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# FORTRAN and MPI

# Message Passing Interface (MPI)

Day 2

## Course plan:

- MPI General concepts
- Communications in MPI
  - Point-to-point communications
  - Collective communications
- Parallel debugging
- Advanced MPI: user-defined data types, functions
   Linear Algebra operations
- Advanced MPI: communicators, virtual topologies
   Parallel sort algorithms
- Parallel performance. Summary. Tendencies

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Communications on parallel architectures

#### Basic notions and definitions

The fundamental characteristics of a communication network are:

network topology	direct (static) or dynamic networks		
routing policy	specifies how messages (respectively, parts of a message, called <i>packages</i> ) choose paths through		
	the network		
flow control policy	deals with allocation of network resources, namely, communication channels (links) and buffers, to packages as they are processed through the network		

A common technique in modern networks is to divide the message in packages, and the packages further in small units, called *flow-control units* (*flits*), and communicate them in a pipelined fashion.

If, while traversing the network, the message requests a resource (a channel or a buffer) which is in use by some other message, the message cannot proceed further and is blocked. When messages are blocked due to waiting for mutually occupied resources, a *deadlock* occurs.

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Communications on parallel architectures



Deadlock situation with four messages.

Deadlocks can be avoided by using appropriate routing techniques.

#### Routing

• **deterministic** routing --- > the message is communicated via a fixed path, connecting the source and the destinations, determined during the initialization of the communication. *Deadlock-free but limits the network performance.* 

• *adaptive* routing —— > the route can change depending on the particular network situation. *Better network performance but higher chance for deadlocks*.

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Communication models

 $T(A, p)(=T_p) = T_{comp} + T_{comm}$  $\max\{T_{comp}, T_{comm}\} \le T_p \le T_{comp} + T_c \parallel \parallel$  $T_{comp} = T_s(A) + \frac{T_p(A)}{p}$ 

 $T_{comm} = \tau + b \, \ell \, N$ , where

- τ startup time, including
  time to establish a connection between the source processor and the router;
  time to determine the route by executing the routing algorithm;
  time to prepare the message by adding a header, trailer and error correction information.
  b the time needed to transfer one word along a connection link (*per-word-transfer* time)
- $\ell$  the links to be traversed
- N the amount of words to be transfered

 $\frac{1}{b}$  - channel bandwidth

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Communication models

#### The basic communication operations

- (i) moving data from one processor to another
- (ii) moving the same data packet from one processor to all others one-to-all broadcast or just a broadcast operation
- (iii) moving a different message from each processor to every other processor *all-to-all* broadcast.
- (iv) scattering (gathering) data from (in) one processor to (from) all others.
   In the scatter operation, a node sends a packet to every other processor.
   Gather is dual to scatter.
- (v) multiscattering or multigathering of data. The multiscatter operation consists of a scatter from every node. Multigather is defined similarly. The difference between the broadcast (ii) and the scatter (iv) is that in the scatter operations a *different data set* is sent to every processor.

# Point-to-point communications

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Point-to-point communications

MPI provides a set of **SEND** and **RECEIVE** functions that allow the communication of **typed** data with an associated **tag**.

Typing of the message contents is necessary for heterogeneous support.

The tag allows selectivity of messages at the receiving end: one can receive on a particular tag, or one can wild-card this quantity, allowing reception of messages with any tag.

MPI provides **blocking** and **nonblocking** send and receive functions.

In the **blocking** version, send call blocks until the send buffer can be reclaimed as well as the receive functions blocks until the receive buffer actually contains the contents of the message.

The **nonblocking send** and **receive** functions allow the possible overlap of message transmittal with computation, or the overlap of multiple message with one-another.

#### Message envelope

Source	for send-operations implicitly determined by the identity of the message sender
Destination	specified by the <b>dest</b> argument; the range of valid values for <b>dest</b> is $0, 1, \ldots, n-1$ ; this range includes the <i>rank</i> of the sender, so each process may send a message to itself
Communicator	specified by <b>comm</b> argument; represents a communication domain; default communication domain is <b>MPI_COMM_WORLD</b>
Tag	specified by the tag argument; the range of valid values for tag is $0, 1, \ldots, impl\_dep$ , where the value of $impl\_dep$ is implementation dependent; MPI requires that $impl\_dep$ be not less than 32767

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Both blocking and nonblocking communications have **modes**, which allow to choose the semantics of the send operation. The four **modes** are:

- **standard** - the completion of the send does not necessarily mean that the matching receive has started, and no assumption should be made in the application program about whether the out-going data is buffered by MPI;

- **buffered** - the user can guarantee that a certain amount of buffering space is available;

- synchronous - rendezvous semantics between sender and receiver is used;

- **ready** - the user asserts that the matching receive already has been posted.

### Standard Send

Using standard send means that the mode of sending may be synchronous or buffered (see below). This means that upon completion, although the send buffer can be safely re-used, the message may or may not have arrived at the destination.

It should not be assumed that sending will complete before receiving begins. Therefore, two machines should not use blocking standard sends to exchange messages as this may cause a deadlock.

Processes need to guarantee to eventually receive all messages that have been sent to them, otherwise a network overload may occur and an error may occur.

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### Synchronous Send

A synchronous send does not complete until acknowledgement of receipt is received. A synchronous send is slower than a standard or buffered send since the send process remains idle until the receive process catches up. However, as an advantage, synchronous sending is safer and more predictable as a network cannot be overloaded as long as processes guarantee they will eventually receive the message.

#### **Buffered Send**

A buffered send copies the message to a system buffer before the message is then received from this buffer.

This mode of sending guarantees to complete immediately and so is quicker than standard sending. It is also more predictable, if the network overloads then an error will be caused. Unfortunately, it cannot be assumed that adequate pre-allocated buffer space will exist and therefore a buffer must be specifically created, attached to (and subsequently detached from) a buffered send.

A buffered send attaches a buffer using the routine "MPI\_Buffer\_attach", called before the send call, and detaches the buffer using "MPI\_Buffer\_detach", called after the send has completed.

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Point-to-point communications

#### **Ready Send**

Similar to a buffered send, a ready send completes immediately. The communication is guaranteed to succeed is a matching receive is already posted.

However, if a matching receive does not exist the outcome is undefined. This distinguishes the ready send mode from all other modes of sending.

Ready sends are mainly used when performance is critical. For the user who is not so concerned about efficiency the mode is not recommended. As with buffered send, the blocking and non-blocking versions are equivalent.

#### RECEIVE

Messages are received by posting a call to MPI\_Recv that matches a posted MPI send. For the receive call to be successful, the datatype argument must be identical to the datatype specified in the equivalent argument in the send call.

A receive call matches a send call through the "source" and "tag" arguments. This means that a process will only receive a message from the specified source, with a specified tag.

It is possible to use the constants MPI\_ANY\_SOURCE and MPI\_ANY\_TAG respectively for these arguments, allowing the receipt of a message from any process, with any tag.

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Point-to-point communications

### **Rules of Point to Point Communication**

- Messages do not overtake each other. If a process sends two messages and another process posts two matching receives, the messages will be received in the order that they were sent.
- It is not possible for a matching send and receive to remain outstanding. Hopefully both the send and receive complete, but for example if two sends (receives) are posted with one matching receive (send), then one send (receive) will fail.
- The message sent by the send call must have the same datatype as the message expected by the receive type. The datatypes posted should be MPI datatypes.

#### **Blocking SEND**

MPI_SEND (buf, count, datatype, dest, tag, comm, status)			
IN	buf	initial address of send buffer	
IN	count	number of entries to send	
IN	datatype	datatype of each entry	
IN	dest	rank of destination	
IN	tag	message tag	
IN	comm	communicator	

int MPI\_SEND(void\* buf, int count, MPI\_Datatype
 datatype, int dest, int tag, MPI\_Comm comm)

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### Blocking RECEIVE

MPI_RECV(buf, count, datatype, source, tag, comm, status)			
IN	buf	initial address of receive buffer	
IN	count	number of entries to receive	
IN	datatype	datatype of each entry	
IN	source	rank of source	
IN	tag	message tag	
IN	comm	communicator	
OUT	status	return status	

MPI\_RECV(buf, count, datatype, source, tag, comm, status, ierror) <type> buf(\*) INTEGER count, datatype, source, tag, comm, status(MPI\_STATUS\_SIZE), ierror

```
if (me.ne.0) then
    call MPI_RECV(nnode,1,MPI_INTEGER,0,1,
                          MPI_COMM_WORLD,status,ierr)
>
    call MPI_RECV(nedge,1,MPI_INTEGER,0,2,
                          MPI_COMM_WORLD,status,ierr)
>
    call MPI_RECV(nface,1,MPI_INTEGER,0,3,
>
                          MPI_COMM_WORLD,status,ierr)
 else
    do iPE=1,nPEs-1
    call MPI_SEND(NodePerProc(iPE),1,MPI_INTEGER,iPE,1,
                          MPI_COMM_WORLD,status,ierr)
>
   call MPI_SEND(EdgePerProc(iPE),1,MPI_INTEGER,iPE,2,
>
                          MPI_COMM_WORLD,status,ierr)
    call MPI_SEND(FacePerProc(iPE),1,MPI_INTEGER,iPE,3,
                          MPI_COMM_WORLD,status,ierr)
>
    enddo
 endif
```

# MATHEMATICS AND MECHANICS MM Point-to-point communications: Combined SEND-RECEI

MPI\_SENDRECV executes a blocking send and receive operation. Both send and receive use the same communicator, but may have distinct tag arguments. The send and receive buffers must be disjoint.

MPI_SENDRECV(sendbuf, sendcount, sendtype, dest, sendtag, recvbuf, recvcount, recvtype, source, recvtag, comm, status)			
IN	sendbuf	initial address of send buffer	
IN	sendcount	number of entries to send	
IN	sendtype	type of entries in the send buffer	
IN	dest	rank of destination	
IN	sendtag	send tag	
OUT	recvbuf	initial address of receive buffer	
IN	recvcount	number of entries to receive	
IN	recvtype	datatype of each entry	
IN	source	rank of source	
IN	recvtag	recv tag	
IN	comm	communicator	
OUT	status	return status	

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```
----- fetch from EAST: [xv(i,j,k) = x(i+distx,j,k)]
С
      if (NEWS27(1) .ne. 999) then
      call MPI_SENDRECV(xv(nanrx+1,1,1),1,type_fixed_x,NEWS27(1),
                        xv(nanrx,1,1), 1,type_fixed_x,NEWS27(1),
     >
     >
                         MPI_COMM_WORLD, status, ierr)
      endif
    ----- fetch from NORTH: [xv(i,j,k) = x(i,j+disty,k)]
С
      if (NEWS27(3) .ne. 999) then
      call MPI_SENDRECV(xv(1,nanry+1,1),1,type_fixed_y,NEWS27(3),
                        xv(1,nanry,1), 1,type_fixed_y,NEWS27(3),
     >
                         MPI COMM WORLD, status, ierr)
     >
      endif
```

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### Nonblocking SEND/RECEIVE

MPI\_ISEND(buf, count, datatype, dest, tag, comm, status, request)

MPI\_IRECV(buf, count, datatype, source, tag, comm, status, request)

OUT request request handle

These calls allocate a request object and return a handle to it in **request** which is used to <u>query the status of the communication</u> or wait for completion.

#### **Completion operations**

MPI_WAIT(request,status)	returns when the operation
	identified by request is completed
MPI_TEST(request,flag,status)	returns flag=true if the operation identified by
	request is completed or flag=false otherwise

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```
...
!start communication
call MPI_ISEND(B(1,1),n,MPI_REAL,left, tag,comm,req(1),ierr)
call MPI_ISEND(B(1,m),n,MPI_REAL,right,tag,comm,req(2),ierr)
call MPI_IRECV(A(1,1),n,MPI_REAL,left, tag,comm,req(3),ierr)
call MPI_IRECV(A(1,m),n,MPI_REAL,right,tag,comm,req(4),ierr)
! do some computational work
...
! Complete communication
do i=1,4
        call MPI_WAIT(req(i),status(1,i),ierr)
end
```



```
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```

```
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```

Point-to-point communications



```
call MPI_COMM_RANK(comm,rank,ierr)
if (rank .eq. 0) then
    call MPI_SEND(sendbuf1, count, MPI_REAL,1,1,comm,ie)
    call MPI_SEND(sendbuf2, count, MPI_REAL,1,2,comm,ie)
else ! ran1 = 1
    call MPI_IRECV(recvbuf2, count, MPI_REAL,0,2,comm,r
    call MPI_IRECV(recvbuf2, count, MPI_REAL,0,1,comm,r
    call MPI_WAIT(req1, status, ierr)
    call MPI_WAIT(req2, status, ierr)
endif
```

If both blocking SEND and RECV were used, the first message has to be copied and buffered before the second SEND can be proceeded.

Persistent communication requests are associated with nonblocking send and receive operations.

**Situation:** communication with the same argument list is repeatedly executed within the inner loop of a parallel computation.

(1) MPI persistent communications can be used to reduce communications overhead in programs which repeatedly call the same point-to-point message passing routines with the same arguments. They minimize the software overhead associated with redundant message setup.

(2) An example of an application which might benefit from persistent communications would be an iterative, data decomposition algorithm that exchanges border elements with its neighbors. The message size, location, tag, communicator and data type remain the same each iteration.

```
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```

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Persistent Communication Requests

#### Step 1: Create persistent requests

The desired routine is called to setup buffer location(s) which will be sent/received. The five available routines are:

MPI_Recv_init	Creates a persistent receive request
MPI_Bsend_init	Creates a persistent buffered send request
MPI_Rsend_init	Creates a persistent ready send request
MPI_Send_init	Creates a persistent standard send request
MPI_Rsend_init	Creates a persistent ready send request
MPI_Ssend_init	Creates a persistent synchronous send request

#### Step 2: Start communication transmission

Data transmission is begun by calling either of the MPI\_Start routines.

MPI\_Start Activates a persistent request operation
MPI\_Startall Activates a collection of persistent request operations

Step 3: Wait for communication completion

Because persistent operations are non-blocking, the appropriate MPI\_Wait or MPI\_Test routine must be used to insure their completion.

Step 4: Deallocate persistent request objects

When there is no longer a need for persistent communications, the programmer should explicitly free the persistent request objects by using the MPI\_Request\_free() routine.

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Persistent Communication Requests

MPI_SEND_INIT(buf, count, type, dest, tag, comm, request) MPI_RECV_INIT(buf, count, type, source, tag, comm, request) MPI_START(request) MPI_STARTALL(count,array-of-requests) MPI_REQUEST_FREE(request)			
IN	buf	initial address of send buffer	
IN	count	number of entries to send	
IN	type	datatype of each entry	
IN	dest	rank of destination	
IN	source	rank of source	
IN	tag	tag	
IN	comm	communicator	
OUT	request	request handle	

```
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                                         Persistents Communication Requests
          i<size
    (i=0:
for
    MPI_SEND_INIT(sendbuf,counts[(rank+1)%size],
                  type, right, i, MPI_COMM_WORLD, &request[2*i] );
    MPI_RECV_INIT(recvbuf,counts[(rank+i-1+size)%size],
                   type, left, i, MPI_COMM_WORLD, &request[2*i+1] );
  }
while (!done)
                                               /* Run pipeline */
      <copy local data into sendbuf>
      for (i=0;i<size; i++) {</pre>
          MPI_STATUS stat[2];
          if (i != size - 1)
             MPI_STARTALL(2,&request[2*i]);
          < compute using sendbuf>
          if (i != size - 1)
             MPI_WAITALL(2, &request[2*i], stat);
          < copy recvbuf into sendbuf>
          }
    <compute new data>
  }
for (i=0; i<2*(size-1); i++) {</pre>
                                                /* Free requests */
    MPI_REQUEST_FREE(&request[i]);
   }
```

```
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```



```
for i=1:n
    do something
    receive from P_src, tag=1
    do something else
    send to P_dest, tag=2
end
```

Use constant tag within a loop: if for one processor it takes longer to finish the current iteration i, it may end up with receiving the data from iteration i + 1 for processor  $P_{src}$ .

The same may happen if the same tag is used in two parts of the code which are not separated explicitly by a barrier.

Result: a nondeterministic code which may finish correctly from time to time, give wrong results some of the time, and other time just crash.

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# Collective communications

 Transmission of data and synchronization among all processes in a group.

Restrictions:

- ◇ amount of data send must match exactly that of data received;
- ◊ collective functions only in blocking version;
- No tag, thus the calls are matched according to the order of execution;
- only 'normal' mode, i.e., a collective function returns as soon as its participation in the overall communication is completed.

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Collective communications

- Barrier synchronization across all processes;
- Global communication functions
  - Broadcast from one to all processes;
  - Gather data from all processes to one process;
  - Scatter data from one to all processes;
  - Scatter/Gather data from all processes to all processes;
- Global reduction operation such as sum, max, min, etc.

All the listed functions (excepts *broadcast*) can be found in two variants:

- $\left(a\right)$  simple where all items are messages of the same size;
- (b) <u>vector</u> where each item may be of a different size.

#### MPI\_BARRIER(comm, ierr)

MPI\_BARRIER blocks the caller until all processes have called it. The call returns at any process only after all processes have entered the call.

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### BROADCAST

MPI\_BCAST(buffer, count, datatype, root, comm)

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MPI\_BCAST broadcasts a message from the process with rank root to all processes in the group. The argument root must have identical value on all processes and comm must represent the same communication domain. On return the contents pf the root's communication buffer is copied to all processes.

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#### **GATHER**

MPI\_GATHER(sendbuf, sendcount, sendtype, recvbuf, recvcount, recvtype, root, comm)



Gather 100 integers from every proc to root.(i) Everybody allocates space for the receive buffer.

```
MPI_COMM comm;
int gsize, sendarray[100];
int root=0, *rbuf;
....
MPI_COMM_SIZE(comm,&gsize);
rbuf = (int*)malloc(gsize*100*sizeof(int));
MPI_GATHER(sendarray,100,MPI_INT,rbuf,100,MPI_INT,root,comm)
....
```

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MPI\_GATHER examples

Gather 100 integers from every proc to root. (ii) Only root allocates space for the receive buffer.

```
MPI_COMM comm;
int gsize, sendarray[100];
int root=0, myrank, *rbuf;
....
MPI_COMM_RANK(comm,myrank);
if ( myrank == root ){
    MPI_COMM_SIZE(comm,&gsize);
    rbuf = (int*)malloc(gsize*100*sizeof(int));
    }
MPI_GATHER(sendarray,100,MPI_INT,rbuf,100,MPI_INT,root,comm)
....
```

Gather 100 integers from every proc to root. (iii) Use derived datatype.

```
MPI_COMM comm;
int gsize, sendarray[100];
int root, *rbuf;
MPI_DATATYPE rtype;
....
MPI_COMM_SIZE(com,&gsize);
MPI_TYPE_CONTIGUOUS(100, MPI_INT, &rtype);
rbuf = (int*)malloc(gsize*100*sizeof(int));
MPI_GATHER(sendarray, 100, MPI_INT, rbuf, 100, rtype,root,comm)
....
```

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Collective communications

### All-GATHER

MPI\_ALLGATHER(sendbuf, sendcount, sendtype, recvbuf,

recvcount, recvtype, comm)



#### **ALL-TO-ALL** communication



MPI\_ALLTOALL(sendbuf, sendcount, sendtype, recvbuf,recvcount, recvtype, comm)

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Collective communications

## **REDUCE and ALL REDUCE**

Name (operation)	Meaning	
MPI_MAX	maximum	
MPI_MIN	minimum	
MPI_SUM	sum	
MPI_PROD	product	
MPI_LAND	logical and	
MPI_LOR	logical or	
MPI_MAXLOC	max value and location	
MPI_MINLOC	min value and location	

MPI\_REDUCE(sendbuf, recvbuf, count, datatype, op, root, comm)

MPI\_ALLREDUCE(sendbuf, recvbuf, count, datatype, op, root, comm)

```
dot_product: compute a scalar product
С
      subroutine dot_product(global,x,y,n)
      implicit none
      include "mpif.h"
      integer n, i, ierr
      double precision global, x(n), y(n)
      double precision tmp, local
      local = 0.0d0
      qlobal = 0.0d0
      do i=1,n
         local = local + x(i) * y(i)
      enddo
      call MPI_ALLREDUCE(local,tmp,1,MPI_DOUBLE_PRECISION,
                          MPI_SUM, MPI_COMM_WORLD, ierr)
     >
      global = tmp
      return
      end
```

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```
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```

Erroneous examples

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```
switch(rank) {
   case 0:
        MPI_BCAST(buf1,count,type,0,comm);
        MPI_BCAST(buf2,count,type,1,comm);
        break;
   case 1:
        MPI_BCAST(buf2,count,type,1,comm);
        MPI_BCAST(buf1,count,type,0,comm);
        break;
}
```

Assume that  $comm = \{0,1\}$ .

The calls do not specify the same root.

**!!!** Collective communications must be executed in the same order at all members of the communication group.

}

```
switch(rank) {
   case 0:
         MPI_BCAST(buf1,count,type,0,comm0);
         \texttt{MPI}\_\texttt{BCAST(buf2,count,type,2,comm2); Say, comm0=\{0,1\}, comm1=\{1,2\}}
                                                      and comm2={2,0}.
         break;
                                                      If the broadcast is a synchronizing
   case 1:
         MPI_BCAST(buf1,count,type,1,comm1); operation, the code will deadlock.
                                                      Reason: there is a cyclic dependency:
         MPI_BCAST(buf2,count,type,0,comm0);
                                                        BCAST in comm2 \longrightarrow BCAST in comm0
         break;
                                                        BCAST in comm0 \longrightarrow BCAST in comm1
   case 2:
                                                        BCAST in comm1 \longrightarrow BCAST in comm2
         MPI BCAST(buf1,count,type,2,comm2);
         MPI_BCAST(buf2,count,type,1,comm1);
         break;
```

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```
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```

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```
switch(rank) {
   case 0:
        MPI_BCAST(buf1,count,type,0,comm);
        MPI_SEND(buf2,count,type,1,tag,comm);
        break;
   case 1:
        MPI_RECV(buf2,count,type,0,tag,comm);
        MPI_BCAST(buf1,count,type,0,comm);
        break;
}
```

The program may deadlock because MPI\_BCAST on P0 may block till PE1 executes the matching MPI\_BCAST. However, PE1 waits to receive data and will never execute BCAST.

```
switch(rank) {
   case 0:
        MPI_BCAST(buf1,count,type,0,comm);
        MPI_SEND(buf2,count,type,1,tag,comm);
        break;
   case 1:
        MPI_RECV(buf2,count,type,MPI_ANY_SOURCE,tag,comm);
        MPI_BCAST(buf1,count,type,0,comm);
        MPI_RECV(buf2,count,type,MPI_ANY_SOURCE,tag,comm);
        break;
   case 2:
        MPI_SEND(buf2,count,type,1,tag,comm);
        MPI_BCAST(buf1,count,type,0,comm);
        MPI_BCAST(buf1,count,type,0,comm);
        break;
   }
}
```

```
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```

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Erroneous examples

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A correct but nondeterministic code. There are two possible scenarios:

Processes			
0	1	2	
	Scenario 1		
	RECV	$\leftarrow$ SEND	
BCAST	BCAST	BCAST	
$SEND \longrightarrow$	RECV		
Scenario 2			
BCAST			
$SEND \longrightarrow$	RECV		
	BCAST		
	RECV	$\leftarrow$ SEND	
		BCAST	

#### **Timing MPI Programs**

MPI\_WTIME() DOUBLE PRECISION MPI\_WTIME()

MPI\_WTIME returns a floating-point number of seconds representing *elapsed wall-clock* time since some arbitrary point of time in the past. This point is guaranteed not to change during the lifetime of the process. Thus, a time interval can be measured by calling this routine at the beginning and end of the program segment has to be measured and subtracting the values returned.

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8 7 + 38 + 42+61 + 55 4 2 2+61 + 53+7+4+83+7+4+8 Σ Σ Σ Σ Σ 1+5+2+6  $\bar{1}+5+2+6$ Σ



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#### MPI environmental management



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Gray codes

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**Theorem** Any  $m_1 \times m_2 \ldots \times m_n$  mesh in the *n*-dimensional space  $\mathbb{R}^n$ , where  $m_i = 2^{r_i}$  can be mapped onto a *d*-cube where  $d = r_1 + r_2 + \cdots + r_n$ , with the proximity property preserved. The mapping of the grid points is the cross product  $G_1 \times G_2 \times \cdots \times G_n$  where  $G_i$ ,  $i = 1, \ldots n$  is any one-dimensional Gray-code mapping of the  $m_i$  points in the *i*th coordinate direction.