CHAPTER 6

Programming Using the Message-Passing Paradigm

Numerous programming languages and libraries have been developed for explicit parallel programming. These differ in their view of the address space that they make available to the programmer, the degree of synchronization imposed on concurrent activities, and the multiplicity of programs. The *message-passing programming paradigm* is one of the oldest and most widely used approaches for programming parallel computers. Its roots can be traced back in the early days of parallel processing and its wide-spread adoption can be attributed to the fact that it imposes minimal requirements on the underlying hardware.

In this chapter, we first describe some of the basic concepts of the message-passing programming paradigm and then explore various message-passing programming techniques using the standard and widely-used Message Passing Interface.

6.1 Principles of Message-Passing Programming

There are two key attributes that characterize the message-passing programming paradigm. The first is that it assumes a partitioned address space and the second is that it supports only explicit parallelization.

The logical view of a machine supporting the message-passing paradigm consists of p processes, each with its own exclusive address space. Instances of such a view come naturally from clustered workstations and non-shared address space multicomputers. There are two immediate implications of a partitioned address space. First, each data element must belong to one of the partitions of the space; hence, data must be explicitly partitioned

and placed. This adds complexity to programming, but encourages locality of access that is critical for achieving high performance on non-UMA architecture, since a processor can access its local data much faster than non-local data on such architectures. The second implication is that all interactions (read-only or read/write) require cooperation of two processes – the process that has the data and the process that wants to access the data. This requirement for cooperation adds a great deal of complexity for a number of reasons. The process that has the data must participate in the interaction even if it has no logical connection to the events at the requesting process. In certain circumstances, this requirement leads to unnatural programs. In particular, for dynamic and/or unstructured interactions the complexity of the code written for this type of paradigm can be very high for this reason. However, a primary advantage of explicit two-way interactions is that the programmer is fully aware of all the costs of non-local interactions, and is more likely to think about algorithms (and mappings) that minimize interactions. Another major advantage of this type of programming paradigm is that it can be efficiently implemented on a wide variety of architectures.

The message-passing programming paradigm requires that the parallelism is coded explicitly by the programmer. That is, the programmer is responsible for analyzing the underlying serial algorithm/application and identifying ways by which he or she can decompose the computations and extract concurrency. As a result, programming using the messagepassing paradigm tends to be hard and intellectually demanding. However, on the other hand, properly written message-passing programs can often achieve very high performance and scale to a very large number of processes.

Structure of Message-Passing Programs Message-passing programs are often written using the *asynchronous* or *loosely synchronous* paradigms. In the asynchronous paradigm, all concurrent tasks execute asynchronously. This makes it possible to implement any parallel algorithm. However, such programs can be harder to reason about, and can have non-deterministic behavior due to race conditions. Loosely synchronous programs are a good compromise between these two extremes. In such programs, tasks or subsets of tasks synchronize to perform interactions. However, between these interactions, tasks execute completely asynchronously. Since the interaction happens synchronously, it is still quite easy to reason about the program. Many of the known parallel algorithms can be naturally implemented using loosely synchronous programs.

In its most general form, the message-passing paradigm supports execution of a different program on each of the *p* processes. This provides the ultimate flexibility in parallel programming, but makes the job of writing parallel programs effectively unscalable. For this reason, most message-passing programs are written using the *single program multiple data* (SPMD) approach. In SPMD programs the code executed by different processes is identical except for a small number of processes (e.g., the "root" process). This does not mean that the processes work in lock-step. In an extreme case, even in an SPMD program, each process could execute a different code (the program contains a large case statement with code for each process). But except for this degenerate case, most processes execute the same code. SPMD programs can be loosely synchronous or completely asynchronous.

6.2 The Building Blocks: Send and Receive Operations

Since interactions are accomplished by sending and receiving messages, the basic operations in the message-passing programming paradigm are send and receive. In their simplest form, the prototypes of these operations are defined as follows:

```
send(void *sendbuf, int nelems, int dest)
receive(void *recvbuf, int nelems, int source)
```

The sendbuf points to a buffer that stores the data to be sent, recvbuf points to a buffer that stores the data to be received, nelems is the number of data units to be sent and received, dest is the identifier of the process that receives the data, and source is the identifier of the process that sends the data.

However, to stop at this point would be grossly simplifying the programming and performance ramifications of how these functions are implemented. To motivate the need for further investigation, let us start with a simple example of a process sending a piece of data to another process as illustrated in the following code-fragment:

1	PO	P1
2		
3	a = 100;	receive(&a, 1, 0)
4	send(&a, 1, 1);	printf("%d n", a);
5	a = 0;	

In this simple example, process P0 sends a message to process P1 which receives and prints the message. The important thing to note is that process P0 changes the value of a to 0 immediately following the send. The semantics of the send operation require that the value received by process P1 must be 100 as opposed to 0. That is, the value of a at the time of the send operation must be the value that is received by process P1.

It may seem that it is quite straightforward to ensure the semantics of the send and receive operations. However, based on how the send and receive operations are implemented this may not be the case. Most message passing platforms have additional hardware support for sending and receiving messages. They may support DMA (direct memory access) and asynchronous message transfer using network interface hardware. Network interfaces allow the transfer of messages from buffer memory to desired location without CPU intervention. Similarly, DMA allows copying of data from one memory location to another (e.g., communication buffers) without CPU support (once they have been programmed). As a result, if the send operation programs the communication hardware and returns before the communication operation has been accomplished, process P1 might receive the value 0 in a instead of 100!

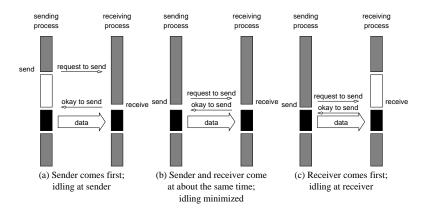


Figure 6.1 Handshake for a blocking non-buffered send/receive operation. It is easy to see that in cases where sender and receiver do not reach communication point at similar times, there can be considerable idling overheads.

While this is undesirable, there are in fact reasons for supporting such send operations for performance reasons. In the rest of this section, we will discuss send and receive operations in the context of such a hardware environment, and motivate various implementation details and message-passing protocols that help in ensuring the semantics of the send and receive operations.

6.2.1 Blocking Message Passing Operations

A simple solution to the dilemma presented in the code fragment above is for the send operation to return only when it is semantically safe to do so. Note that this is not the same as saying that the send operation returns only after the receiver has received the data. It simply means that the sending operation blocks until it can guarantee that the semantics will not be violated on return irrespective of what happens in the program subsequently. There are two mechanisms by which this can be achieved.

Blocking Non-Buffered Send/Receive

In the first case, the send operation does not return until the matching receive has been encountered at the receiving process. When this happens, the message is sent and the send operation returns upon completion of the communication operation. Typically, this process involves a handshake between the sending and receiving processes. The sending process sends a request to communicate to the receiving process. When the receiving process encounters the target receive, it responds to the request. The sending process upon receiving this response initiates a transfer operation. The operation is illustrated in Figure 6.1. Since there are no buffers used at either sending or receiving ends, this is also referred to as a *non-buffered blocking operation*.

Idling Overheads in Blocking Non-Buffered Operations In Figure 6.1, we illustrate three scenarios in which the send is reached before the receive is posted, the send and receive are posted around the same time, and the receive is posted before the send is reached. In cases (a) and (c), we notice that there is considerable idling at the sending and receiving process. It is also clear from the figures that a blocking non-buffered protocol is suitable when the send and receive are posted at roughly the same time. However, in an asynchronous environment, this may be impossible to predict. This idling overhead is one of the major drawbacks of this protocol.

Deadlocks in Blocking Non-Buffered Operations Consider the following simple exchange of messages that can lead to a deadlock:

1	PO	P1
2		
3	send(&a, 1, 1);	send(&a, 1, 0);
4	receive(&b, 1, 1);	receive(&b, 1, 0);

The code fragment makes the values of a available to both processes P0 and P1. However, if the send and receive operations are implemented using a blocking non-buffered protocol, the send at P0 waits for the matching receive at P1 whereas the send at process P1 waits for the corresponding receive at P0, resulting in an infinite wait.

As can be inferred, deadlocks are very easy in blocking protocols and care must be taken to break cyclic waits of the nature outlined. In the above example, this can be corrected by replacing the operation sequence of one of the processes by a receive and a send as opposed to the other way around. This often makes the code more cumbersome and buggy.

Blocking Buffered Send/Receive

A simple solution to the idling and deadlocking problem outlined above is to rely on buffers at the sending and receiving ends. We start with a simple case in which the sender has a buffer pre-allocated for communicating messages. On encountering a send operation, the sender simply copies the data into the designated buffer and returns after the copy operation has been completed. The sender process can now continue with the program knowing that any changes to the data will not impact program semantics. The actual communication can be accomplished in many ways depending on the available hardware resources. If the hardware supports asynchronous communication (independent of the CPU), then a network transfer can be initiated after the message has been copied into the buffer. Note that at the receiving end, the data cannot be stored directly at the target location since this would violate program semantics. Instead, the data is copied into a buffer at the receiver as well. When the receiving process encounters a receive operation, it checks to see if the message is available in its receive buffer. If so, the data is copied into the target location. This operation is illustrated in Figure 6.2(a).

In the protocol illustrated above, buffers are used at both sender and receiver and communication is handled by dedicated hardware. Sometimes machines do not have such

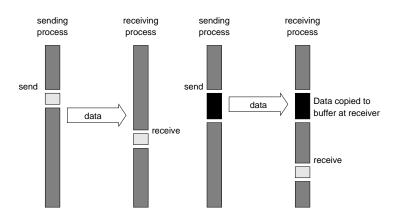


Figure 6.2 Blocking buffered transfer protocols: (a) in the presence of communication hardware with buffers at send and receive ends; and (b) in the absence of communication hardware, sender interrupts receiver and deposits data in buffer at receiver end.

communication hardware. In this case, some of the overhead can be saved by buffering only on one side. For example, on encountering a send operation, the sender interrupts the receiver, both processes participate in a communication operation and the message is deposited in a buffer at the receiver end. When the receiver eventually encounters a receive operation, the message is copied from the buffer into the target location. This protocol is illustrated in Figure 6.2(b). It is not difficult to conceive a protocol in which the buffering is done only at the sender and the receiver initiates a transfer by interrupting the sender.

It is easy to see that buffered protocols alleviate idling overheads at the cost of adding buffer management overheads. In general, if the parallel program is highly synchronous (i.e., sends and receives are posted around the same time), non-buffered sends may perform better than buffered sends. However, in general applications, this is not the case and buffered sends are desirable unless buffer capacity becomes an issue.

Example 6.1 Impact of finite buffers in message passing Consider the following code fragment:

```
1
       P0
                                            Ρ1
2
3
       for (i = 0; i < 1000; i++) {
                                            for (i = 0; i < 1000; i++) {
4
         produce data(&a);
                                              receive(&a, 1, 0);
5
         send(&a, 1, 1);
                                              consume_data(&a);
6
       }
                                            }
```

In this code fragment, process P0 produces 1000 data items and process P1 consumes them. However, if process P1 was slow getting to this loop, process P0 might have sent all of its data. If there is enough buffer space, then both processes can proceed; however, if the buffer is not sufficient (i.e., buffer overflow), the sender

would have to be blocked until some of the corresponding receive operations had been posted, thus freeing up buffer space. This can often lead to unforeseen overheads and performance degradation. In general, it is a good idea to write programs that have bounded buffer requirements.

Deadlocks in Buffered Send and Receive Operations While buffering alleviates many of the deadlock situations, it is still possible to write code that deadlocks. This is due to the fact that as in the non-buffered case, receive calls are always blocking (to ensure semantic consistency). Thus, a simple code fragment such as the following deadlocks since both processes wait to receive data but nobody sends it.

Once again, such circular waits have to be broken. However, deadlocks are caused only by waits on receive operations in this case.

6.2.2 Non-Blocking Message Passing Operations

In blocking protocols, the overhead of guaranteeing semantic correctness was paid in the form of idling (non-buffered) or buffer management (buffered). Often, it is possible to require the programmer to ensure semantic correctness and provide a fast send/receive operation that incurs little overhead. This class of non-blocking protocols returns from the send or receive operation before it is semantically safe to do so. Consequently, the user must be careful not to alter data that may be potentially participating in a communication operation. Non-blocking operations are generally accompanied by a check-status operation, which indicates whether the semantics of a previously initiated transfer may be violated or not. Upon return from a non-blocking send or receive operation, the process is free to perform any computation that does not depend upon the completion of the operation. Later in the program, the process can check whether or not the non-blocking operation has completed, and, if necessary, wait for its completion.

As illustrated in Figure 6.3, non-blocking operations can themselves be buffered or non-buffered. In the non-buffered case, a process wishing to send data to another simply posts a pending message and returns to the user program. The program can then do other useful work. At some point in the future, when the corresponding receive is posted, the communication operation is initiated. When this operation is completed, the check-status operation indicates that it is safe for the programmer to touch this data. This transfer is indicated in Figure 6.4(a).

Comparing Figures 6.4(a) and 6.1(a), it is easy to see that the idling time when the process is waiting for the corresponding receive in a blocking operation can now be utilized for computation, provided it does not update the data being sent. This alleviates the major bottleneck associated with the former at the expense of some program restructuring.

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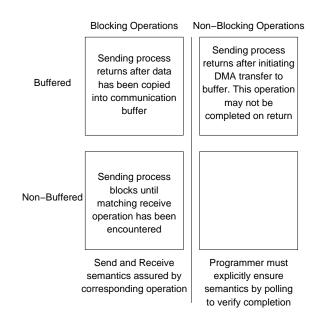


Figure 6.3 Space of possible protocols for send and receive operations.

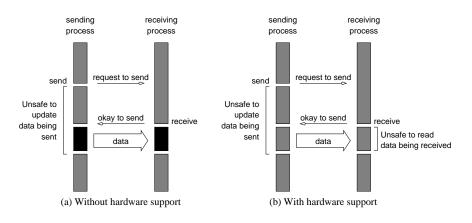
The benefits of non-blocking operations are further enhanced by the presence of dedicated communication hardware. This is illustrated in Figure 6.4(b). In this case, the communication overhead can be almost entirely masked by non-blocking operations. In this case, however, the data being received is unsafe for the duration of the receive operation.

Non-blocking operations can also be used with a buffered protocol. In this case, the sender initiates a DMA operation and returns immediately. The data becomes safe the moment the DMA operation has been completed. At the receiving end, the receive operation initiates a transfer from the sender's buffer to the receiver's target location. Using buffers with non-blocking operation has the effect of reducing the time during which the data is unsafe.

Typical message-passing libraries such as Message Passing Interface (MPI) and Parallel Virtual Machine (PVM) implement both blocking and non-blocking operations. Blocking operations facilitate safe and easier programming and non-blocking operations are useful for performance optimization by masking communication overhead. One must, however, be careful using non-blocking protocols since errors can result from unsafe access to data that is in the process of being communicated.

6.3 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. Since



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Figure 6.4 Non-blocking non-buffered send and receive operations (a) in absence of communication hardware; (b) in presence of communication hardware.

message-passing is the natural programming paradigm for these machines, this resulted in the development of many different message-passing libraries. In fact, message-passing became the modern-age form of assembly language, in which every hardware vendor provided its own library, that 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 reengineering to port a message-passing program from one library to another.

The message-passing interface, or MPI as it is commonly known, was created to essentially solve this problem. MPI defines a standard library for message-passing that can be used to develop portable message-passing programs using either C or Fortran. The MPI standard defines both the syntax as well as the semantics of a core set of library routines that are very useful in writing message-passing programs. MPI was developed by a group of researchers from academia and industry, and has enjoyed wide support by almost all the hardware vendors. Vendor implementations of MPI are available on almost all commercial parallel computers.

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 the six routines shown in Table 6.1. These routines are used to initialize and terminate the MPI library, to get information about the parallel computing environment, and to send and receive messages.

In this section we describe these routines as well as some basic concepts that are essential in writing correct and efficient message-passing programs using MPI.

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.

 Table 6.1
 The minimal set of MPI routines.

6.3.1 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, and 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. Both MPI_Init and MPI_Finalize must be called by all the processes, otherwise MPI's behavior will be undefined. The exact calling sequences of these two routines for C are as follows:

```
int MPI_Init(int *argc, char ***argv)
int MPI Finalize()
```

The arguments argc and argv of MPI_Init are the command-line arguments of the C program. An MPI implementation is expected to remove from the argv array any command-line arguments that should be processed by the implementation before returning back to the program, and to decrement argc accordingly. Thus, command-line processing should be performed only after MPI_Init has been called. Upon successful execution, MPI_Init and MPI_Finalize return MPI_SUCCESS; otherwise they return an implementation-defined error code.

The bindings and calling sequences of these two functions are illustrative of the naming practices and argument conventions followed by MPI. All MPI routines, data-types, and constants are prefixed by "MPI_". The return code for successful completion is MPI_SUCCESS. This and other MPI constants and data-structures are defined for C in the file "mpi.h". This header file must be included in each MPI program.

6.3.2 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 and they uniquely identify the processes participating in the message transfer operation. Note that each process can belong to many different (possibly overlapping) communication domains.

The communicator is used to define a set of processes that can communicate with each other. This set of processes form a *communication domain*. 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 in the parallel execution. However, in many cases we want to perform communicator 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. How to create and use such communicators is described at a later point in this chapter. For now, it suffices to use MPI_COMM_WORLD as the communicator argument to all the MPI functions that require a communicator.

6.3.3 Getting Information

The MPI_Comm_size and MPI_Comm_rank functions are used to determine the number of processes and the label of the calling process, respectively. 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)
```

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 using the MPI_Comm_rank function that takes two arguments: the communicator and an integer variable rank. Up on return, the variable rank stores the rank of the process. Note that each process that calls either one of these functions must belong in the supplied communicator, otherwise an error will occur.

Example 6.2 Hello World

We can use the four MPI functions just described to write a program that prints out a "Hello World" message from each processor.

```
1 #include <mpi.h>
2
3 main(int argc, char *argv[])
4 {
5 int npes, myrank;
6
7 MPI_Init(&argc, &argv);
8 MPI_Comm_size(MPI_COMM_WORLD, &npes);
```

```
9 MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
10 printf("From process %d out of %d, Hello World!\n",
11 myrank, npes);
12 MPI_Finalize();
13 }
```

6.3.4 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:

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. The correspondence between MPI datatypes and those provided by C is shown in Table 6.2. Note that for all C datatypes, an equivalent MPI datatype is provided. However, 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) and 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.

The destination of the message sent by MPI_Send is uniquely specified by the dest and comm arguments. The dest argument is the rank of the destination process in the communication domain specified by the communicator comm. Each message has an integervalued 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. Even though the value of MPI_TAG_UB is implementation specific, it is at least 32,767.

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 wildcard 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

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	

 Table 6.2
 Correspondence between the datatypes supported by MPI and those supported by C.

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 datastructure. 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 of this function is as follows:

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. In the first implementation, MPI_Send returns only after the corresponding MPI_Recv have been issued and the message has been sent to the receiver. In the second implementation, 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.

Avoiding Deadlocks The semantics of MPI_Send and MPI_Recv place some restrictions on how we can mix and match send and receive operations. For example, consider the following piece of code in which process 0 sends two messages with different tags to process 1, and process 1 receives them in the reverse order.

```
1
   int a[10], b[10], myrank;
2 MPI Status status;
3
4 MPI Comm rank(MPI COMM WORLD, &myrank);
5
  if (myrank == 0) {
     MPI Send(a, 10, MPI INT, 1, 1, MPI COMM WORLD);
6
     MPI Send(b, 10, MPI INT, 1, 2, MPI COMM WORLD);
7
8
  }
9
  else if (myrank == 1) {
10
    MPI Recv(b, 10, MPI INT, 0, 2, MPI COMM WORLD);
11
     MPI_Recv(a, 10, MPI_INT, 0, 1, MPI_COMM_WORLD);
12 }
13 ...
```

If MPI_Send is implemented using buffering, then this code will run correctly provided that 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 is because process zero (i.e., myrank == 0) will wait until process one issues the matching MPI_Recv (i.e., the one with tag equal to 1), and at the same time process one will wait until process zero performs the matching MPI_Send (i.e., the one with tag equal to 2). 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. Even though this is legal, its behavior is implementation dependent and must be avoided. 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 piece of code, in which process *i* sends a message to process i + 1 (modulo the number of processes) and receives a message from process i - 1 (module the number of processes).

```
1 int a[10], b[10], npes, myrank;
2 MPI_Status status;
3 ...
4 MPI_Comm_size(MPI_COMM_WORLD, &npes);
5 MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
6 MPI_Send(a, 10, MPI_INT, (myrank+1)%npes, 1, MPI_COMM_WORLD);
7 MPI_Recv(b, 10, MPI_INT, (myrank-1+npes)%npes, 1, MPI_COMM_WORLD);
8 ...
```

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 neighboring 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:

```
int a[10], b[10], npes, myrank;
2
  MPI_Status status;
3
   . . .
4
  MPI Comm size (MPI COMM WORLD, &npes);
5 MPI Comm rank (MPI COMM WORLD, &myrank);
6
  if (myrank%2 == 1) {
7
    MPI_Send(a, 10, MPI_INT, (myrank+1)%npes, 1, MPI_COMM_WORLD);
8
    MPI Recv(b, 10, MPI INT, (myrank-1+npes)%npes, 1, MPI COMM WORLD);
 }
9
10 else {
11
   MPI Recv(b, 10, MPI INT, (myrank-1+npes)%npes, 1, MPI COMM WORLD);
12
    MPI Send(a, 10, MPI INT, (myrank+1)%npes, 1, MPI COMM WORLD);
13 }
14
   . . .
```

This new implementation partitions the processes into two groups. One consists of the oddnumbered processes and the other of the even-numbered processes. The odd-numbered processes perform a send followed by a receive, and the even-numbered processes perform a receive followed by a send. Thus, when an odd-numbered process calls MPI_Send, the target process (which has an even number) will call MPI_Recv to receive that message, before attempting to send its own message.

Sending and Receiving Messages Simultaneously The above communication pattern appears frequently in many message-passing programs, and 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 the following:

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 earlier example using MPI Sendrecv is as follows.

```
1 int a[10], b[10], npes, myrank;
2 MPI_Status status;
3 ...
4 MPI_Comm_size(MPI_COMM_WORLD, &npes);
5 MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
6 MPI_SendRecv(a, 10, MPI_INT, (myrank+1)%npes, 1,
7 b, 10, MPI_INT, (myrank+1+npes)%npes, 1,
8 MPI_COMM_WORLD, &status);
9 ...
```

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. The calling sequence of this function is the following:

Note that both the send and receive operations must transfer data of the same datatype.

6.3.5 Example: Odd-Even Sort

We will now use the MPI functions described in the previous sections to write a complete message-passing program that will sort a list of numbers using the odd-even sorting algorithm. Recall from Section 9.3.1 that the odd-even sorting algorithm sorts a sequence of n elements using p processes in a total of p phases. During each of these phases, the odd-or even-numbered processes perform a compare-split step with their right neighbors. The MPI program for performing the odd-even sort in parallel is shown in Program 6.1. To simplify the presentation, this program assumes that n is divisible by p.

```
Program 6.1 Odd-Even Sorting
```

```
#include <stdlib.h>
 1
    #include <mpi.h> /* Include MPI's header file */
 2
 3
 4
    main(int argc, char *argv[])
 5
                         /* The total number of elements to be sorted */
 6
       int n;
                         /* The total number of processes */
 7
       int npes;
                         /* The rank of the calling process */
 8
       int myrank;
                         /* The local number of elements, and the array that stores them */
 9
       int nlocal;
                         /* The array that stores the local elements */
10
       int *elmnts;
       int *relmnts; /* The array that stores the received elements */
11
                       /* The rank of the process during odd-phase communication */
12
       int oddrank;
       int evenrank; /* The rank of the process during even-phase communication */
13
                        /* Working space during the compare-split operation */
14
       int *wspace;
15
       int i;
      MPI Status status;
16
17
18
       /* Initialize MPI and get system information */
19
       MPI_Init(&argc, &argv);
       MPI Comm size (MPI COMM WORLD, &npes);
20
21
       MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
22
      n = atoi(argv[1]);
nlocal = n/npes; /* Compute the number of elements to be stored locally. */
23
24
25
       /* Allocate memory for the various arrays */
26
27
       elmnts = (int *)malloc(nlocal*sizeof(int));
28
       relmnts = (int *)malloc(nlocal*sizeof(int));
29
       wspace = (int *)malloc(nlocal*sizeof(int));
30
       /* Fill-in the elmnts array with random elements */
31
       srandom(mvrank);
32
33
       for (i=0; i<nlocal; i++)</pre>
34
         elmnts[i] = random();
35
36
       /* Sort the local elements using the built-in quicksort routine */
37
       gsort(elmnts, nlocal, sizeof(int), IncOrder);
38
       /* Determine the rank of the processors that myrank needs to communicate during the */
39
40
       /* odd and even phases of the algorithm */
41
       if (myrank%2 == 0) {
42
         oddrank = myrank-1;
43
         evenrank = myrank+1;
44
       else {
45
46
         oddrank = myrank+1;
47
         evenrank = myrank-1;
       }
48
49
       /* Set the ranks of the processors at the end of the linear */
50
       if (oddrank == -1 || oddrank == npes)
51
52
         oddrank = MPI PROC NULL;
       if (evenrank == -1 || evenrank == npes)
53
         evenrank = MPI_PROC_NULL;
54
55
56
       /* Get into the main loop of the odd-even sorting algorithm */
      for (i=0; i<npes-1; i++) {
    if (i%2 == 1) /* Odd phase */</pre>
57
58
           MPI Sendrecv(elmnts, nlocal, MPI INT, oddrank, 1, relmnts,
59
```

```
60
                nlocal, MPI INT, oddrank, 1, MPI COMM WORLD, &status);
 61
         else /* Even phase */
 62
           MPI_Sendrecv(elmnts, nlocal, MPI_INT, evenrank, 1, relmnts,
 63
                nlocal, MPI INT, evenrank, 1, MPI COMM WORLD, &status);
 64
 65
         CompareSplit(nlocal, elmnts, relmnts, wspace,
 66
                        myrank < status.MPI SOURCE);</pre>
 67
       }
 68
 69
       free(elmnts); free(relmnts); free(wspace);
 70
       MPI Finalize();
 71 }
 72
 73
    /* This is the CompareSplit function */
 74
    CompareSplit(int nlocal, int *elmnts, int *relmnts, int *wspace,
 75
                    int keepsmall)
 76
     {
 77
       int i, j, k;
 78
 79
       for (i=0; i<nlocal; i++)</pre>
 80
         wspace[i] = elmnts[i]; /* Copy the elmnts array into the wspace array */
 81
       if (keepsmall) { /* Keep the nlocal smaller elements */
 82
 83
         for (i=j=k=0; k<nlocal; k++) {</pre>
            if (j == nlocal || (i < nlocal && wspace[i] < relmnts[j]))</pre>
 84
 85
              elmnts[k] = wspace[i++];
 86
            else
 87
              elmnts[k] = relmnts[j++];
         }
 88
 89
       }
       else { /* Keep the nlocal larger elements */
 90
 91
         for (i=k=nlocal-1, j=nlocal-1; k>=0; k--) {
 92
            if (j == 0 || (i >= 0 && wspace[i] >= relmnts[j]))
              elmnts[k] = wspace[i--];
 93
 94
            else
 95
              elmnts[k] = relmnts[j--];
 96
          }
 97
       }
 98
     }
 99
100 /* The IncOrder function that is called by qsort is defined as follows */
     int IncOrder(const void *e1, const void *e2)
101
102
     {
       return (*((int *)e1) - *((int *)e2));
103
104
```

6.4 Topologies and Embedding

MPI views the processes as being arranged in a one-dimensional topology and uses a linear ordering to number the processes. However, in many parallel programs, processes are naturally arranged in higher-dimensional topologies (e.g., two- or three-dimensional). In such programs, both the computation and the set of interacting processes are naturally identified by their coordinates in that topology. For example, in a parallel program in which the processes are arranged in a two-dimensional topology, process (i, j) may need to send message to (or receive message from) process (k, l). To implement these programs

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0	1	2	3		0	4	8	12		0	3	4	5		0	1	3	2
4	5	6	7		1	5	9	13		1	- 2	7	6		4	5	7	6
8	9	10	11		2	6	10	14		14	13	8	9		12	13	15	14
12	13	14	15		3	7	11	15		15	12	1.1	10		8	9	11	10
(a	(a) Row-major mapping		(b) Column-major mapping			(c) Space–filling curve mapping			1	(d) Hypercube mapping								

Figure 6.5 Different ways to map a set of processes to a two-dimensional grid. (a) and (b) show a row- and column-wise mapping of these processes, (c) shows a mapping that follows a space-filling curve (dotted line), and (d) shows a mapping in which neighboring processes are directly connected in a hypercube.

in MPI, we need to map each MPI process to a process in that higher-dimensional topology.

Many such mappings are possible. Figure 6.5 illustrates some possible mappings of eight MPI processes onto a 4×4 two-dimensional topology. For example, for the mapping shown in Figure 6.5(a), an MPI process with rank *rank* corresponds to process (*row*, *col*) in the grid such that *row* = *rank*/4 and *col* = *rank*%4 (where '%' is C's module operator). As an illustration, the process with rank 7 is mapped to process (1, 3) in the grid.

In general, the goodness of a mapping is determined by the pattern of interaction among the processes in the higher-dimensional topology, the connectivity of physical processors, and the mapping of MPI processes to physical processors. For example, consider a program that uses a two-dimensional topology and each process needs to communicate with its neighboring processes along the x and y directions of this topology. Now, if the processors of the underlying parallel system are connected using a hypercube interconnection network, then the mapping shown in Figure 6.5(d) is better, since neighboring processes in the grid are also neighboring processors in the hypercube topology.

However, the mechanism used by MPI to assign ranks to the processes in a communication domain does not use any information about the interconnection network, making it impossible to perform topology embeddings in an intelligent manner. Furthermore, even if we had that information, we will need to specify different mappings for different interconnection networks, diminishing the architecture independent advantages of MPI. A better approach is to let the library itself compute the most appropriate embedding of a given topology to the processors of the underlying parallel computer. This is exactly the approach facilitated by MPI. MPI provides a set of routines that allows the programmer to arrange the processes in different topologies without having to explicitly specify how these processes are mapped onto the processors. It is up to the MPI library to find the most appropriate mapping that reduces the cost of sending and receiving messages.

6.4.1 Creating and Using Cartesian Topologies

MPI provides routines that allow the specification of virtual process topologies of arbitrary connectivity in terms of a graph. Each node in the graph corresponds to a process and two

nodes are connected if they communicate with each other. Graphs of processes can be used to specify any desired topology. However, most commonly used topologies in message-passing programs are one-, two-, or higher-dimensional grids, that are also referred to as *Cartesian topologies*. For this reason, MPI provides a set of specialized routines for specifying and manipulating this type of multi-dimensional grid topologies.

MPI's function for describing Cartesian topologies is called MPI_Cart_create. Its calling sequence is as follows.

This function takes the group of processes that belong to the communicator comm old and creates a virtual process topology. The topology information is attached to a new communicator comm cart that is created by MPI Cart create. Any subsequent MPI routines that want to take advantage of this new Cartesian topology must use comm cart as the communicator argument. Note that all the processes that belong to the comm old communicator must call this function. The shape and properties of the topology are specified by the arguments ndims, dims, and periods. The argument ndims specifies the number of dimensions of the topology. The array dims specify the size along each dimension of the topology. The *i*th element of this array stores the size of the *i*th dimension of the topology. The array periods is used to specify whether or not the topology has wraparound connections. In particular, if periods [i] is true (non-zero in C), then the topology has wraparound connections along dimension i, otherwise it does not. Finally, the argument reorder is used to determine if the processes in the new group (i.e., communicator) are to be reordered or not. If reorder is false, then the rank of each process in the new group is identical to its rank in the old group. Otherwise, MPI Cart create may reorder the processes if that leads to a better embedding of the virtual topology onto the parallel computer. If the total number of processes specified in the dims array is smaller than the number of processes in the communicator specified by comm old, then some processes will not be part of the Cartesian topology. For this set of processes, the value of comm cart will be set to MPI COMM NULL (an MPI defined constant). Note that it will result in an error if the total number of processes specified by dims is greater than the number of processes in the comm old communicator.

Process Naming When a Cartesian topology is used, each process is better identified by its coordinates in this topology. However, all MPI functions that we described for sending and receiving messages require that the source and the destination of each message be specified using the rank of the process. For this reason, MPI provides two functions, MPI_Cart_rank and MPI_Cart_coord, for performing coordinate-to-rank and rank-to-coordinate translations, respectively. The calling sequences of these routines are the following:

The MPI_Cart_rank takes the coordinates of the process as argument in the coords array and returns its rank in rank. The MPI_Cart_coords takes the rank of the process rank and returns its Cartesian coordinates in the array coords, of length maxdims. Note that maxdims should be at least as large as the number of dimensions in the Cartesian topology specified by the communicator comm cart.

Frequently, the communication performed among processes in a Cartesian topology is that of shifting data along a dimension of the topology. MPI provides the function MPI_Cart_shift, that can be used to compute the rank of the source and destination processes for such operation. The calling sequence of this function is the following:

The direction of the shift is specified in the dir argument, and is one of the dimensions of the topology. The size of the shift step is specified in the s_step argument. The computed ranks are returned in rank_source and rank_dest. If the Cartesian topology was created with wraparound connections (i.e., the periods [dir] entry was set to true), then the shift wraps around. Otherwise, a MPI_PROC_NULL value is returned for rank source and/or rank dest for those processes that are outside the topology.

6.4.2 Example: Cannon's Matrix-Matrix Multiplication

To illustrate how the various topology functions are used we will implement Cannon's algorithm for multiplying two matrices *A* and *B*, described in Section 8.2.2. Cannon's algorithm views the processes as being arranged in a virtual two-dimensional square array. It uses this array to distribute the matrices *A*, *B*, and the result matrix *C* in a block fashion. That is, if $n \times n$ is the size of each matrix and *p* is the total number of process, then each matrix is divided into square blocks of size $n/\sqrt{p} \times n/\sqrt{p}$ (assuming that *p* is a perfect square). Now, process $P_{i,j}$ in the grid is assigned the $A_{i,j}$, $B_{i,j}$, and $C_{i,j}$ blocks of each matrix. After an initial data alignment phase, the algorithm proceeds in \sqrt{p} steps. In each step, every process multiplies the locally available blocks of matrices *A* and *B*, and then sends the block of *A* to the leftward process, and the block of *B* to the upward process.

Program 6.2 shows the MPI function that implements Cannon's algorithm. The dimension of the matrices is supplied in the parameter n. The parameters a, b, and c point to the locally stored portions of the matrices A, B, and C, respectively. The size of these arrays is $n/\sqrt{p} \times n/\sqrt{p}$, where p is the number of processes. This routine assumes that p is a perfect square and that n is a multiple of \sqrt{p} . The parameter comm stores the communicator describing the processes that call the MatrixMatrixMultiply function. Note that the remaining programs in this chapter will be provided in the form of a function, as opposed to complete stand-alone programs.

```
Program 6.2 Cannon's Matrix-Matrix Multiplication with MPI's Topologies
```

```
1 MatrixMatrixMultiply(int n, double *a, double *b, double *c,
 2
                            MPI Comm comm)
 3
    {
      int i;
 4
 5
      int nlocal;
 6
      int npes, dims[2], periods[2];
      int myrank, my2drank, mycoords[2];
 7
 8
      int uprank, downrank, leftrank, rightrank, coords[2];
 9
      int shiftsource, shiftdest;
10
      MPI_Status status;
      MPI_Comm comm_2d;
11
12
      /* Get the communicator related information */
13
      MPI_Comm_size(comm, &npes);
14
15
      MPI Comm rank (comm, &myrank);
16
17
      /* Set up the Cartesian topology */
18
      dims[0] = dims[1] = sqrt(npes);
19
      /* Set the periods for wraparound connections */
20
21
      periods[0] = periods[1] = 1;
22
      /* Create the Cartesian topology, with rank reordering */
23
24
      MPI_Cart_create(comm, 2, dims, periods, 1, &comm_2d);
25
      /* Get the rank and coordinates with respect to the new topology */
26
27
      MPI_Comm_rank(comm_2d, &my2drank);
      MPI_Cart_coords(comm_2d, my2drank, 2, mycoords);
28
29
30
      /* Compute ranks of the up and left shifts */
      MPI_Cart_shift(comm_2d, 0, -1, &rightrank, &leftrank);
MPI_Cart_shift(comm_2d, 1, -1, &downrank, &uprank);
31
32
33
34
      /* Determine the dimension of the local matrix block */
35
      nlocal = n/dims[0];
36
37
      /* Perform the initial matrix alignment. First for A and then for B */
38
      MPI_Cart_shift(comm_2d, 0, -mycoords[0], &shiftsource, &shiftdest);
      MPI_Sendrecv_replace(a, nlocal*nlocal, MPI_DOUBLE, shiftdest,
39
40
           1, shiftsource, 1, comm_2d, &status);
41
      MPI_Cart_shift(comm_2d, 1, -mycoords[1], &shiftsource, &shiftdest);
42
43
      MPI Sendrecv replace(b, nlocal*nlocal, MPI DOUBLE,
           shiftdest, 1, shiftsource, 1, comm_2d, &status);
44
45
46
      /* Get into the main computation loop */
47
      for (i=0; i<dims[0]; i++) {
        MatrixMultiply(nlocal, a, b, c); /* c = c + a*b*/
48
49
50
        /* Shift matrix a left by one */
51
        MPI_Sendrecv_replace(a, nlocal*nlocal, MPI_DOUBLE,
52
             leftrank, 1, rightrank, 1, comm 2d, &status);
53
        /* Shift matrix b up by one */
54
        MPI_Sendrecv_replace(b, nlocal*nlocal, MPI_DOUBLE,
55
             uprank, 1, downrank, 1, comm_2d, &status);
56
57
      }
58
      /* Restore the original distribution of a and b */
59
```

```
60
      MPI Cart shift(comm 2d, 0, +mycoords[0], &shiftsource, &shiftdest);
61
      MPI Sendrecv replace(a, nlocal*nlocal, MPI DOUBLE,
          shiftdest, 1, shiftsource, 1, comm_2d, &status);
62
63
64
      MPI Cart shift(comm 2d, 1, +mycoords[1], &shiftsource, &shiftdest);
      MPI_Sendrecv_replace(b, nlocal*nlocal, MPI_DOUBLE,
65
66
          shiftdest, 1, shiftsource, 1, comm 2d, &status);
67
     MPI Comm free (&comm 2d); /* Free up communicator */
68
   }
69
70
   /* This function performs a serial matrix-matrix multiplication c = a^*b^*/
71
72
   MatrixMultiply(int n, double *a, double *b, double *c)
73
74
      int i, j, k;
75
      for (i=0; i<n; i++)</pre>
76
77
        for (j=0; j<n; j++)</pre>
          for (k=0; k<n; k++)
78
79
            c[i*n+j] += a[i*n+k]*b[k*n+j];
80
   }
```

6.5 Overlapping Communication with Computation

The MPI programs we developed so far used blocking send and receive operations whenever they needed to perform point-to-point communication. Recall that a blocking send operation remains blocked until the message has been copied out of the send buffer (either into a system buffer at the source process or sent to the destination process). Similarly, a blocking receive operation returns only after the message has been received and copied into the receive buffer. For example, consider Cannon's matrix-matrix multiplication program described in Program 6.2. During each iteration of its main computational loop (lines 47– 57), it first computes the matrix multiplication of the sub-matrices stored in a and b, and then shifts the blocks of a and b, using MPI Sendrecv replace which blocks until the specified matrix block has been sent and received by the corresponding processes. In each iteration, each process spends $O(n^3/p^{1.5})$ time for performing the matrix-matrix multiplication and $O(n^2/p)$ time for shifting the blocks of matrices A and B. Now, since the blocks of matrices A and B do not change as they are shifted among the processors, it will be preferable if we can overlap the transmission of these blocks with the computation for the matrix-matrix multiplication, as many recent distributed-memory parallel computers have dedicated communication controllers that can perform the transmission of messages without interrupting the CPUs.

6.5.1 Non-Blocking Communication Operations

In order to overlap communication with computation, MPI provides a pair of functions for performing non-blocking send and receive operations. These functions are MPI_Isend and MPI Irecv. MPI Isend starts a send operation but does not complete, that is, it

returns before the data is copied out of the buffer. Similarly, MPI_Irecv starts a receive operation but returns before the data has been received and copied into the buffer. With the support of appropriate hardware, the transmission and reception of messages can proceed concurrently with the computations performed by the program upon the return of the above functions.

However, at a later point in the program, a process that has started a non-blocking send or receive operation must make sure that this operation has completed before it proceeds with its computations. This is because a process that has started a non-blocking send operation may want to overwrite the buffer that stores the data that are being sent, or a process that has started a non-blocking receive operation may want to use the data it requested. To check the completion of non-blocking send and receive operations, MPI provides a pair of functions MPI_Test and MPI_Wait. The first tests whether or not a non-blocking operation has finished and the second waits (i.e., gets blocked) until a nonblocking operation actually finishes.

The calling sequences of MPI Isend and MPI Irecv are the following:

Note that these functions have similar arguments as the corresponding blocking send and receive functions. The main difference is that they take an additional argument request. MPI_Isend and MPI_Irecv functions allocate a *request object* and return a pointer to it in the request variable. This request object is used as an argument in the MPI_Test and MPI_Wait functions to identify the operation whose status we want to query or to wait for its completion.

Note that the MPI_Irecv function does not take a status argument similar to the blocking receive function, but the status information associated with the receive operation is returned by the MPI Test and MPI Wait functions.

int MPI_Test(MPI_Request *request, int *flag, MPI_Status *status)
int MPI_Wait(MPI_Request *request, MPI_Status *status)

MPI_Test tests whether or not the non-blocking send or receive operation identified by its request has finished. It returns flag = {true} (non-zero value in C) if it completed, otherwise it returns {false} (a zero value in C). In the case that the nonblocking operation has finished, the request object pointed to by request is deallocated and request is set to MPI_REQUEST_NULL. Also the status object is set to contain information about the operation. If the operation has not finished, request is not modified and the value of the status object is undefined. The MPI_Wait function blocks until the non-blocking operation identified by request completes. In that case it deallocates the request object, sets it to MPI_REQUEST_NULL, and returns information about the completed operation in the status object. For the cases that the programmer wants to explicitly deallocate a request object, MPI provides the following function.

int MPI_Request_free(MPI_Request *request)

Note that the deallocation of the request object does not have any effect on the associated non-blocking send or receive operation. That is, if it has not yet completed it will proceed until its completion. Hence, one must be careful before explicitly deallocating a request object, since without it, we cannot check whether or not the non-blocking operation has completed.

A non-blocking communication operation can be matched with a corresponding blocking operation. For example, a process can send a message using a non-blocking send operation and this message can be received by the other process using a blocking receive operation.

Avoiding Deadlocks By using non-blocking communication operations we can remove most of the deadlocks associated with their blocking counterparts. For example, as we discussed in Section 6.3 the following piece of code is not safe.

```
1
   int a[10], b[10], myrank;
2
  MPI Status status;
3
4
  MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
5
   if (myrank == 0) {
6
    MPI_Send(a, 10, MPI_INT, 1, 1, MPI_COMM_WORLD);
7
    MPI_Send(b, 10, MPI_INT, 1, 2, MPI_COMM_WORLD);
8
  }
9
  else if (myrank == 1) {
    MPI Recv(b, 10, MPI INT, 0, 2, &status, MPI COMM WORLD);
10
     MPI Recv(a, 10, MPI INT, 0, 1, &status, MPI COMM WORLD);
11
12 }
13 ...
```

However, if we replace either the send or receive operations with their non-blocking counterparts, then the code will be safe, and will correctly run on any MPI implementation.

```
int a[10], b[10], myrank;
1
2 MPI Status status;
3 MPI_Request requests [2];
4
   . . .
5
   MPI Comm rank (MPI COMM WORLD, &myrank);
6
   if (myrank == 0) {
7
    MPI Send(a, 10, MPI INT, 1, 1, MPI COMM WORLD);
8
    MPI_Send(b, 10, MPI_INT, 1, 2, MPI_COMM_WORLD);
9
   }
10 else if (myrank == 1) {
   MPI_Irecv(b, 10, MPI_INT, 0, 2, &requests[0], MPI_COMM_WORLD);
11
12
     MPI Irecv(a, 10, MPI INT, 0, 1, &requests[1], MPI COMM WORLD);
13 }
14 ...
```

This example also illustrates that the non-blocking operations started by any process can finish in any order depending on the transmission or reception of the corresponding messages. For example, the second receive operation will finish before the first does.

Example: Cannon's Matrix-Matrix Multiplication (Using Non-Blocking Operations)

Program 6.3 shows the MPI program that implements Cannon's algorithm using nonblocking send and receive operations. The various parameters are identical to those of Program 6.2.

Program 6.3 Non-Blocking Cannon's Matrix-Matrix Multiplication

```
1
   MatrixMatrixMultiply_NonBlocking(int n, double *a, double *b,
                                         double *c, MPI_Comm comm)
 2
 3
      int i, j, nlocal;
 4
 5
      double *a_buffers[2], *b_buffers[2];
 6
      int npes, dims[2], periods[2];
 7
      int myrank, my2drank, mycoords[2];
 8
      int uprank, downrank, leftrank, rightrank, coords[2];
 9
      int shiftsource, shiftdest;
10
      MPI_Status status;
11
      MPI Comm comm 2d;
12
      MPI_Request reqs[4];
13
      /* Get the communicator related information */
14
15
      MPI Comm size(comm, &npes);
      MPI Comm rank(comm, &myrank);
16
17
18
      /* Set up the Cartesian topology */
      dims[0] = dims[1] = sqrt(npes);
19
20
21
      /* Set the periods for wraparound connections */
22
      periods[0] = periods[1] = 1;
23
24
      /* Create the Cartesian topology, with rank reordering */
25
      MPI Cart create(comm, 2, dims, periods, 1, &comm 2d);
26
27
      /* Get the rank and coordinates with respect to the new topology */
28
      MPI Comm rank(comm 2d, &my2drank);
      MPI_Cart_coords(comm_2d, my2drank, 2, mycoords);
29
30
31
      /* Compute ranks of the up and left shifts */
      MPI_Cart_shift(comm_2d, 0, -1, &rightrank, &leftrank);
32
33
      MPI_Cart_shift(comm_2d, 1, -1, &downrank, &uprank);
34
      /* Determine the dimension of the local matrix block */
35
36
      nlocal = n/dims[0];
37
      /* Setup the a_buffers and b_buffers arrays */
38
39
      a buffers[0] = a;
40
      a buffers[1] = (double *)malloc(nlocal*nlocal*sizeof(double));
41
      b buffers[0] = b;
42
      b buffers[1] = (double *)malloc(nlocal*nlocal*sizeof(double));
43
      /* Perform the initial matrix alignment. First for A and then for B */
44
```

```
45
     MPI Cart shift(comm 2d, 0, -mycoords[0], &shiftsource, &shiftdest);
     MPI Sendrecv replace(a buffers[0], nlocal*nlocal, MPI_DOUBLE,
46
          shiftdest, 1, shiftsource, 1, comm_2d, &status);
47
48
49
     MPI Cart shift(comm 2d, 1, -mycoords[1], &shiftsource, &shiftdest);
     MPI_Sendrecv_replace(b_buffers[0], nlocal*nlocal, MPI_DOUBLE,
50
51
          shiftdest, 1, shiftsource, 1, comm 2d, &status);
52
53
     /* Get into the main computation loop */
54
     for (i=0; i<dims[0]; i++)</pre>
55
       MPI Isend(a buffers[i%2], nlocal*nlocal, MPI DOUBLE,
56
            leftrank, 1, comm_2d, &reqs[0]);
        MPI_Isend(b_buffers[i%2], nlocal*nlocal, MPI DOUBLE,
57
            uprank, 1, comm 2d, &reqs[1]);
58
59
       MPI_Irecv(a_buffers[(i+1)%2], nlocal*nlocal, MPI_DOUBLE,
60
            rightrank, 1, comm_2d, &reqs[2]);
       MPI Irecv(b buffers[(i+1)%2], nlocal*nlocal, MPI DOUBLE,
61
            downrank, 1, comm 2d, &reqs[3]);
62
63
       /* c = c + a*b*/
64
65
       MatrixMultiply(nlocal, a buffers[i%2], b buffers[i%2], c);
66
67
        for (j=0; j<4; j++)
68
          MPI Wait(&regs[j], &status);
     }
69
70
      /* Restore the original distribution of a and b */
71
     MPI Cart_shift(comm_2d, 0, +mycoords[0], &shiftsource, &shiftdest);
72
73
     MPI Sendrecv replace(a buffers[i%2], nlocal*nlocal, MPI DOUBLE,
74
          shiftdest, 1, shiftsource, 1, comm 2d, &status);
75
76
     MPI_Cart_shift(comm_2d, 1, +mycoords[1], &shiftsource, &shiftdest);
     MPI Sendrecv replace (b buffers [i%2], nlocal*nlocal, MPI DOUBLE,
77
78
          shiftdest, 1, shiftsource, 1, comm 2d, &status);
79
80
     MPI Comm free (&comm 2d); /* Free up communicator */
81
82
      free(a_buffers[1]);
      free(b buffers[1]);
83
84 }
```

There are two main differences between the blocking program (Program 6.2) and this non-blocking one. The first difference is that the non-blocking program requires the use of the additional arrays $a_buffers$ and $b_buffers$, that are used as the buffer of the blocks of A and B that are being received while the computation involving the previous blocks is performed. The second difference is that in the main computational loop, it first starts the non-blocking send operations to send the locally stored blocks of A and B to the processes left and up the grid, and then starts the non-blocking receive operations to receive the blocks for the next iteration from the processes right and down the grid. Having initiated these four non-blocking operations, it proceeds to perform the matrix-matrix multiplication of the blocks it currently stores. Finally, before it proceeds to the next iteration, it uses MPI Wait to wait for the send and receive operations to complete.

Note that in order to overlap communication with computation we have to use two auxiliary arrays – one for A and one for B. This is to ensure that incoming messages never overwrite the blocks of A and B that are used in the computation, which proceeds concurrently with the data transfer. Thus, increased performance (by overlapping communication with computation) comes at the expense of increased memory requirements. This is a trade-off that is often made in message-passing programs, since communication overheads can be quite high for loosely coupled distributed memory parallel computers.

6.6 Collective Communication and Computation Operations

MPI provides an extensive set of functions for performing many commonly used collective communication operations. In particular, the majority of the basic communication operations described in Chapter 4 are supported by MPI. All of the collective communication functions provided by MPI take as an argument a communicator that defines the group of processes that participate in the collective operation. All the processes that belong to this communicator participate in the operation, and all of them must call the collective communication function. Even though collective communication operations do not act like barriers (i.e., it is possible for a processor to go past its call for the collective communication operation even before other processes have reached it), it acts like a virtual synchronization step in the following sense: the parallel program should be written such that it behaves correctly even if a global synchronization is performed before and after the collective call. Since the operations are virtually synchronous, they do not require tags. In some of the collective functions data is required to be sent from a single process (source-process) or to be received by a single process (target-process). In these functions, the source- or targetprocess is one of the arguments supplied to the routines. All the processes in the group (i.e., communicator) must specify the same source- or target-process. For most collective communication operations, MPI provides two different variants. The first transfers equalsize data to or from each process, and the second transfers data that can be of different sizes.

6.6.1 Barrier

The barrier synchronization operation is performed in MPI using the MPI_Barrier function.

int MPI_Barrier(MPI_Comm comm)

The only argument of MPI_Barrier is the communicator that defines the group of processes that are synchronized. The call to MPI_Barrier returns only after all the processes in the group have called this function.

6.6.2 Broadcast

The one-to-all broadcast operation described in Section 4.1 is performed in MPI using the MPI Bcast function.

 Table 6.3
 Predefined reduction operations.

Operation	Meaning	Datatypes
MPI_MAX	Maximum	C integers and floating point
MPI_MIN	Minimum	C integers and floating point
MPI_SUM	Sum	C integers and floating point
MPI_PROD	Product	C integers and floating point
MPI_LAND	Logical AND	C integers
MPI_BAND	Bit-wise AND	C integers and byte
MPI_LOR	Logical OR	C integers
MPI_BOR	Bit-wise OR	C integers and byte
MPI_LXOR	Logical XOR	C integers
MPI_BXOR	Bit-wise XOR	C integers and byte
MPI_MAXLOC	max-min value-location	Data-pairs
MPI_MINLOC	min-min value-location	Data-pairs

MPI_Bcast sends the data stored in the buffer buf of process source to all the other processes in the group. The data received by each process is stored in the buffer buf. The data that is broadcast consist of count entries of type datatype. The amount of data sent by the source process must be equal to the amount of data that is being received by each process; i.e., the count and datatype fields must match on all processes.

6.6.3 Reduction

The all-to-one reduction operation described in Section 4.1 is performed in MPI using the MPI Reduce function.

MPI_Reduce combines the elements stored in the buffer sendbuf of each process in the group, using the operation specified in op, and returns the combined values in the buffer recvbuf of the process with rank target. Both the sendbuf and recvbuf must have the same number of count items of type datatype. Note that all processes must provide a recvbuf array, even if they are not the *target* of the reduction operation. When count is more than one, then the combine operation is applied element-wise on each entry of the sequence. All the processes must call MPI_Reduce with the same value for count, datatype, op, target, and comm.

MPI provides a list of predefined operations that can be used to combine the elements stored in sendbuf. MPI also allows programmers to define their own operations, which is

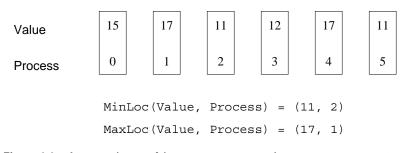


Figure 6.6 An example use of the MPI_MINLOC and MPI_MAXLOC operators.

not covered in this book. The predefined operations are shown in Table 6.3. For example, in order to compute the maximum of the elements stored in sendbuf, the MPI_MAX value must be used for the op argument. Not all of these operations can be applied to all possible data-types supported by MPI. For example, a bit-wise OR operation (i.e., *op* = MPI_BOR) is not defined for real-valued data-types such as MPI_FLOAT and MPI_REAL. The last column of Table 6.3 shows the various data-types that can be used with each operation.

The operation MPI_MAXLOC combines pairs of values (v_i, l_i) and returns the pair (v, l) such that v is the maximum among all v_i 's and l is the smallest among all l_i 's such that $v = v_i$. Similarly, MPI_MINLOC combines pairs of values and returns the pair (v, l) such that v is the minimum among all v_i 's and l is the smallest among all l_i 's such that $v = v_i$. One possible application of MPI_MAXLOC or MPI_MINLOC is to compute the maximum or minimum of a list of numbers each residing on a different process and also the rank of the first process that stores this maximum or minimum, as illustrated in Figure 6.6. Since both MPI_MAXLOC and MPI_MINLOC require datatypes that correspond to pairs of values, a new set of MPI datatypes have been defined as shown in Table 6.4. In C, these datatypes are implemented as structures containing the corresponding types.

When the result of the reduction operation is needed by all the processes, MPI provides the MPI_Allreduce operation that returns the result to all the processes. This function provides the functionality of the all-reduce operation described in Section 4.3.

MPI Datatype	C Datatype
MPI_2INT	pair of ints
MPI_SHORT_INT	short and int
MPI_LONG_INT	long and int
MPI_LONG_DOUBLE_INT	long double and int
MPI_FLOAT_INT	float and int
MPI_DOUBLE_INT	double and int

 Table 6.4
 MPI datatypes for data-pairs used with the MPI_MAXLOC and MPI_MINLOC reduction operations.

Note that there is no target argument since all processes receive the result of the operation.

6.6.4 Prefix

The prefix-sum operation described in Section 4.3 is performed in MPI using the MPI_Scan function.

MPI_Scan performs a prefix reduction of the data stored in the buffer sendbuf at each process and returns the result in the buffer recvbuf. The receive buffer of the process with rank i will store, at the end of the operation, the reduction of the send buffers of the processes whose ranks range from 0 up to and including i. The type of supported operations (i.e., op) as well as the restrictions on the various arguments of MPI_Scan are the same as those for the reduction operation MPI_Reduce.

6.6.5 Gather

The gather operation described in Section 4.4 is performed in MPI using the MPI_Gather function.

Each process, including the target process, sends the data stored in the array sendbuf to the target process. As a result, if p is the number of processors in the communication comm, the target process receives a total of p buffers. The data is stored in the array recvbuf of the target process, in a rank order. That is, the data from process with rank iare stored in the recvbuf starting at location i * sendcount (assuming that the array recvbuf is of the same type as recvdatatype).

The data sent by each process must be of the same size and type. That is, MPI_Gather must be called with the sendcount and senddatatype arguments having the same values at each process. The information about the receive buffer, its length and type applies only for the target process and is ignored for all the other processes. The argument recvcount specifies the number of elements received by each process and not the total number of elements it receives. So, recvcount must be the same as sendcount and their datatypes must be matching.

MPI also provides the MPI_Allgather function in which the data are gathered to all the processes and not only at the target process.

The meanings of the various parameters are similar to those for MPI_Gather; however, each process must now supply a recvbuf array that will store the gathered data.

In addition to the above versions of the gather operation, in which the sizes of the arrays sent by each process are the same, MPI also provides versions in which the size of the arrays can be different. MPI refers to these operations as the *vector* variants. The vector variants of the MPI_Gather and MPI_Allgather operations are provided by the functions MPI Gatherv and MPI Allgatherv, respectively.

These functions allow a different number of data elements to be sent by each process by replacing the recvcount parameter with the array recvcounts. The amount of data sent by process *i* is equal to recvcounts [i]. Note that the size of recvcounts is equal to the size of the communicator comm. The array parameter displs, which is also of the same size, is used to determine where in recvbuf the data sent by each process will be stored. In particular, the data sent by process *i* are stored in recvbuf starting at location displs[i]. Note that, as opposed to the non-vector variants, the sendcount parameter can be different processes.

6.6.6 Scatter

The scatter operation described in Section 4.4 is performed in MPI using the $MPI_Scatter$ function.

The source process sends a different part of the send buffer sendbuf to each processes, including itself. The data that are received are stored in recvbuf. Process ireceives sendcount contiguous elements of type senddatatype starting from the i * sendcount location of the sendbuf of the source process (assuming that sendbuf is of the same type as senddatatype). MPI_Scatter must be called by all the processes with the same values for the sendcount, senddatatype, recvcount, recvdatatype, source, and comm arguments. Note again that sendcount is the number of elements sent to each individual process.

Similarly to the gather operation, MPI provides a vector variant of the scatter operation, called MPI_Scatterv, that allows different amounts of data to be sent to different processes.

As we can see, the parameter sendcount has been replaced by the array sendcounts that determines the number of elements to be sent to each process. In particular, the target process sends sendcounts [i] elements to process *i*. Also, the array displs is used to determine where in sendbuf these elements will be sent from. In particular, if sendbuf is of the same type is senddatatype, the data sent to process *i* start at location displs[i] of array sendbuf. Both the sendcounts and displs arrays are of size equal to the number of processes in the communicator. Note that by appropriately setting the displs array we can use MPI_Scatterv to send overlapping regions of sendbuf.

6.6.7 All-to-All

The all-to-all personalized communication operation described in Section 4.5 is performed in MPI by using the MPI Alltoall function.

Each process sends a different portion of the sendbuf array to each other process, including itself. Each process sends to process i sendcount contiguous elements of type senddatatype starting from the i * sendcount location of its sendbuf array. The data that are received are stored in the recvbuf array. Each process receives from process i recvcount elements of type recvdatatype and stores them in its recvbuf array starting at location i * recvcount. MPI_Alltoall must be called by all the processes with the same values for the sendcount, senddatatype, recvcount, recvdatatype, and comm arguments. Note that sendcount and recvcount are the number of elements sent to, and received from, each individual process.

MPI also provides a vector variant of the all-to-all personalized communication operation called MPI_Alltoallv that allows different amounts of data to be sent to and received from each process.

The parameter sendcounts is used to specify the number of elements sent to each process, and the parameter sdispls is used to specify the location in sendbuf in which these elements are stored. In particular, each process sends to process *i*, starting at location sdispls[i] of the array sendbuf, sendcounts[i] contiguous elements. The parameter recvcounts is used to specify the number of elements received by each process, and the parameter rdispls is used to specify the location in recvbuf in which these elements are stored. In particular, each process receives from process *i* recvcounts[i] elements that are stored in contiguous locations of recvbuf starting at location rdispls[i]. MPI_Alltoallv must be called by all the processes with the same values for the senddatatype, recvdatatype, and comm arguments.

6.6.8 Example: One-Dimensional Matrix-Vector Multiplication

Our first message-passing program using collective communications will be to multiply a dense $n \times n$ matrix A with a vector b, i.e., x = Ab. As discussed in Section 8.1, one way of performing this multiplication in parallel is to have each process compute different portions of the product-vector x. In particular, each one of the p processes is responsible for computing n/p consecutive elements of x. This algorithm can be implemented in MPI by distributing the matrix A in a row-wise fashion, such that each process receives the n/p rows that correspond to the portion of the product-vector x it computes. Vector b is distributed in a fashion similar to x.

Program 6.4 shows the MPI program that uses a row-wise distribution of matrix A. The dimension of the matrices is supplied in the parameter n, the parameters a and b point to the locally stored portions of matrix A and vector b, respectively, and the parameter x points to the local portion of the output matrix-vector product. This program assumes that n is a multiple of the number of processors.

Program 6.4 Row-wise Matrix-Vector Multiplication

```
1
    RowMatrixVectorMultiply(int n, double *a, double *b, double *x,
 2
                                MPI Comm comm)
 3
    {
      int i, j;
 4
                             /* Number of locally stored rows of A */
 5
      int nlocal;
 6
      double *fb;
                             /* Will point to a buffer that stores the entire vector b */
 7
      int npes, myrank;
 8
      MPI_Status status;
 9
10
      /* Get information about the communicator */
      MPI_Comm_size(comm, &npes);
11
12
      MPI Comm rank(comm, &myrank);
13
      /* Allocate the memory that will store the entire vector b */
14
15
      fb = (double *)malloc(n*sizeof(double));
16
      nlocal = n/npes;
17
18
      /* Gather the entire vector b on each processor using MPI's ALLGATHER operation */
19
      MPI_Allgather(b, nlocal, MPI_DOUBLE, fb, nlocal, MPI_DOUBLE,
20
```

```
21
            comm);
22
      /* Perform the matrix-vector multiplication involving the locally stored submatrix */
23
24
      for (i=0; i<nlocal; i++) {</pre>
25
         x[i] = 0.0;
         for (j=0; j<n; j++)
26
           x[i] += a[i*n+j]*fb[j];
27
28
29
30
       free(fb);
31 }
```

An alternate way of computing x is to parallelize the task of performing the dot-product for each element of x. That is, for each element x_i , of vector x, all the processes will compute a part of it, and the result will be obtained by adding up these partial dot-products. This algorithm can be implemented in MPI by distributing matrix A in a column-wise fashion. Each process gets n/p consecutive columns of A, and the elements of vector b that correspond to these columns. Furthermore, at the end of the computation we want the product-vector x to be distributed in a fashion similar to vector b. Program 6.5 shows the MPI program that implements this column-wise distribution of the matrix.

Program 6.5 Column-wise Matrix-Vector Multiplication

```
1
    ColMatrixVectorMultiply(int n, double *a, double *b, double *x,
 2
                                MPI Comm comm)
 3
    {
      int i, j;
 4
 5
      int nlocal;
 6
      double *px;
 7
      double *fx:
 8
      int npes, myrank;
 9
      MPI Status status;
10
      /* Get identity and size information from the communicator */
11
      MPI Comm size(comm, &npes);
12
13
      MPI Comm rank (comm, &myrank);
14
15
      nlocal = n/npes;
16
      /* Allocate memory for arrays storing intermediate results. */
17
18
      px = (double *)malloc(n*sizeof(double));
      fx = (double *)malloc(n*sizeof(double));
19
20
21
      /* Compute the partial-dot products that correspond to the local columns of A. */
      for (\hat{i}=0; i< n; i++)^{-}
22
         px[i] = 0.0;
23
24
         for (j=0; j<nlocal; j++)</pre>
25
           px[i] += a[i*nlocal+j]*b[j];
26
27
28
      /* Sum-up the results by performing an element-wise reduction operation */
      MPI_Reduce(px, fx, n, MPI_DOUBLE, MPI_SUM, 0, comm);
29
30
      /* Redistribute fx in a fashion similar to that of vector b */
31
      MPI_Scatter(fx, nlocal, MPI_DOUBLE, x, nlocal, MPI_DOUBLE, 0,
32
33
           comm);
34
```

35 free(px); free(fx); 36 }

Comparing these two programs for performing matrix-vector multiplication we see that the row-wise version needs to perform only a MPI_Allgather operation whereas the column-wise program needs to perform a MPI_Reduce and a MPI_Scatter operation. In general, a row-wise distribution is preferable as it leads to small communication overhead (see Problem 6.6). However, many times, an application needs to compute not only Ax but also $A^T x$. In that case, the row-wise distribution can be used to compute Ax, but the computation of $A^T x$ requires the column-wise distribution (a row-wise distribution of A is a column-wise distribution of its transpose A^T). It is much cheaper to use the program for the column-wise distribution than to transpose the matrix and then use the row-wise program. We must also note that using a dual of the all-gather operation, it is possible to develop a parallel formulation for column-wise distribution that is as fast as the program using row-wise distribution (see Problem 6.7). However, this dual operation is not available in MPI.

6.6.9 Example: Single-Source Shortest-Path

Our second message-passing program that uses collective communication operations computes the shortest paths from a source-vertex s to all the other vertices in a graph using Dijkstra's single-source shortest-path algorithm described in Section 10.3. This program is shown in Program 6.6.

The parameter n stores the total number of vertices in the graph, and the parameter source stores the vertex from which we want to compute the single-source shortest path. The parameter wgt points to the locally stored portion of the weighted adjacency matrix of the graph. The parameter lengths points to a vector that will store the length of the shortest paths from source to the locally stored vertices. Finally, the parameter comm is the communicator to be used by the MPI routines. Note that this routine assumes that the number of vertices is a multiple of the number of processors.

Program 6.6 Dijkstra's Single-Source Shortest-Path

```
SingleSource(int n, int source, int *wgt, int *lengths, MPI_Comm comm)
1
2
3
      int i, j;
      int nlocal; /* The number of vertices stored locally */
4
      int *marker; /* Used to mark the vertices belonging to V_o */
5
      int firstvtx; /* The index number of the first vertex that is stored locally */
6
      int lastvtx; /* The index number of the last vertex that is stored locally */
7
8
      int u, udist;
9
      int lminpair[2], gminpair[2];
10
      int npes, myrank;
11
      MPI Status status;
12
13
      MPI Comm size(comm, &npes);
14
      MPI Comm rank(comm, &myrank);
```

```
16
      nlocal = n/npes;
      firstvtx = myrank*nlocal;
17
18
      lastvtx = firstvtx+nlocal-1;
19
       /* Set the initial distances from source to all the other vertices */
20
      for (j=0; j<nlocal; j++)</pre>
21
22
         lengths[j] = wgt[source*nlocal + j];
23
      /* This array is used to indicate if the shortest part to a vertex has been found or not. */
24
25
      /* if marker[v] is one, then the shortest path to v has been found, otherwise it has not. */
26
      marker = (int *)malloc(nlocal*sizeof(int));
       for (j=0; j<nlocal; j++)
27
28
         marker[j] = 1;
29
      /* The process that stores the source vertex, marks it as being seen */
30
31
      if (source >= firstvtx && source <= lastvtx)
         marker[source-firstvtx] = 0;
32
33
34
      /* The main loop of Dijkstra's algorithm */
35
       for (i=1; i<n; i++) {
         /* Step 1: Find the local vertex that is at the smallest distance from source */
36
37
         lminpair[0] = MAXINT; /* set it to an architecture dependent large number */
38
         lminpair[1] = -1;
         for (j=0; j<nlocal; j++) {
39
40
            if (marker[j] && lengths[j] < lminpair[0]) {</pre>
              lminpair[0] = lengths[j];
41
              lminpair[1] = firstvtx+j;
42
43
            }
         }
44
45
         /* Step 2: Compute the global minimum vertex, and insert it into V_c */
46
         MPI Allreduce(lminpair, gminpair, 1, MPI 2INT, MPI MINLOC,
47
48
              comm);
         udist = gminpair[0];
49
50
         u = gminpair[1];
51
         /* The process that stores the minimum vertex, marks it as being seen */
52
         if (u == lminpair[1])
53
           marker[u-firstvtx] = 0;
54
55
         /* Step 3: Update the distances given that u got inserted */
56
         for (j=0; j<nlocal; j++) {
57
            if (marker[j] && udist + wgt[u*nlocal+j] < lengths[j])</pre>
58
59
              lengths[j] = udist + wgt[u*nlocal+j];
60
         }
      }
61
62
63
      free(marker);
64
    }
```

15

The main computational loop of Dijkstra's parallel single-source shortest path algorithm performs three steps. First, each process finds the locally stored vertex in V_o that has the smallest distance from the source. Second, the vertex that has the smallest distance over all processes is determined, and it is included in V_c . Third, all processes update their distance arrays to reflect the inclusion of the new vertex in V_c .

The first step is performed by scanning the locally stored vertices in V_o and determining the one vertex v with the smaller *lengths*[v] value. The result of this computation is

stored in the array *lminpair*. In particular, *lminpair*[0] stores the distance of the vertex, and *lminpair*[1] stores the vertex itself. The reason for using this storage scheme will become clear when we consider the next step, in which we must compute the vertex that has the smallest overall distance from the source. We can find the overall shortest distance by performing a min-reduction on the distance values stored in *lminpair*[0]. However, in addition to the shortest distance, we also need to know the vertex that is at that shortest distance. For this reason, the appropriate reduction operation is the MPI_MINLOC which returns both the minimum as well as an index value associated with that minimum. Because of MPI_MINLOC we use the two-element array *lminpair* to store the distance as well as the vertex that achieves this distance. Also, because the result of the reduction operation is needed by all the processes to perform the third step, we use the MPI_Allreduce operation to perform the reduction. The result of the reduction is returned in the *gminpair* array. The third and final step during each iteration is performed by scanning the local vertices that belong in V_o and updating their shortest distances from the source vertex.

Avoiding Load Imbalances Program 6.6 assigns n/p consecutive columns of W to each processor and in each iteration it uses the MPI_MINLOC reduction operation to select the vertex v to be included in V_c . Recall that the MPI_MINLOC operation for the pairs (a, i) and (a, j) will return the one that has the smaller index (since both of them have the same value). Consequently, among the vertices that are equally close to the source vertex, it favors the smaller numbered vertices. This may lead to load imbalances, because vertices stored in lower-ranked processes will tend to be included in V_c faster than vertices in higher-ranked processes (especially when many vertices in V_o are at the same minimum distance from the source). Consequently, the size of the set V_o will be larger in higher-ranked processes, dominating the overall runtime.

One way of correcting this problem is to distribute the columns of W using a cyclic distribution. In this distribution process i gets every pth vertex starting from vertex i. This scheme also assigns n/p vertices to each process but these vertices have indices that span almost the entire graph. Consequently, the preference given to lower-numbered vertices by MPI MINLOC does not lead to load-imbalance problems.

6.6.10 Example: Sample Sort

The last problem requiring collective communications that we will consider is that of sorting a sequence A of n elements using the sample sort algorithm described in Section 9.5. The program is shown in Program 6.7.

The SampleSort function takes as input the sequence of elements stored at each process and returns a pointer to an array that stores the sorted sequence as well as the number of elements in this sequence. The elements of this SampleSort function are integers and they are sorted in increasing order. The total number of elements to be sorted is specified by the parameter n and a pointer to the array that stores the local portion of

these elements is specified by elmnts. On return, the parameter nsorted will store the number of elements in the returned sorted array. This routine assumes that n is a multiple of the number of processes.

Program 6.7 Samplesort

```
int *SampleSort(int n, int *elmnts, int *nsorted, MPI Comm comm)
 1
 2
    {
 3
      int i, j, nlocal, npes, myrank;
      int *sorted_elmnts, *splitters, *allpicks;
 4
 5
      int *scounts, *sdispls, *rcounts, *rdispls;
 6
      /* Get communicator-related information */
 7
 8
      MPI_Comm_size(comm, &npes);
 9
      MPI Comm rank (comm, &myrank);
10
11
      nlocal = n/npes;
12
13
      /* Allocate memory for the arrays that will store the splitters */
14
      splitters = (int *)malloc(npes*sizeof(int));
15
      allpicks = (int *)malloc(npes*(npes-1)*sizeof(int));
16
17
      /* Sort local array */
18
      qsort(elmnts, nlocal, sizeof(int), IncOrder);
19
      /* Select local npes-1 equally spaced elements */
20
21
      for (i=1; i<npes; i++)</pre>
22
         splitters[i-1] = elmnts[i*nlocal/npes];
23
      /* Gather the samples in the processors */
24
25
      MPI_Allgather(splitters, npes-1, MPI_INT, allpicks, npes-1,
26
           MPI INT, comm);
27
28
      /* sort these samples */
      qsort(allpicks, npes*(npes-1), sizeof(int), IncOrder);
29
30
31
      /* Select splitters */
      for (i=1; i<npes; i++)</pre>
32
         splitters[i-1] = allpicks[i*npes];
33
34
      splitters[npes-1] = MAXINT;
35
      /* Compute the number of elements that belong to each bucket */
36
37
      scounts = (int *)malloc(npes*sizeof(int));
      for (i=0; i<npes; i++)</pre>
38
39
         scounts[i] = 0;
40
      for (j=i=0; i<nlocal; i++) {</pre>
41
         if (elmnts[i] < splitters[j])</pre>
42
43
           scounts[j]++;
44
         else
           scounts[++j]++;
45
46
      }
47
      /* Determine the starting location of each bucket's elements in the elmnts array */
48
49
      sdispls = (int *)malloc(npes*sizeof(int));
50
      sdispls[0] = 0;
      for (i=1; i<npes; i++)</pre>
51
52
         sdispls[i] = sdispls[i-1]+scounts[i-1];
53
      /* Perform an all-to-all to inform the corresponding processes of the number of elements */
54
```

```
/* they are going to receive. This information is stored in rcounts array */
55
56
      rcounts = (int *)malloc(npes*sizeof(int));
57
      MPI_Alltoall(scounts, 1, MPI_INT, rcounts, 1, MPI_INT, comm);
58
59
      /* Based on rcounts determine where in the local array the data from each processor */
      /* will be stored. This array will store the received elements as well as the final */
60
      /* sorted sequence */
61
62
      rdispls = (int *)malloc(npes*sizeof(int));
63
      rdispls[0] = 0;
64
      for (i=1; i<npes; i++)</pre>
65
         rdispls[i] = rdispls[i-1]+rcounts[i-1];
66
67
       *nsorted = rdispls[npes-1]+rcounts[i-1];
68
      sorted elmnts = (int *)malloc((*nsorted)*sizeof(int));
69
70
      /* Each process sends and receives the corresponding elements, using the MPI_Alltoallv */
71
      /* operation. The arrays scounts and sdispls are used to specify the number of elements */
72
      /* to be sent and where these elements are stored, respectively. The arrays rcounts */
      /* and rdispls are used to specify the number of elements to be received, and where these */
73
74
      /* elements will be stored, respectively. */
75
      MPI_Alltoallv(elmnts, scounts, sdispls, MPI_INT, sorted_elmnts,
76
           rcounts, rdispls, MPI_INT, comm);
77
78
      /* Perform the final local sort */
79
      qsort(sorted_elmnts, *nsorted, sizeof(int), IncOrder);
80
      free(splitters); free(allpicks); free(scounts); free(sdispls);
81
82
      free(rcounts); free(rdispls);
83
84
      return sorted elmnts;
85 }
```

6.7 Groups and Communicators

In many parallel algorithms, communication operations need to be restricted to certain subsets of processes. MPI provides several mechanisms for partitioning the group of processes that belong to a communicator into subgroups each corresponding to a different communicator. A general method for partitioning a graph of processes is to use MPI_Comm_split that is defined as follows:

This function is a collective operation, and thus needs to be called by all the processes in the communicator comm. The function takes color and key as input parameters in addition to the communicator, and partitions the group of processes in the communicator comm into disjoint subgroups. Each subgroup contains all processes that have supplied the same value for the color parameter. Within each subgroup, the processes are ranked in the order defined by the value of the key parameter, with ties broken according to their rank in the old communicator (i.e., comm). A new communicator for each subgroup is returned in the newcomm parameter. Figure 6.7 shows an example of splitting a communicator using the MPI Comm split function. If each process called MPI Comm split using the

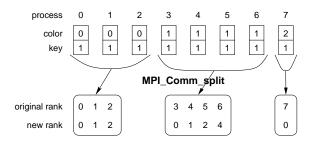


Figure 6.7 Using MPI_Comm_split to split a group of processes in a communicator into subgroups.

values of parameters color and key as shown in Figure 6.7, then three communicators will be created, containing processes $\{0, 1, 2\}$, $\{3, 4, 5, 6\}$, and $\{7\}$, respectively.

Splitting Cartesian Topologies In many parallel algorithms, processes are arranged in a virtual grid, and in different steps of the algorithm, communication needs to be restricted to a different subset of the grid. MPI provides a convenient way to partition a Cartesian topology to form lower-dimensional grids.

MPI provides the MPI_Cart_sub function that allows us to partition a Cartesian topology into sub-topologies that form lower-dimensional grids. For example, we can partition a two-dimensional topology into groups, each consisting of the processes along the row or column of the topology. The calling sequence of MPI_Cart_sub is the following:

The array keep_dims is used to specify how the Cartesian topology is partitioned. In particular, if keep_dims[i] is true (non-zero value in C) then the ith dimension is retained in the new sub-topology. For example, consider a three-dimensional topology of size $2 \times 4 \times 7$. If keep_dims is {true, false, true}, then the original topology is split into four two-dimensional sub-topologies of size 2×7 , as illustrated in Figure 6.8(a). If keep_dims is {false, false, true}, then the original topology is split one-dimensional topologies of size seven, illustrated in Figure 6.8(b). Note that the number of sub-topologies created is equal to the product of the number of processes along the dimensions that are not being retained. The original topology is specified by the communicator comm_cart, and the returned communicator comm_subcart stores information about the created sub-topology. Only a single communicator is returned to each process, and for processes that do not belong to the same sub-topology, the group specified by the returned communicator is different.

The processes belonging to a given sub-topology can be determined as follows. Consider a three-dimensional topology of size $d_1 \times d_2 \times d_3$, and assume that keep_dims is set to {true, false, true}. The group of processes that belong to the same sub-topology as the

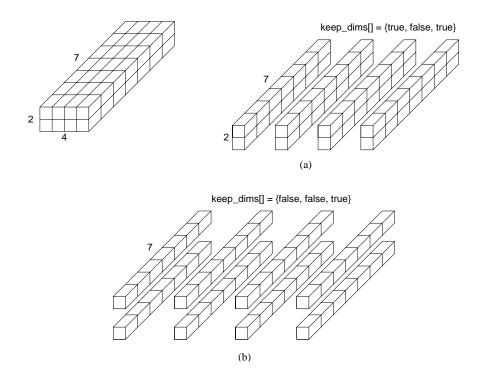


Figure 6.8 Splitting a Cartesian topology of size $2 \times 4 \times 7$ into (a) four subgroups of size $2 \times 1 \times 7$, and (b) eight subgroups of size $1 \times 1 \times 7$.

process with coordinates (x, y, z) is given by (*, y, *), where a '*' in a coordinate denotes all the possible values for this coordinate. Note also that since the second coordinate can take d_2 values, a total of d_2 sub-topologies are created.

Also, the coordinate of a process in a sub-topology created by MPI_Cart_sub can be obtained from its coordinate in the original topology by disregarding the coordinates that correspond to the dimensions that were not retained. For example, the coordinate of a process in the column-based sub-topology is equal to its row-coordinate in the twodimensional topology. For instance, the process with coordinates (2, 3) has a coordinate of (2) in the sub-topology that corresponds to the third column of the grid.

6.7.1 Example: Two-Dimensional Matrix-Vector Multiplication

In Section 6.6.8, we presented two programs for performing the matrix-vector multiplication x = Ab using a row- and column-wise distribution of the matrix. As discussed in Section 8.1.2, an alternative way of distributing matrix A is to use a two-dimensional distribution, giving rise to the two-dimensional parallel formulations of the matrix-vector multiplication algorithm.

Program 6.8 shows how these topologies and their partitioning are used to implement

the two-dimensional matrix-vector multiplication. The dimension of the matrix is supplied in the parameter n, the parameters a and b point to the locally stored portions of matrix *A* and vector *b*, respectively, and the parameter x points to the local portion of the output matrix-vector product. Note that only the processes along the first column of the process grid will store b initially, and that upon return, the same set of processes will store the result x. For simplicity, the program assumes that the number of processes *p* is a perfect square and that *n* is a multiple of \sqrt{p} .

Program 6.8 Two-Dimensional Matrix-Vector Multiplication

```
MatrixVectorMultiply_2D(int n, double *a, double *b, double *x,
 1
                               MPI Comm comm)
 2
 3
    {
      int ROW=0, COL=1; /* Improve readability */
 4
 5
      int i, j, nlocal;
      double *px; /* Will store partial dot products */
 6
 7
      int npes, dims[2], periods[2], keep_dims[2];
 8
      int myrank, my2drank, mycoords[2];
 9
      int other_rank, coords[2];
10
      MPI Status status;
      MPI_Comm comm_2d, comm_row, comm_col;
11
12
13
      /* Get information about the communicator */
      MPI Comm size(comm, &npes);
14
15
      MPI_Comm_rank(comm, &myrank);
16
17
      /* Compute the size of the square grid */
18
      dims[ROW] = dims[COL] = sqrt(npes);
19
      nlocal = n/dims[ROW];
20
21
22
      /* Allocate memory for the array that will hold the partial dot-products */
      px = malloc(nlocal*sizeof(double));
23
24
25
      /* Set up the Cartesian topology and get the rank & coordinates of the process in this topology */
      periods [ROW] = periods [COL] = 1; /* Set the periods for wrap-around connections */
26
27
28
      MPI_Cart_create(MPI_COMM_WORLD, 2, dims, periods, 1, &comm_2d);
29
      MPI_Comm_rank (comm_2d, &my2drank); /* Get my rank in the new topology */
30
31
      MPI_Cart_coords (comm_2d, my2drank, 2, mycoords); /* Get my coordinates */
32
      /* Create the row-based sub-topology */
33
34
      keep_dims[ROW] = 0;
      keep_dims[COL] = 1;
35
      MPI_Cart_sub(comm_2d, keep_dims, &comm_row);
36
37
38
      /* Create the column-based sub-topology */
      keep_dims[ROW] = 1;
39
40
      keep dims[COL] = 0;
      MPI Cart_sub(comm_2d, keep_dims, &comm_col);
41
42
      /* Redistribute the b vector. */
43
44
      /* Step 1. The processors along the 0th column send their data to the diagonal processors */
      if (mycoords [COL] == 0 && mycoords [ROW] != 0) { /* I'm in the first column */
45
46
         coords[ROW] = mycoords[ROW];
47
         coords[COL] = mycoords[ROW];
        MPI Cart_rank(comm_2d, coords, &other_rank);
48
```

```
49
         MPI Send(b, nlocal, MPI DOUBLE, other rank, 1, comm 2d);
50
      if (mycoords[ROW] == mycoords[COL] && mycoords[ROW] != 0) {
51
52
         coords [ROW] = mycoords [ROW];
53
         coords[COL] = 0;
54
         MPI_Cart_rank(comm_2d, coords, &other_rank);
55
         MPI Recv(b, nlocal, MPI DOUBLE, other rank, 1, comm 2d,
56
              &status);
57
      }
58
59
      /* Step 2. The diagonal processors perform a column-wise broadcast */
      coords[0] = mycoords[COL];
60
61
      MPI_Cart_rank(comm_col, coords, &other_rank);
      MPI Bcast(b, nlocal, MPI DOUBLE, other rank, comm col);
62
63
      /* Get into the main computational loop */
64
65
      for (i=0; i<nlocal; i++)</pre>
         px[i] = 0.0;
66
67
         for (j=0; j<nlocal; j++)
68
           px[i] += a[i*nlocal+j]*b[j];
69
70
71
      /* Perform the sum-reduction along the rows to add up the partial dot-products */
72
      coords[0] = 0;
      MPI_Cart_rank(comm_row, coords, &other rank);
73
74
      MPI_Reduce(px, x, nlocal, MPI_DOUBLE, MPI_SUM, other_rank,
75
           comm row);
76
      MPI_Comm_free(&comm_2d); /* Free up communicator */
MPI_Comm_free(&comm_row); /* Free up communicator */
MPI_Comm_free(&comm_col); /* Free up communicator */
77
78
79
80
81
      free(px);
82
    }
```

6.8 Bibliographic Remarks

The best source for information about MPI is the actual reference of the library itself [Mes94]. At the time of writing of this book, there have been two major releases of the MPI standard. The first release, version 1.0, was released in 1994 and its most recent revision, version 1.2, has been implemented by the majority of hardware vendors. The second release of the MPI standard, version 2.0 [Mes97], contains numerous significant enhancements over version 1.x, such as one-sided communication, dynamic process creation, and extended collective operations. However, despite the fact that the standard was voted in 1997, there are no widely available MPI-2 implementations that support the entire set of features specified in that standard. In addition to the above reference manuals, a number of books have been written that focus on parallel programming using MPI [Pac98, GSNL98, GLS99].

In addition to MPI implementations provided by various hardware vendors, there are a number of publicly available MPI implementations that were developed by various government research laboratories and universities. Among them, the MPICH [GLDS96, GL96b] (available at http://www-unix.mcs.anl.gov/mpi/mpich) distributed by Argonne National

Laboratories and the LAM-MPI (available at http://www.lam-mpi.org) distributed by Indiana University are widely used and are portable to a number of different architectures. In fact, these implementations of MPI have been used as the starting point for a number of specialized MPI implementations that are suitable for off-the-shelf high-speed interconnection networks such as those based on gigabit Ethernet and Myrinet networks.

Problems

- **6.1** Describe a message-transfer protocol for buffered sends and receives in which the buffering is performed only by the sending process. What kind of additional hardware support is needed to make these types of protocols practical?
- **6.2** One of the advantages of non-blocking communication operations is that they allow the transmission of the data to be done concurrently with computations. Discuss the type of restructuring that needs to be performed on a program to allow for the maximal overlap of computation with communication. Is the sending process in a better position to benefit from this overlap than the receiving process?
- **6.3** As discussed in Section 6.3.4 the MPI standard allows for two different implementations of the MPI_Send operation one using buffered-sends and the other using blocked-sends. Discuss some of the potential reasons why MPI allows these two different implementations. In particular, consider the cases of different message-sizes and/or different architectural characteristics.
- **6.4** Consider the various mappings of 16 processors on a 4 × 4 two-dimensional grid shown in Figure 6.5. Show how $n = \sqrt{p} \times \sqrt{p}$ processors will be mapped using each one of these four schemes.
- **6.5** Consider Cannon's matrix-matrix multiplication algorithm. Our discussion of Cannon's algorithm has been limited to cases in which *A* and *B* are square matrices, mapped onto a square grid of processes. However, Cannon's algorithm can be extended for cases in which *A*, *B*, and the process grid are not square. In particular, let matrix *A* be of size $n \times k$ and matrix *B* be of size $k \times m$. The matrix *C* obtained by multiplying *A* and *B* is of size $n \times m$. Also, let $q \times r$ be the number of processes in the grid arranged in *q* rows and *r* columns. Develop an MPI program for multiplying two such matrices on a $q \times r$ process grid using Cannon's algorithm.
- **6.6** Show how the row-wise matrix-vector multiplication program (Program 6.4) needs to be changed so that it will work correctly in cases in which the dimension of the matrix does not have to be a multiple of the number of processes.
- **6.7** Consider the column-wise implementation of matrix-vector product (Program 6.5). An alternate implementation will be to use MPI_Allreduce to perform the required reduction operation and then have each process copy the locally stored elements of vector x from the vector fx. What will be the cost of this implementation? Another implementation can be to perform p single-node reduction

operations using a different process as the root. What will be the cost of this implementation?

- **6.8** Consider Dijkstra's single-source shortest-path algorithm described in Section 6.6.9. Describe why a column-wise distribution is preferable to a row-wise distribution of the weighted adjacency matrix.
- **6.9** Show how the two-dimensional matrix-vector multiplication program (Program 6.8) needs to be changed so that it will work correctly for a matrix of size $n \times m$ on a $q \times r$ process grid.