1 MPI: the Message Passing Interface

- Many early generation commercial parallel computers were based on the message-passing architecture due to its lower cost relative to shared-address-space architectures.
- Message-passing became the modern-age form of assembly language, in which every hardware vendor provided its own library.
- Performed very well on its own hardware, but was incompatible with the parallel computers offered by other vendors.
- Many of the differences between the various vendor-specific message-passing libraries were only syntactic.
- However, often enough there were some *serious semantic differences* that required significant re-engineering to port a message-passing program from one library to another.
- The message-passing interface (MPI) was created to essentially solve this problem.
- MPI defines
  - a standard library for message-passing,
  - can be used to develop **portable** message-passing programs.
- The MPI standard defines both the syntax as well as the semantics of a core set of library routines.
- The MPI library contains over 125 routines, but the number of key concepts is much smaller.
- In fact, it is possible to write fully-functional message-passing programs by using only six routines (see table 1).

1.1 Starting and Terminating the MPI Library

- **MPI_Init** is called prior to any calls to other MPI routines.
  - Its purpose is to initialize the mpi environment.
  - Calling **MPI_Init** more than once during the execution of a program will lead to an error.
- **MPI_Finalize** is called at the end of the computation.

Table 1: The minimal set of MPI routines.

MPI_Init	Initializes MPI
MPI_Finalize	Terminates MPI
MPI_Comm_size	Determines the number of processes
MPI_Comm_rank	Determines the label of the calling process
MPI_Send	Sends a message
MPI_Recv	Receives a message

  - It performs various clean-up tasks to terminate the MPI environment.
  - No MPI calls may be performed after **MPI_Finalize** has been called, not even **MPI_Init.**

- Upon successful execution, **MPI_Init** and **MPI_Finalize** return *MPI_SUCCESS*; otherwise they return an implementation-defined error code.

1.2 Communicators

- A key concept used throughout MPI is that of the communication domain.
- A communication domain is a set of processes that are allowed to communicate with each other.
- Information about communication domains is stored in variables of type *MPI_Comm*, that are called *communicators*.
- These communicators are used as arguments to all message transfer MPI routines.
- They uniquely identify the processes participating in the message transfer operation.
- In general, all the processes may need to communicate with each other.
- For this reason, MPI defines a default communicator called *MPI_COMM_WORLD* which includes all the processes involved.
- However, in many cases we want to perform communication only within (possibly overlapping) groups of processes.

- By using a different communicator for each such group, we can ensure that no messages will ever interfere with messages destined to any other group.

1.3 Getting Information

- **MPI_Comm_size** function ⟹ number of processes
- **MPI_Comm_rank** function ⟹ label of the calling process
- The calling sequences of these routines are as follows:

  ```
  int MPI_Comm_size(MPI_Comm comm, int *size)
  int MPI_Comm_rank(MPI_Comm comm, int *rank)
  ```

- Note that each process that calls either one of these functions must belong in the supplied communicator, otherwise an error will occur.
- The function MPI_Comm_size returns in the variable size the number of processes that belong to the communicator *comm*.
- So, when there is a single process per processor, the call

  ```
  MPI_Comm_size(MPI_COMM_WORLD, &size)
  ```

  will return in *size* the number of processors used by the program.

- Every process that belongs to a communicator is uniquely identified by its *rank*.
- The rank of a process is an integer that ranges from zero up to the size of the communicator minus one.
- A process can determine its rank in a communicator by calling

  ```
  MPI_Comm_rank(MPI_COMM_WORLD, &rank)
  ```

  that takes two arguments:

  1. the communicator,
  2. an integer variable rank.

- Up on return, the variable *rank* stores the rank of the process.

1.4 Sending and Receiving Messages

- The basic functions for sending and receiving messages in MPI are the **MPI_Send** and **MPI_Recv**, respectively.
- The calling sequences of these routines are as follows:

```
int MPI_Send(void *buf, int count,
             MPI_Datatype datatype,
             int dest, int tag,
             MPI_Comm comm)
int MPI_Recv(void *buf, int count,
             MPI_Datatype datatype,
             int source, int tag,
             MPI_Comm comm,
             MPI_Status *status)
```

- **MPI_Send** sends the data stored in the buffer pointed by *buf*.
- This buffer consists of consecutive entries of the type specified by the parameter datatype.
- The number of entries in the buffer is given by the parameter *count*.

Note that for all C datatypes, an equivalent MPI datatype is provided.

- MPI allows two additional datatypes that are not part of the C language.
- These are *MPI_BYTE* and *MPI_PACKED*.
    - *MPI_BYTE* corresponds to a byte (8 bits)
    - *MPI_PACKED* corresponds to a collection of data items that has been created by packing non-contiguous data.
- Note that the length of the message in **MPI_Send**, as well as in other MPI routines, is specified *in terms of the number of entries* being sent and *not in terms of the number of bytes.*
- Specifying the length in terms of the number of entries has the advantage of making the MPI code *portable*,
- since the number of bytes used to store various datatypes can be different for different architectures.

Table 2: Correspondence between the datatypes supported by MPI and those supported by C.

MPI Datatype	C Datatype
MPI_CHAR	signed char
MPI_SHORT	signed short int
MPI_INT	signed int
MPI_LONG	signed long int
MPI_UNSIGNED_CHAR	unsigned char
MPI_UNSIGNED_SHORT	unsigned short int
MPI_UNSIGNED	unsigned int
MPI_UNSIGNED_LONG	unsigned long int
MPI_FLOAT	float
MPI_DOUBLE	double
MPI_LONG_DOUBLE	long double
MPI_BYTE	
MPI_PACKED	

- The destination of the message sent by **MPI_Send** is uniquely specified by
  - *dest* argument. This argument is the *rank* of the destination process in the communication domain specified by the communicator *comm*.
  - *comm* argument.
- Each message has an integer-valued *tag* associated with it.
- This is used to distinguish different types of messages.
- The message-tag can take values ranging from zero up to the MPI defined constant *MPI_TAG_UB* (implementation specific, at least 32767).
- **MPI_Recv** receives a message sent by a process whose *rank* is given by the *source* in the communication domain specified by the *comm* argument.
- The *tag* of the sent message must be that specified by the tag argument.
- If there are many messages with identical tag from the same process, then any one of these messages is received.

- MPI allows specification of wild card arguments for both source and tag.
  - If source is set to *MPI_ANY_SOURCE*, then any process of the communication domain can be the source of the message.
  - Similarly, if tag is set to *MPI_ANY_TAG*, then messages with any tag are accepted.
- The received message is stored in continuous locations in the buffer pointed to by *buf*.
- The *count* and *datatype* arguments of **MPI_Recv** are used to specify the length of the supplied buffer.
- The received message should be of length equal to or less than this length.
- This allows the receiving process to not know the exact size of the message being sent.
- If the received message is larger than the supplied buffer, then an overflow error will occur, and the routine will return the error *MPI_ERR_TRUNCATE*.
- After a message has been received, the status variable can be used to get information about the **MPI_Recv** operation.
- In C, status is stored using the *MPI_Status* data-structure.
- This is implemented as a structure with three fields, as follows:

```
typedef struct MPI_Status {
  int MPI_SOURCE;
  int MPI_TAG;
  int MPI_ERROR;
};
```

- *MPI_SOURCE* and *MPI_TAG* store the source and the tag of the received message.
- They are particularly useful when *MPI_ANY_SOURCE* and *MPI_ANY_TAG* are used for the source and tag arguments.
- *MPI_ERROR* stores the error-code of the received message.

- The status argument also returns information about the length of the received message.

- This information is not directly accessible from the status variable, but it can be retrieved by calling the **MPI_Get_count** function.

- The calling sequence:

```
int MPI_Get_count(MPI_Status *status,
                  MPI_Datatype datatype,
                  int *count)
```

- **MPI_Get_count** takes as arguments the status returned by **MPI_Recv** and the type of the received data in *datatype*, and returns the number of entries that were actually received in the *count* variable.

- The **MPI_Recv** returns only after the requested message has been received and copied into the buffer.

- That is, **MPI_Recv** is a **blocking** receive operation.

- However, MPI allows two different implementations for **MPI_Send**.

1 **MPI_Send** returns only after the corresponding **MPI_Recv** have been issued and the message has been sent to the receiver.

2 **MPI_Send** first copies the message into a **buffer** and then returns, without waiting for the corresponding **MPI_Recv** to be executed.

- In either implementation, the buffer that is pointed by the *buf* argument of **MPI_Send** *can be safely reused and overwritten.*

- MPI programs must be able to run correctly regardless of which of the two methods is used for implementing **MPI_Send**.

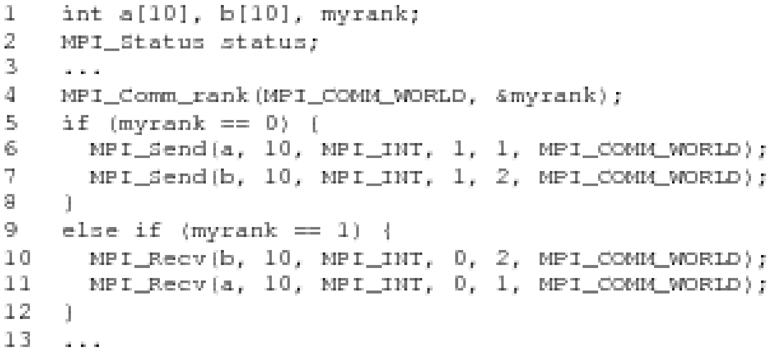
- Such programs are called safe.

- In writing safe MPI programs, sometimes it is helpful to forget about the alternate implementation of **MPI_Send** and just think of it as being a blocking send operation.

1.5 Avoiding Deadlocks

- The semantics of **MPI_Send** and **MPI_Recv** place some restrictions on how we can mix and match send and receive operations.

- Consider the following not complete code in which process 0 sends two messages with different tags to process 1, and process 1 receives them in the reverse order.



```
int a[10], b[10], myrank;
MPI_Status status;
...
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
if (myrank == 0) {
  MPI_Send(a, 10, MPI_INT, 1, 1, MPI_COMM_WORLD);
  MPI_Send(b, 10, MPI_INT, 1, 2, MPI_COMM_WORLD);
}
else if (myrank == 1) {
  MPI_Recv(b, 10, MPI_INT, 0, 2, MPI_COMM_WORLD);
  MPI_Recv(a, 10, MPI_INT, 0, 1, MPI_COMM_WORLD);
}
...
```

- If **MPI_Send** is implemented using buffering, then this code will run correctly (if sufficient buffer space is available).

- However, if **MPI_Send** is implemented by blocking until the matching receive has been issued, then neither of the two processes will be able to proceed.

- This code fragment is not safe, as its behavior is implementation dependent.

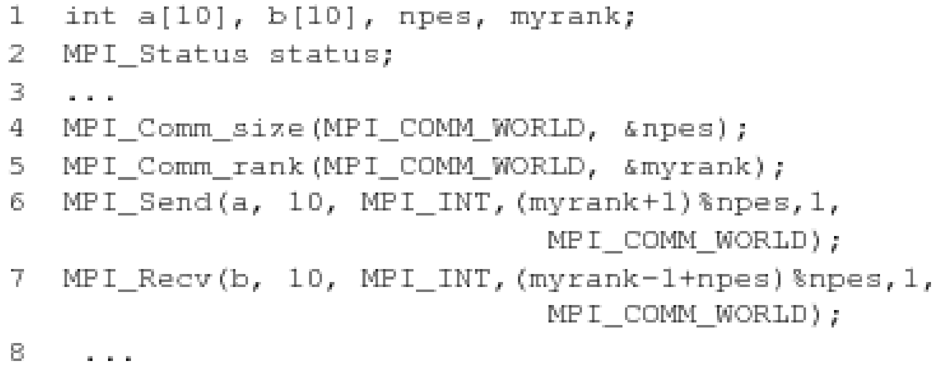
- It is up to the programmer to ensure that his or her program will run correctly on any MPI implementation.

- The problem in this program can be corrected by matching the order in which the send and receive operations are issued.

- Similar deadlock situations can also occur when a process sends a message to itself.

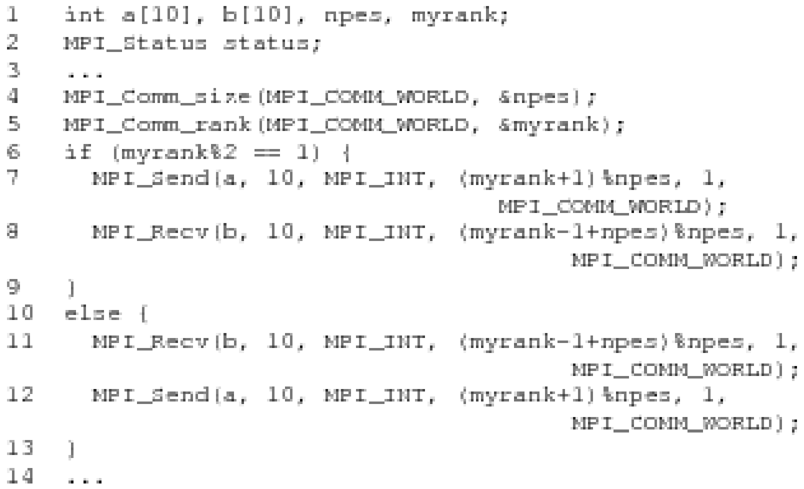
- Improper use of **MPI_Send** and **MPI_Recv** can also lead to deadlocks in situations when each processor needs to send and receive a message in a circular fashion.

- Consider the following not complete code, in which
  - process i sends a message to process $i+1$ (modulo the number of processes),
  - process i receives a message from process $i-1$ (module the number of processes).



```
int a[10], b[10], npes, myrank;
MPI_Status status;
...
MPI_Comm_size(MPI_COMM_WORLD, &npes);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
MPI_Send(a, 10, MPI_INT,(myrank+1)%npes,1,
                              MPI_COMM_WORLD);
MPI_Recv(b, 10, MPI_INT,(myrank-1+npes)%npes,1,
                              MPI_COMM_WORLD);
 ...
```

- When **MPI_Send** is implemented using buffering, the program will work correctly,
  - since every call to **MPI_Send** will get buffered, allowing the call of the **MPI_Recv** to be performed, which will transfer the required data.
- However, if **MPI_Send** blocks until the matching receive has been issued,
  - all processes will enter an infinite wait state, waiting for the neighbouring process to issue a **MPI_Recv** operation.
- Note that the deadlock still remains even when we have only two processes.
- Thus, when pairs of processes need to exchange data, the above method leads to an unsafe program.
- The above example can be made safe, by rewriting it as follows:
- This new implementation partitions the processes into two groups.
- One consists of the odd-numbered processes and the other of the even-numbered processes.



```
int a[10], b[10], npes, myrank;
MPI_Status status;
...
MPI_Comm_size(MPI_COMM_WORLD, &npes);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
if (myrank%2 == 1) {
  MPI_Send(a, 10, MPI_INT, (myrank+1)%npes, 1,
                              MPI_COMM_WORLD);
  MPI_Recv(b, 10, MPI_INT, (myrank-1+npes)%npes, 1,
                                   MPI_COMM_WORLD);
}
else {
  MPI_Recv(b, 10, MPI_INT, (myrank-1+npes)%npes, 1,
                                   MPI_COMM_WORLD);
  MPI_Send(a, 10, MPI_INT, (myrank+1)%npes, 1,
                                   MPI_COMM_WORLD);
}
...
```

1.6 Sending and Receiving Messages Simultaneously

- The above communication pattern appears frequently in many message-passing programs,
- For this reason MPI provides the **MPI_Sendrecv** function that both sends and receives a message.
- **MPI_Sendrecv** does not suffer from the circular deadlock problems of **MPI_Send** and **MPI_Recv**.
- You can think of **MPI_Sendrecv** as allowing data to travel for both send and receive simultaneously.
- The calling sequence of **MPI_Sendrecv** is as the following:

```
int MPI_Sendrecv(void *sendbuf, int sendcount,
        MPI_Datatype senddatatype, int dest,
                             int sendtag,
        void *recvbuf, int recvcount,
        MPI_Datatype recvdatatype, int source,
                   int recvtag, MPI_Comm comm,
        MPI_Status *status)
```

- The arguments of **MPI_Sendrecv** are essentially the combination of the arguments of **MPI_Send** and **MPI_Recv**.
- The send and receive buffers must be disjoint, and the source and destination of the messages can be the same or different.

- The safe version of our previous example using **MPI_Sendrecv** is as the following;

```
int a[10], b[10], npes, myrank;
MPI_Status status;
...
MPI_Comm_size(MPI_COMM_WORLD, &npes);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
MPI_SendRecv(a, 10, MPI_INT, (myrank+1)%npes, 1,
             b, 10, MPI_INT, (myrank-1+npes)%npes, 1,
             MPI_COMM_WORLD, &status);
...
```

- In many programs, the requirement for the send and receive buffers of **MPI_Sendrecv** be disjoint may force us to use a temporary buffer.
- This increases the amount of memory required by the program and also increases the overall run time due to the extra copy.
- This problem can be solved by using that **MPI_Sendrecv_replace** MPI function.
- This function performs a blocking send and receive, but it uses a single buffer for both the send and receive operation.
- That is, the received data replaces the data that was sent out of the buffer.