

```
myrank=0
size=4
leftid=3
rightid=1

myrank=1
size=4
leftid=0
rightid=2

myrank=2
size=4
leftid=1
rightid=3

myrank=3
size=4
leftid=2
rightid=0
```
Example: Ring (Non-blocking Communication) – C

```c
#include <stdio.h>
#include "mpi.h"
main(int argc, char *argv[]) {
    int myrank, nprocs, leftid, rightid, val, sum, tmp;
    MPI_Status recv_status, send_status;
    MPI_request send_request;
    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
    MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
    if((leftid=(myrank-1)) < 0) leftid = nprocs -1;
    if((rightid=(myrank+1) == nprocs) rightid = 0;
    val = myrank
    sum = 0;
    do {
        MPI_Issend(&val,1,MPI_INT,right,99, MPI_COMM_WORLD,&send_request);
        MPI_Recv(&tmp,1, MPI_INT, left, 99, MPI_COMM_WORLD, &recv_status);
        MPI_Wait(&send_request,&send_status);
        val = tmp;sum += val;
    } while (val != myrank);
    printf("proc %d sum = %d \n", myrank, sum);
    MPI_Finalize();
}
```
Example: Ring (Non-blocking Communication) – Fortran

PROGRAM ring
IMPLICIT NONE
include "mpif.h"
INTEGER ierror, val, my_rank, nprocs, rightid, leftid, tmp, sum
INTEGER send_status(MPI_STATUS_SIZE), recv_status(MPI_STATUS_SIZE)
INTEGER request
CALL MPI_INIT(ierror)
CALL MPI_COMM_RANK(MPI_COMM_WORLD, my_rank, ierror)
CALL MPI_COMM_SIZE(MPI_COMM_WORLD, nprocs, ierror)
rightid = my_rank + 1
IF (rightid .EQ. nprocs) rightid = 0
leftid = my_rank – 1
IF (leftid .EQ. -1) leftid = nprocs-1
sum = 0
val = my_rank
100 CONTINUE
CALL MPI_ISSEND(val, 1, MPI_INTEGER, rightid, 99, $     MPI_COMM_WORLD, request, ierror)
CALL MPI_RECV(tmp, 1, MPI_INTEGER, leftid, 99, $     MPI_COMM_WORLD, recv_status, ierror)
CALL MPI_WAIT(request, send_status, ierror)
sum = sum + tmp
val = tmp
IF(tmp .NE. my_rank) GOTO 100
PRINT *, 'Proc ', my_rank, ' Sum = ',sum
CALL MPI_FINALIZE(ierr)
STOP
END
Example: Simple Array

- This is a simple array assignment used to demonstrate the distribution of data among multiple tasks and the communications required to accomplish that distribution.

- The master distributes an equal portion of the array to each worker. Each worker receives its portion of the array and performs a simple value assignment to each of its elements. Each worker then sends its portion of the array back to the master. As the master receives a portion of the array from each worker, selected elements are displayed.

- Note: For this example, the number of processes should be set to an odd number, to ensure even distribution of the array to numtasks-1 worker tasks.
Example: MPI Communication Timing Test

• The objective of this exercise is to investigate the amount of time required for message passing between two processes, i.e. an MPI communication timing test is performed.

• In this exercise different size messages are sent back and forth between two processes a number of times. Timings are made for each message before it is sent and after it has been received. The difference is computed to obtain the actual communication time. Finally, the average communication time and the bandwidth are calculated and output to the screen.

• For example, one can run this code on two nodes (one process on each node) passing messages of length 1, 100, 10,000, and 1,000,000 and record the results in a table.
Example: $\pi$ -calculation

- This program calculates $\pi$ -number by integrating $f(x) = \frac{4}{1+x^2}$
- Area under the curve is divided into rectangles and the rectangles are distributed to the processors.
- Let $f(x) = \frac{4}{1+x^2}$ then integrate $f(x)$ from $x = 0$ to $1$
Example: $\pi$ -calculation – Using Rectangles

- Method: Divide area under curve into rectangles and distribute the rectangles to the processors
- Suppose there are 3 processors, how should the distribution be done?
Example: Simple Matrix Multiplication Algorithm

- Matrix A is copied to every processor (FORTRAN)
- Matrix B is divided into blocks and distributed among processors
- Perform matrix multiplication simultaneously
- Output solutions

\[
\begin{array}{c}
\text{proc} \\
1, 2, 3, 4
\end{array} \quad * \quad \begin{array}{cccc}
p1 & p2 & p3 & p4
\end{array} = \begin{array}{cccc}
p1 & p2 & p3 & p4
\end{array}
\]

\[
A \quad * \quad B = C
\]
Example: Parallel Processing, matrix dimension n=8

Obtain
A(1:8, 1-8)
B(1:8, 1:8)
A(1:8, 1-8)

B(1:8, 7-8)
B(1:8, 5-6)
B(1:8, 3-4)
B(1:8, 1-2)

C(1:8, 7-8)
C(1:8, 5-6)
C(1:8, 3-4)
C(1:8, 1-2)

C=A*B
C=A*B
C=A*B
C=A*B

P0
P1
P2
P3
P4

Go to Menu
Example: Matrix Multiplication, steps 1-2

**step 1**

```
  p1
  p2
  p3
  p4
```

```
  p1  p2  p3  p4
  p2
  p4
```

```
  p1
  p2
  p3
  p4
```

**step 2**

```
  p4
  p1
  p2
  p3
```

```
  p1  p2  p3  p4
  p2
  p3
```

```
  p1
  p2
  p3
  p4
```

```
  p1
  p2
  p3
```

```
  p1
  p2
  p3
  p4
```

Go to Menu
Example: Matrix Multiplication, steps 3-4

**step 3**

<table>
<thead>
<tr>
<th></th>
<th>p3</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>p4</td>
</tr>
<tr>
<td></td>
<td>p1</td>
</tr>
<tr>
<td></td>
<td>p2</td>
</tr>
</tbody>
</table>

| p1 | p2 | p3 | p4 |

<table>
<thead>
<tr>
<th></th>
<th>p3</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>p4</td>
</tr>
<tr>
<td>p1</td>
<td>p2</td>
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</tbody>
</table>

**step 4**

<table>
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</thead>
<tbody>
<tr>
<td></td>
<td>p1</td>
</tr>
<tr>
<td></td>
<td>p2</td>
</tr>
<tr>
<td></td>
<td>p3</td>
</tr>
</tbody>
</table>

| p1 | p2 | p3 | p4 |

<table>
<thead>
<tr>
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</tr>
</tbody>
</table>
### Fox’s Algorithm (1)

Broadcast the diagonal element of block A in rows, perform multiplication.

<table>
<thead>
<tr>
<th>A(0,0)</th>
<th>A(0,0)</th>
<th>A(0,0)</th>
<th>B(0,0)</th>
<th>B(0,1)</th>
<th>B(0,2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A(1,1)</td>
<td>A(1,1)</td>
<td>A(1,1)</td>
<td>B(1,0)</td>
<td>B(1,1)</td>
<td>B(1,2)</td>
</tr>
<tr>
<td>A(2,2)</td>
<td>A(2,2)</td>
<td>A(2,2)</td>
<td>B(2,0)</td>
<td>B(2,1)</td>
<td>B(2,2)</td>
</tr>
</tbody>
</table>

\[
\begin{align*}
C(0,0) &= A(0,0) \times B(0,0) + A(0,1) \times B(1,0) + A(0,2) \times B(2,0) \\
C(0,1) &= A(0,0) \times B(0,1) + A(0,1) \times B(1,1) + A(0,2) \times B(2,1) \\
C(0,2) &= A(0,0) \times B(0,2) + A(0,1) \times B(1,2) + A(0,2) \times B(2,2) \\
C(1,0) &= A(1,0) \times B(0,0) + A(1,1) \times B(1,0) + A(1,2) \times B(2,0) \\
C(1,1) &= A(1,0) \times B(0,1) + A(1,1) \times B(1,1) + A(1,2) \times B(2,1) \\
C(1,2) &= A(1,0) \times B(0,2) + A(1,1) \times B(1,2) + A(1,2) \times B(2,2) \\
C(2,0) &= A(2,0) \times B(0,0) + A(2,1) \times B(1,0) + A(2,2) \times B(2,0) \\
C(2,1) &= A(2,0) \times B(0,1) + A(2,1) \times B(1,1) + A(2,2) \times B(2,1) \\
C(2,2) &= A(2,0) \times B(0,2) + A(2,1) \times B(1,2) + A(2,2) \times B(2,2)
\end{align*}
\]
Fox’s Algorithm (2)

Broadcast next element of block A in rows, shift Bij in column, perform multiplication

\[
\begin{align*}
C(0,0) &= A(0,0)B(0,0) + A(0,1)B(1,0) + A(0,2)B(2,0) \\
C(0,1) &= A(0,0)B(0,1) + A(0,1)B(1,1) + A(0,2)B(2,1) \\
C(0,2) &= A(0,0)B(0,2) + A(0,1)B(1,2) + A(2,0)B(0,1) + A(2,1)B(1,1) + A(2,2)B(2,1) \\
C(1,0) &= A(1,0)B(0,0) + A(1,1)B(1,0) + A(1,2)B(2,0) \\
C(1,1) &= A(1,0)B(0,1) + A(1,1)B(1,1) + A(1,2)B(2,1) \\
C(1,2) &= A(1,0)B(0,2) + A(1,1)B(1,2) + A(1,2)B(2,2) \\
C(2,0) &= A(2,0)B(0,0) + A(2,1)B(1,0) + A(2,2)B(2,0) \\
C(2,1) &= A(2,0)B(0,1) + A(2,1)B(1,1) + A(2,2)B(2,1) \\
C(2,2) &= A(2,0)B(0,2) + A(2,1)B(1,2) + A(2,2)B(2,2)
\end{align*}
\]
Fox’s Algorithm (3)

Broadcast next element of block A in rows, shift Bij in column, perform multiplication.

\[
\begin{array}{ccc}
A(0,2) & A(0,2) & A(0,2) \\
A(1,0) & A(1,0) & A(1,0) \\
A(2,1) & A(2,1) & A(2,1) \\
\end{array}
\times
\begin{array}{ccc}
B(2,0) & B(2,1) & B(2,2) \\
B(0,0) & B(0,1) & B(0,2) \\
B(1,0) & B(1,1) & B(1,2) \\
\end{array}
= \begin{array}{c}
C(0,0) \\
C(1,1) \\
C(2,2) \\
\end{array}
\]

\[
\begin{align*}
C(0,0) &= A(0,0) \cdot B(0,0) + A(0,1) \cdot B(1,0) + A(0,2) \cdot B(2,0) \\
C(0,1) &= A(0,0) \cdot B(0,1) + A(0,1) \cdot B(1,1) + A(0,2) \cdot B(2,1) \\
C(0,2) &= A(0,0) \cdot B(0,2) + A(0,1) \cdot B(1,2) + A(0,2) \cdot B(2,2) \\
C(1,0) &= A(1,0) \cdot B(0,0) + A(1,1) \cdot B(1,0) + A(1,2) \cdot B(2,0) \\
C(1,1) &= A(1,0) \cdot B(0,1) + A(1,1) \cdot B(1,1) + A(1,2) \cdot B(2,1) \\
C(1,2) &= A(1,0) \cdot B(0,2) + A(1,1) \cdot B(1,2) + A(1,2) \cdot B(2,2) \\
C(2,0) &= A(2,0) \cdot B(0,0) + A(2,1) \cdot B(1,0) + A(2,2) \cdot B(2,0) \\
C(2,1) &= A(2,0) \cdot B(0,1) + A(2,1) \cdot B(1,1) + A(2,2) \cdot B(2,1) \\
C(2,2) &= A(2,0) \cdot B(0,2) + A(2,1) \cdot B(1,2) + A(2,2) \cdot B(2,2)
\end{align*}
\]
Outline: Collective Communications

- Overview
- Barrier Synchronization Routines
- Broadcast Routines
- MPI_Scatterv and MPI_Gatherv
- MPI_Allgather
- MPI_Alltoall
- Global Reduction Routines
- Reduce and Allreduce
- Predefined Reduce Operations
Overview

- Substitutes for a more complex sequence of point-to-point calls
- Involve all the processes in a process group
- Called by all processes in a communicator
- All routines block until they are locally complete
- Receive buffers must be exactly the right size
- No message tags are needed
- Divided into three subsets:
  - synchronization
  - data movement
  - global computation
Barrier Synchronization Routines

- To synchronize all processes within a communicator
- A node calling it will be blocked until all nodes within the group have called it.

- C:
  ```c
  ierr = MPI_BARRIER(comm)
  ```

- Fortran:
  ```fortran
  call MPI_BARRIER(comm, ierr)
  ```

- C++:
  ```cpp
  void MPI::Comm::Barrier() const;
  ```
Broadcast Routines

- One processor sends some data to all processors in a group

**C:**

```c
ierr = MPI_Bcast(buffer, count, datatype, root, comm)
```

**Fortran:**

```fortran
call MPI_Bcast(buffer, count, datatype, root, comm, ierr)
```

**C++:**

```cpp
void MPI::Comm::Bcast(void* buffer, int count, const MPI::Datatype& datatype, int root) const;
```

- The `MPI_Bcast` must be called by each node in a group, specifying the same communicator and root. The message is sent from the root process to all processes in the group, including the root process.
Scatter

- Data are distributed into \( n \) equal segments, where the \( i^{th} \) segment is sent to the \( i^{th} \) process in the group which has \( n \) processes.

C:
\[
ierr = \text{MPI	extunderscore Scatter}(&\text{sbuff, scount, sdatatype,} \\
&\text{&rbuf, rcount, rdatatype, root, comm})
\]

Fortran:
\[
call \text{MPI	extunderscore Scatter}(\text{sbuff, scount, sdatatype, rbuf,} \\
\text{rcount, rdatatype, root, comm, ierr})
\]

C++:
\[
void \text{MPI	extasciitilde Comm	extasciitilde Scatter(const void* sendbuf, int} \\
\text{sendcount, const MPI	extasciitilde Datatype& sendtype, void*} \\
\text{recvbuf, int recvcount, const MPI	extasciitilde Datatype&} \\
\text{recvtype, int root) const;}
\]
Example: MPI_Scatter

real sbuf(12), rbuf(2)
call MPI_Scatter(sbuf, 2, MPI_INT, rbuf, 2, MPI_INT, 3, MPI_COMM_WORLD, ierr)
Scatter and Gather

**DATA**

<table>
<thead>
<tr>
<th>PE 0</th>
<th>A0</th>
<th>A1</th>
<th>A2</th>
<th>A3</th>
<th>A4</th>
<th>A5</th>
</tr>
</thead>
<tbody>
<tr>
<td>PE 1</td>
<td></td>
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<tr>
<td>PE 2</td>
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<td>PE 3</td>
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<td>PE 4</td>
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<tr>
<td>PE 5</td>
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</tr>
</tbody>
</table>

**scatter**

**DATA**

<table>
<thead>
<tr>
<th>A0</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
</tr>
<tr>
<td>A2</td>
</tr>
<tr>
<td>A3</td>
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<tr>
<td>A4</td>
</tr>
<tr>
<td>A5</td>
</tr>
</tbody>
</table>

**gather**

<table>
<thead>
<tr>
<th>PE 0</th>
</tr>
</thead>
<tbody>
<tr>
<td>PE 1</td>
</tr>
<tr>
<td>PE 2</td>
</tr>
<tr>
<td>PE 3</td>
</tr>
<tr>
<td>PE 4</td>
</tr>
<tr>
<td>PE 5</td>
</tr>
</tbody>
</table>
Gather

- Data are collected into a specified process in the order of process rank, reverse process of scatter.

- C:
  
  ```c
  ierr = MPI_Gather(&sbuf, scount, sdatatype, &rbuf, rcount, rdatatype, root, comm)
  ```

- Fortran:
  
  ```fortran
  call MPI_Gather(sbuff, scount, sdatatype, rbuff, rcount, rdtatatype, root, comm, ierr)
  ```

- C++:
  
  ```cpp
  void MPI::Comm::Gather(const void* sendbuf, int sendcount, const MPI::Datatype& sendtype, void* recvbuf, int recvccount, const MPI::Datatype& recvtype, int root) const;
  ```
Example: MPI_Gather

```fortran
real sbuf(2), rbuf(12)
call MPI_Gather(sbuf, 2, MPI_INT, rbuf, 2, MPI_INT, 3, MPI_COMM_WORLD, ierr)
```

ROOT PROCESSOR: 3
MPI_Scatterv and MPI_Gatherv

- allow varying count of data and flexibility for data placement

- C:
  
  ```c
  ierr = MPI_Scatterv( &sbuf, &scount, &displace, sdatatype, &rbuf, rcount, rdatatype, root, comm)
  ierr = MPI_Gatherv(&sbuf, scount, sdatatype, &rbuf, &rcount, &displace, rdatatype, root, comm)
  ```

- Fortran:
  
  ```fortran
  call MPI_Scatterv(sbuf,scount,displace,sdatatype, rbuf, rcount, rdatatype, root, comm, ierr)
  ```

- C++:
  
  ```cpp
  void MPI::Comm::Scatterv(const void* sendbuf, const int sendcounts[], const int displs[], const MPI::Datatype& sendtype, void* recvbuf, int recvcount, const MPI::Datatype& recvtype, int root, comm, const)
  ```
MPI_Allgather

```c
ierr = MPI_Allgather(&sbuf, scount, stype, &rbuf, rcount, rtype, comm)
```
MPI_Alltoall

MPI_Alltoall(sbuf, scount, stype, rbuf, rcount, rtype, comm)

sbuf: starting address of send buffer (*)
scount: number of elements sent to each process
stype: data type of send buffer
rbuf: address of receive buffer (*)
rcount: number of elements received from any process
rtype: data type of receive buffer elements
comm: communicator
## All to All

<table>
<thead>
<tr>
<th>DATA</th>
<th>alltoall</th>
</tr>
</thead>
<tbody>
<tr>
<td>PE 0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>A0</td>
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<tr>
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<td>F5</td>
</tr>
</tbody>
</table>
Global Reduction Routines

• The partial result in each process in the group is combined together using some desired function.

• The operation function passed to a global computation routine is either a predefined MPI function or a user supplied function

• Examples:
  – global sum or product
  – global maximum or minimum
  – global user-defined operation
Reduce and Allreduce

MPI_Reduce(sbuf, rbuf, count, stype, op, root, comm)
MPI_Allreduce(sbuf, rbuf, count, stype, op, comm)

sbuf: address of send buffer
rbuf: address of receive buffer
count: the number of elements in the send buffer
stype: the datatype of elements of send buffer
op: the reduce operation function, predefined or user-defined
root: the rank of the root process
comm: communicator

MPI_Reduce returns results to single process
MPI_Allreduce returns results to all processes in the group
## Predefined Reduce Operations

<table>
<thead>
<tr>
<th>MPI NAME</th>
<th>FUNCTION</th>
<th>MPI NAME</th>
<th>FUNCTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>MPI_MAX</td>
<td>Maximum</td>
<td>MPI_LOR</td>
<td>Logical OR</td>
</tr>
<tr>
<td>MPI_MIN</td>
<td>Minimum</td>
<td>MPI_BOR</td>
<td>Bitwise OR</td>
</tr>
<tr>
<td>MPI_SUM</td>
<td>Sum</td>
<td>MPI_LXOR</td>
<td>Logical exclusive OR</td>
</tr>
<tr>
<td>MPI_PROD</td>
<td>Product</td>
<td>MPI_BXOR</td>
<td>Bitwise exclusive OR</td>
</tr>
<tr>
<td>MPI_LAND</td>
<td>Logical AND</td>
<td>MPI_MAXLOC</td>
<td>Maximum and location</td>
</tr>
<tr>
<td>MPI_LOR</td>
<td>Bitwise AND</td>
<td>MPI_MINLOC</td>
<td>Minimum and location</td>
</tr>
</tbody>
</table>
Example: MPI Collective Communication Functions

- Collective communication routines are a group of MPI message passing routines to perform one (processor)-to-many (processors) and many-to-one communications.

- The first four columns on the left denote the contents of respective send buffers (e.g., arrays) of four processes. The content of each buffer, shown here as alphabets, is assigned a unique color to identify its origin. For instance, the alphabets in blue indicate that they originated from process 1. The middle column shows the MPI routines with which the send buffers are operated on. The four columns on the right represent the contents of the processes' receive buffers resulting from the MPI operations.
Outline: Derived Datatypes

- Overview
- Datatypes
- Defining Datatypes
- MPI_Type_vector
- MPI_Type_struct
Overview

• To provide a portable and efficient way of communicating mixed types, or non-contiguous types in a single message
  – Datatypes are built from the basic MPI datatypes
  – MPI datatypes are created at run-time through calls to MPI library

• Steps required
  – construct the datatype : define shapes and handle
  – allocate the datatype : commit types
  – use the datatype : use constructors
  – deallocate the datatype : free space
Datatypes

- Basic datatypes:
  \[ \text{MPI\_INT, MPI\_REAL, MPI\_DOUBLE, MPI\_COMPLEX, MPI\_LOGICAL, MPI\_CHARACTER, MPI\_BYTE, ...} \]

- MPI also supports array sections and structures through general datatypes. A general datatypes is a sequence of basic datatypes and integer byte displacements. These displacements are taken to be relative to the buffer that the basic datatype is describing. \( \Rightarrow \) typemap

\[ \text{Datatype} = \{ (\text{type0, disp0}) , (\text{type1, disp1}) , \ldots , (\text{typeN, dispN}) \} \]
Defining Datatypes

MPI_Type_contiguous(count, oldtype, newtype, ierr)

'count' copies of 'oldtype' are concatenated

MPI_Type_vector(count, buffer, strides, oldtype, newtype, ierr)

'count' blocks with 'blen' elements of 'oldtype' spaced by 'stride'

MPI_Type_indexed(count, buffer, strides, oldtype, newtype, ierr)

Extension of vector: varying 'blens' and 'strides'

MPI_Type_struct(count, buffer, strides, oldtype, newtype, ierr)

extension of indexed: varying data types allowed
MPI_Type_vector

- It replicates a datatype, taking blocks at fixed offsets.

\[
\text{MPI\_Type\_vector(count, blocklen, stride, oldtype, newtype)}
\]

- The new datatype consists of:
  - \text{count: number of blocks}
  - each block is a repetition of blocklen items of oldtype
  - the start of successive blocks is offset by stride items of oldtype

If \text{count = 2, stride = 4, blocklen = 3, oldtype = \{(double,0), (char,8)\}}
\text{newtype = \{(double,0), (char,8), (double,16), (char,24),}
\text{(double,32), (char,40), (double,64),}
\text{(char,72), (double,80), (char,88),}
\text{(double,96), (char,104)\}}
Example: Datatypes

```c
#include <mpi.h>
{
    float mesh[10][20];
    int dest, tag;
    MPI_Datatype newtype;
    /* Do this once */
    MPI_Type_vector( 10, /* # column elements */
                    1,   /* 1 column only */
                    20,  /* skip 20 elements */
                    MPI_FLOAT, /* elements are float */
                    &newtype); /* MPI derived datatype */
    MPI_Type_commit(&newtype); /* Do this for every new message */
    MPI_Send(&mesh[0][19], 1, newtype, dest, tag, MPI_COMM_WORLD);
}
```
MPI_Type_struct

- To gather a mix of different datatypes scattered at many locations in space into one datatype

\[
\text{MPI\_Type\_struct}(\text{count}, \text{array\_of\_blocklength}, \text{array\_of\_displacements}, \text{array\_of\_types}, \text{newtype}, \text{ierr})
\]

- \text{count} : number of blocks
- \text{array\_of\_blocklength} (B) : number of elements in each block
- \text{array\_of\_displacements} (I) : byte of displacement of each block
- \text{array\_of\_type} (T) : type of elements in each block

If \text{count} = 3

\[
\begin{align*}
T & = \{\text{MPI\_FLOAT}, \text{type1}, \text{MPI\_CHAR}\} \\
I & = \{0, 16, 26\} \\
B & = \{2, 1, 3\} \\
\text{type1} & = \{(\text{double}, 0), (\text{char}, 8)\} \\
\text{newtype} & = \{(\text{float}, 0), (\text{float}, 4), (\text{double}, 16), (\text{char}, 24), \ (\text{char}, 26), (\text{char}, 27), (\text{char}, 28)\}
\end{align*}
\]
Example

```c
Struct{ char display[50];
    int maxiter;
    double xmin, ymin, xmax, ymax;
    int width, height; } cmdline;

/* set up 4 blocks */
int blockcounts[4] = {50, 1, 4, 2};
MPI_Datatype types[4];
MPI_Aint displs[4];
MPI_Datatype cmdtype;

/* initialize types and displacements with addresses of items */

MPI_Address(&cmdline.display, &displs[0]);
MPI_Address(&cmdline.maxiter, &displs[1]);
MPI_Address(&cmdline.xmin, &displs[2]);
MPI_Address(&cmdline.width, &displs[3]);
types[0] = MPI_CHAR; types[1]=MPI_INT;

for ( i = 3 ; i >= 0; i-- ) displs[i] -= displs[0]
MPI_Type_struct(4, blockcounts, displs, types, &cmdtype);
MPI_Type_commit(&cmdtype);
```
Outline: Resources for Users

– Getting Started

– Advanced Topics

– More Information

– man pages and MPI web-sites

– MPI Books
Resources for Users: Getting Started

- About Jaguar
  
  http://www.nccs.gov/computing-resources/jaguar/

- Quad Core AMD Opteron Processor Overview
  

- PGI Compilers for XT5
  

- NCCS Training & Education – archives of NCCS workshops and seminar series, HPC/parallel computing references
  
  http://www.nccs.gov/user-support/training-education/

- 2009 Cray XT5 Quad-core Workshop
  
  http://www.nccs.gov/user-support/training-education/workshops/2008-cray-xt5-quad-core-workshop/
Resources for Users: Advanced Topics

- Debugging Applications Using TotalView
  
  http://www.nccs.gov/user-support/general-support/software/totalview

- Using Cray Performance Tools - CrayPat
  
  http://www.nccs.gov/computing-resources/jaguar/debugging-optimization/cray-pat/

- I/O Tips for Cray XT4
  
  http://www.nccs.gov/computing-resources/jaguar/debugging-optimization/io-tips/

- NCCS Software
  
  http://www.nccs.gov/computing-resources/jaguar/software/
Resources for Users: More Information

- NCCS website
  
  http://www.nccs.gov/

- Cray Documentation
  
  http://docs.cray.com/

- Contact us
  
  help@nccs.gov
Resources for Users: man pages and MPI web-sites

- There are man pages available for MPI which should be installed in your MANPATH. The following man pages have some introductory information about MPI.
  
  ```
  % man MPI
  % man cc
  % man ftn
  % man qsub
  % man MPI_Init
  % man MPI_Finalize
  ```

- MPI man pages are also available online.

- Main MPI web page at Argonne National Laboratory

- Set of guided exercises

- MPI tutorial at Lawrence Livermore National Laboratory
  [https://computing.llnl.gov/tutorials/mpi/](https://computing.llnl.gov/tutorials/mpi/)

- MPI Forum home page contains the official copies of the MPI standard.
Resources for Users: MPI Books

- Books on and about MPI
  - Designing and Building Parallel Programs is Ian Foster's online book that includes a chapter on MPI. It provides a succinct introduction to an MPI subset. (ISBN 0-201-57594-9; Published by Addison-Wesley)
  - Parallel Programming With MPI, by Peter S. Pacheco, published by Morgan Kaufmann.
  - RS/6000 SP: Practical MPI Programming, by Yukiya Aoyama and Jun Nakano (IBM Japan), and available as an IBM Redbook.