IN3200/IN4200: Chapter 9 Distributed-memory parallel programming with MPI

 ${\it Textbook: Hager \& Wellein, Introduction to High Performance Computing for Scientists and } \\ Engineers$

Objective

- The concept of explicit "message passing"
- Introduction to MPI (the Message Passing Interface)

Message passing

- Shared-memory programming (such as OpenMP) does not work for distributed-memory parallel computers
 - There is no way for one processor to directly access the address space of another process
- Explicit "message passing" is required
 - This can also be a programming model for shared-memory or hybrid systems

Basic features of message-passing programming

- The same program runs on all processes (Single Program Multiple Data, or SPMD)—no difference from OpenMP programing in this regard
- The work of each process is implementation in a sequential language (such as C)
 - Data exchange (sending and receiving messages) is done via calls to an appropriate library
- All variables in a process are local to this process (nothing is shared)

"Messages" carry data to be exchanged between processes

Information needed about a message:

- Which process is sending the message?
- Where is the data on the sending process?
- What kind of data is being sent?
- How much data constitutes the message?
- Which process is going to receive the message?
- Where should the data be placed on the receiving process?
- What amount of data is the receiving process prepared to accept?

MPI (Message Passing Interface)

MPI is a *library standard* for programming distributed memory

- MPI implementation(s) available on almost every major parallel platform (also on shared-memory machines)
- Portability, good performance & functionality
- Collaborative computing by a group of individual processes
- Each process has its own local memory
- Explicit message passing enables information exchange and collaboration between processes

MPI C language binding

```
#include <mpi.h>
rv = MPI_Xxxxx(parameter, ... )
```

Beware of the case-sensitive naming pattern.

The return value (rv) transports information about the success of the MPI operation. (MPI_SUCCESS is returned if the MPI routine completed successfully.)

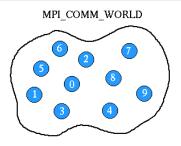
MPI_Init

The MPI_Init function initializes the parallel environment.

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

The MPI_Init function takes pointers to the main() function's arguments so that the library can evaluate and remove any additional command line arguments that may have been added by the MPI startup process.

MPI communicator



- An MPI communicator is a "communication universe" for a group of processes
- MPI_COMM_WORLD name of the default MPI communicator, i.e., the collection of all processes
- Each process in a communicator is identified by its rank
- Almost every MPI command needs to provide a communicator as input argument

MPI process rank

- Each process has a unique rank, i.e. an integer identifier, within a communicator
- The rank value is between 0 and #procs-1
- The rank value is used to distinguish one process from another
- Commands MPI_Comm_size & MPI_Comm_rank are very useful int size, my_rank;
 MPI_Comm_size (MPI_COMM_WORLD, &size);
 MPI_Comm_rank (MPI_COMM_WORLD, &my_rank);

MPI_Finalize

An MPI parallel program is shut down by a call to MPI_Finalize().

Note that no MPI process except rank 0 is guaranteed to execute any code beyond MPI_Finalize().

Example running result of "Hello world"

- Example of compilation: mpicc hello_world_mpi.c
- Example of parallel execution: mpirun -np 4 ./a.out
- Example running result (note: no deterministic order of the output):

```
Hello world, I've rank 2 out of 4 procs.
Hello world, I've rank 1 out of 4 procs.
Hello world, I've rank 3 out of 4 procs.
Hello world, I've rank 0 out of 4 procs.
```

Note: Compilation and execution can vary from system to system.

The abstract "picture" of parallel execution

Process 0 Process 1 \cdots Process P-1

```
#in clude < stdio .h>
                                                                #include < std io.h>
#in clude cmp i.h>
                                                                #include cmpi.b>
int main (int margs, char ** args)
                                                                int main (int margs, char** args)
  int size, my_rank;
                                                                 int size, ny_renk;
 MPI_Init (Roarge, Rarge);
                                                                 MP L_In it (Roarge, Rarge);
 MPI_Comm_wise (MPI_COMM_WORLD, & wise);
                                                                 MPI_Comm_size (MPI_COMM_WORLD, &size);
 MPI Comm rank (MPI COMM WORLD, key rank):
                                                                 MP I Comm rank (MPI COMM WORLD, Rmy rank):
 printf("Hello world, I've rank %d out of %d proce.\n",
                                                                 printf("Hello world, I've rank %d out of %d proce.\n",
         my_rank, size);
                                                                        my_rank, size);
 MPI_Finalize ();
                                                                 MPI_Finalize ();
 return 0:
                                                                 return 0:
```

```
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```

MPI message

An MPI message is simply an array of elements of a particular MPI data type.

Data types can either be standard types (pre-defined) or *derived* types, which must be defined by appropriate MPI calls.

MPI type	C type
MPI_CHAR	signed char
MPI_INT	signed int
MPI_LONG	signed long
MPI_FLOAT	float
MPI_DOUBLE	double
MPI_BYTE	N/A

Table 9.2: A selection of the standard MPI data types for C. Unsigned variants exist where applicable.

Point-to-point communication

- One "sender" and one "receiver": point-to-point communication
- Both the sender and receiver are identified by their ranks (within an MPI communicator)
- Each point-to-point message can carry an additional integer label, the so-called tag

The simplest MPI send command

This *blocking* send function returns when the data has been delivered to the system and the buffer can be reused. The message may not have been received by the destination process.

The simplest MPI receive command

- This blocking receive function waits until a matching message is received from the system so that the buffer contains the incoming message.
- Match of data type, source process (or MPI_ANY_SOURCE), message tag (or MPI_ANY_TAG).
- Receiving fewer datatype elements than count is ok, but receiving more elements is an error.

MPI_Status

The MPI_Recv function has an additional output argument: the status object, which can be used to determine "unknown" parameters (if any).

For example, the source or tag of a received message may not be known if wildcard values were used in the receive function.

To query the information stored in a status object:

MPI parallelization of numerical integration

```
int rank. size:
double a=0.0, b=1.0, mya, myb, psum;
MPI_Status;
MPI_Init (&nargs, &args);
MPI_Comm_size (MPI_COMM_WORLD, &size);
MPI_Comm_rank (MPI_COMM_WORLD, &rank);
mva = a + rank*(b-a)/size;
mvb = mva + (b-a)/size:
psum = integrate(mya,myb); // integrate over its "subinterval"
if (rank==0) {
 double res = psum;
 for (i=1; i<size; i++) {
   MPI_Recv(&psum,1,MPI_DOUBLE,i,0,MPI_COMM_WORLD,&status);
   res += psum;
 printf("Result: %g\n", res);
else {
 MPI_Send(&psum,1,MPI_DOUBLE,0,0,MPI_COMM_WORLD);
MPI Finalize():
```

Some explanations

- Each MPI process is assigned a "subinterval": [mya, myb] to work on.
- Each MPI process then computes its partial result (psum)
- Thereafter, the partial results need to be summed up
- The strategy chosen by the preceding MPI example is to let each process (except rank 0) send its partial result to process rank 0, which sums up all the partial results

Additional remarks

The preceding MPI example can be improved in several ways:

- Rank 0 receives in total size-1 messages, one from each of the other processes. The order of receiving the messages is fixed, probably not the same as the incoming order of the messages. Using MPI_ANY_SOURCE (wildcard) instead of a prescribed sender rank is more appropriate.
- Rank 0 calls MPI_Recv after its own calculation (integrate(mya,myb)). If some of the other processes finish their computation earlier, communication cannot proceed, and it cannot be overlapped with computation on rank 0. (Non-blocking point-to-point communication will be more appropriate, see Section 9.2.4.)
- Rank 0 can easily become a "bottleneck", because it is responsible for receiving all the partial results. (Use of collective communication, such as that specifically designed for "reduction", will be more appropriate, see Section 9.2.3.)

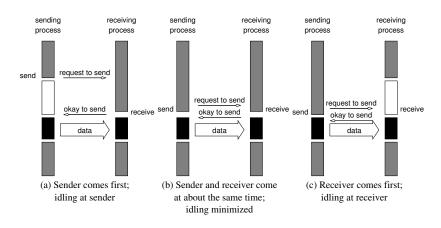
"Uncertainties/risks" with MPI_Send

While MPI_Send is easy to use, one should be aware that the MPI standard allows for a considerable amount of freedom in its actual implementation.

- Internally it may work completely synchronously, meaning that the call can not return until a message transfer has at least started after a "handshake" with the receiver.
- However, it may also copy the message to an intermediate buffer and return right away, leaving the "handshake" and data transmission to another mechanism, like a background thread.
- It may even change its behavior depending on any explicit or hidden parameters.

Scenarios of "handshake"

Non-Buffered Blocking Message Passing Operations



Source: A. Grama, A. Gupta, G. Karypis, and V. Kumar. Introduction to Parallel Computing. Addison

Wesley, 2003

Possibilities for deadlock

Deadlocks may occur if the possible synchronousness of MPI_Send is not taken into account. A typical communication pattern where this may become crucial is a "ring shift":

```
int rank, size, left, right,in_buf[N], out_buf[N];
MPI_Status;

// ......

MPI_Comm_size (MPI_COMM_WORLD, &size);
MPI_Comm_rank (MPI_COMM_WORLD, &rank);

left = rank==size-1 ? 0 : rank+1;
right = rank==0 ? size-1 : rank-1;

MPI_Send(out_buf,N,MPI_INT,left,0,MPI_COMM_WORLD);
MPI_Recv(in_buf,N,MPI_INT,right,0,MPI_COMM_WORLD,&status);
```

Depiction of the "ring shift" pattern

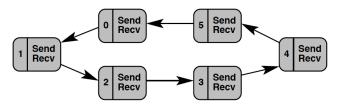


Figure 9.1: A ring shift communication pattern. If sends and receives are performed in the order shown, a deadlock can occur because MPI Send() may be synchronous.

- If MPI_Send is synchronous (and there is no buffering), all processes call it first and then wait forever for a matching receive to be posted—deadlock.
- However, the ring shift may run without problems if the messages are sufficiently short. In fact, most MPI implementations provide a (small) internal buffer for short messages and switch to synchronous mode when the buffer is full or too small.

One simple solution

```
int rank, size, left, right,in_buf[N], out_buf[N];
MPI_Status;
// ......
MPI Comm size (MPI COMM WORLD, &size):
MPI Comm rank (MPI COMM WORLD, &rank);
left = rank==size-1 ? 0 : rank+1:
right = rank==0 ? size-1 : rank-1;
if (rank%2) {
 MPI_Recv(in_buf,N,MPI_INT,right,0,MPI_COMM_WORLD,&status);
 MPI Send(out buf.N.MPI INT.left.O.MPI COMM WORLD):
else {
 MPI Send(out buf.N.MPI INT.left.O.MPI COMM WORLD):
 MPI_Recv(in_buf,N,MPI_INT,right,0,MPI_COMM_WORLD,&status);
```

Depiction of the simple solution

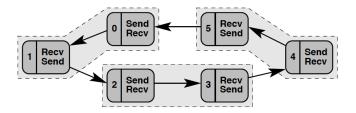


Figure 9.2: A possible solution for the deadlock problem with the ring shift: By changing the order of MPI_Send() and MPI_Recv() on all odd-numbered ranks, pairs of processes can communicate without deadlocks because there is now a matching receive for every send operation (dashed boxes).

Special MPI functions for "ring shifts"

Both routines use blocking communication, are guaranteed to not be subject to the deadlock effects that may occur with separate send and receive.

Collective communication in MPI

Recall the numerical integration example: summing up the partial sums is a *reduction* operation.

MPI has mechanisms that make reductions much simpler and in most cases more efficient than looping over all ranks and collecting results.

Since a reduction is a procedure involves all ranks in a communicator, it belongs to the so-called **collective** communication operations in MPI.

A collective MPI routine must be called by all ranks in a communicator.

$MPI_Barrier$

MPI_Barrier is the simplest collective in MPI, it does not actually perform any real data transfer.

```
int MPI_Barrier(MPI_Comm comm)
```

The barrier *synchronizes* the members of the communicator, i.e., all processes must call it before they are allowed to return to the user code.

Don't over-use MPI_Barrier! There are other MPI routines that allow for implicit or explicit synchronization with finer control.

MPI_Bcast

MPI_Bcast sends a message from one process (the "root") to all others in the communicator.

The **buffer** argument to MPI_Bcast() is a send buffer on the root and a receive buffer on any other process.

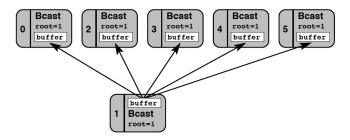


Figure 9.3: An MPI broadcast: The "root" process (rank 1 in this example) sends the same message to all others. Every rank in the communicator must call MPI_Bcast() with the same root argument.

MPI_Gather & MPI_Scatter

Examples of more advanced MPI collective calls that are concerned with global data distribution:

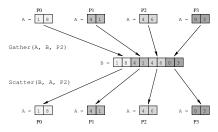
- MPI_Gather() collects the send buffer contents of all processes and concatenates them in rank order into the receive buffer of the root process
- MPI_Scatter() does the reverse, distributing equal-sized chunks of the root's send buffer
- MPI_Gatherv() and MPI_Scatterv() support arbitrary per-rank chunk sizes

MPI_Gather & MPI_Scatter syntax

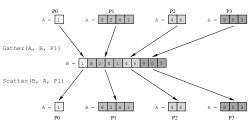
The syntax of MPI_Gatherv() and MPI_Scatterv() is more complex, not listed here.

Depiction of MPI_Gather & MPI_Scatter

(a) Equal-Size Gather and Scatter Operations



(b) Unequal-Size Gather and Scatter Operations



MPI_Reduce

MPI_Reduce() combines the contents of the sendbuf array on all processes, element-wise, using an operator encoded by the op argument, and stores the result in recvbuf on root

Examples of predefined operators: MPI_MAX, MPI_MIN, MPI_SUM and MPI_PROD

Depiction of MPI_Reduce

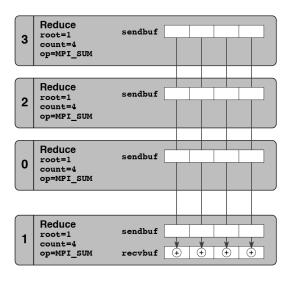


Figure 9.4: A reduction on an array of length count (a sum in this example) is performed by MPI_Reduce(). Every process must provide a send buffer. The receive buffer argument is only used on the root process. The local copy on root can be prevented by specifying MPI_IN_PLACE instead of a send buffer address.

Rewrite of the "numerical integration" example

```
int rank, size;
double a=0.0, b=1.0, mya, myb, psum, res=0.;
MPI_Status;
MPI_Init (&nargs, &args);
MPI Comm size (MPI COMM WORLD, &size):
MPI Comm rank (MPI_COMM_WORLD, &rank);
mva = a + rank*(b-a)/size:
myb = mya + (b-a)/size;
psum = integrate(mya,myb); // integrate over its "subinterval"
MPI_Reduce(&psum,&res,1,MPI_DOUBLE,MPI_SUM,0,MPI_COMM_WORLD);
if (rank==0)
 printf("Result: %g\n", res);
MPI Finalize():
```

MPI_Allreduce

The result of the reduction operation (recvbuf) is available on all MPI ranks.

Nonblocking point-to-point communication

Point-to-point communication can be performed with nonblocking semantics.

- A nonblocking point-to-point call merely initiates a message transmission and returns very quickly to the user code.
- In an efficient implementation, waiting for data to arrive and the actual data transfer occur in the background, leaving resources free for computation.
- In other words, nonblocking MPI is a way in which communication may be overlapped with computation if implemented efficiently.
- The message buffer must not be used as long as the user program has not been notified that it is safe to do so (which can be checked by suitable MPI calls).
- Nonblocking and blocking MPI calls are mutually compatible, i.e., a message sent via a blocking send can be matched by a nonblocking receive.

- As opposed to the blocking send (MPI_Send()), MPI_Isend()
 has an additional output argument, the request handle (of type
 struct MPI_Request).
- It serves as an identifier by which the program can later refer to the "pending" communication request.

MPI_Irecv

 The status object known from MPI_Recv() is not needed for MPI_Irecv.

MPI_Test & MPI_Wait

Checking a pending communication for completion can be done via the MPI_Test() and MPI_Wait() functions. The former only tests for completion and returns a flag, while the latter blocks until the buffer can be used.

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

The status object contains useful information only if the pending communication is a completed receive (i.e., in the case of MPI_Test() the value of flag must be true).

MPI_Waitall

In the case of multiple non-blocking communication operations (multiple requests pending), it is more convenient to use the MPI_Waitall function:

The "numerical integration" example, yet again

```
// ...
double *tmp;
MPI_Request *request_array;
MPI_Status *status_array;
if (rank==0) {
 // allocate arrays of tmp, request_array & status_array...
 for (i=1; i<size; i++)
   MPI_Irecv(&tmp[i-1],1,MPI_DOUBLE,i,0,MPI_COMM_WORLD,&request_array[i-1]);
mva = a + rank*(b-a)/size;
myb = mya + (b-a)/size;
psum = integrate(mya,myb); // integrate over its "subinterval"
if (rank==0) {
 double res = psum;
 MPI_Waitall (size-1,request_array,status_array);
 for (i=1: i<size: i++)
   res += tmp[i-1];
 printf("Result: %g\n", res);
else {
 MPI_Send(&psum,1,MPI_DOUBLE,0,0,MPI_COMM_WORLD);
```

Benefits of nonblocking communication

- Nonblocking communication provides an obvious way to overlap communication, i.e., overhead, with useful work.
- The possible performance advantage, however, depends on many factors, and may even be nonexistent.
- But even if there is no real overlap, multiple outstanding nonblocking requests may improve performance because the MPI library can decide which of them gets serviced first.
- Nonblocking communication helps to avoid deadlock.

A short summary

	Point-to-point	Collective
Blocking	<pre>MPI_Send() MPI_Ssend() MPI_Bsend() MPI_Recv()</pre>	MPI_Barrier() MPI_Bcast() MPI_Scatter()/ MPI_Gather() MPI_Reduce() MPI_Reduce_scatter() MPI_Allreduce()
Nonblocking	<pre>MPI_Isend() MPI_Irecv() MPI_Wait()/MPI_Test() MPI_Waitany()/ MPI_Testany() MPI_Waitsome()/ MPI_Testsome() MPI_Testsome() MPI_Waitall()/ MPI_Testall()</pre>	N/A

Table 9.3: MPI's communication modes and a nonexhaustive overview of the corresponding subroutines.

Virtual topologies

- MPI suits very well for implementing domain decomposition (Section 5.2.1) on distributed-memory parallel computers.
- However, setting up the process grid and keeping track of which ranks have to exchange halo data is nontrivial.
- MPI contains some functionality to support this recurring task in the form of virtual topologies.
- These provide a convenient process naming scheme, which fits the required communication pattern.

Cartesian topologies

Example: a 2D global Cartesian mesh of size 3000×4000 . Suppose we want to use $3 \times 4 = 12$ MPI processes to divide the global mesh, each holding a piece of 1000×1000 .

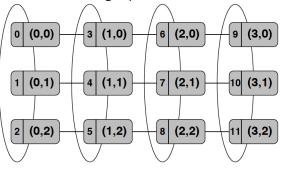


Figure 9.6: Two-dimensional Cartesian topology: 12 processes form a 3×4 grid, which is periodic in the second dimension but not in the first. The mapping between MPI ranks and Cartesian coordinates is shown

Cartesian topologies (2)

- As shown in the preceding figure, each process can either be identified by its rank or its Cartesian coordinates.
- Each process has a number of neighbors, which depends on the grid's dimensionality. (In our example, the number of dimensions is two, which leads to at most four neighbors per process.)
- MPI can help with establishing the mapping between ranks and Cartesian coordinates in the process grid.

MPI_Cart_create

- A new, "Cartesian" communicator comm_cart is generated, which can be used later to refer to the topology.
- The periods array specifies which Cartesian directions are periodic, and the reorder parameter allows, if true, for rank reordering so that the rank of a process in communicators comm_old and comm_cart may differ.
- Here, MPI merely keeps track of the topology information.

MPI_Cart_coords & MPI_Cart_rank

```
int MPI_Cart_coords(MPI_Comm comm, int rank, int maxdims, int coords[])
int MPI_Cart_rank(MPI_Comm comm, const int coords[], int *rank)
```

- These are two "service" functions responsible for the translation between Cartesian process coordinates and an MPI rank.
- MPI_Cart_coords() calculates the Cartesian coordinates for a given rank.
- The reverse mapping, i.e., from Cartesian coordinates to an MPI rank, is performed by MPI_Cart_rank().

Example of 2D Cartesian grid

```
int rank, size;
MPI_Comm comm;
int dim[2], period[2], reorder;
int coord[2], id;
// ....
dim[0]=4; dim[1]=3;
period[0]=0; period[1]=1;
reorder=1:
MPI_Cart_create(MPI_COMM_WORLD, 2, dim, period, reorder, &comm);
if (rank == 5) {
    MPI_Cart_coords(comm, rank, 2, coord);
    printf("Rank %d coordinates are %d %d\n", rank, coord[0], coord[1]);
if(rank==0) {
    coord[0]=3: coord[1]=1:
    MPI Cart rank(comm, coord, &id):
    printf("The processor at position (%d, %d) has rank %d\n", coord[0], coord[1], id);
}
```

MPI_Cart_shift

A regular task with domain decomposition is to find out who the next neighbors of a certain process are along a certain Cartesian dimension.

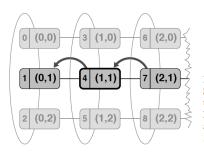


Figure 9.7: Example for the result of MPI_Cart_shift() on a part of the Cartesian topology from Figure 9.6. Executed by rank 4 with direction=0 and disp=-1, the function returns rank source=7 and rank dest=1.

1D example

```
// ....
dims[0] = size:
periods[0] = 1:
MPI_Cart_create( MPI_COMM_WORLD, 1, dims, periods, 0, &comm );
MPI Cart shift( comm. 0. 1. &source. &dest ):
if (source != ((rank - 1 + size) % size)) {
    errs++;
    printf( "source for shift 1 is %d\n", source ):fflush(stdout):
if (dest != ((rank + 1) % size)) {
    errs++;
    printf( "dest for shift 1 is %d\n", dest ):fflush(stdout):
MPI Cart shift( comm. 0. -1. &source. &dest ):
if (source != ((rank + 1) % size)) {
    errs++;
    printf( "source for shift -1 is %d\n", source ):fflush(stdout);
if (dest != ((rank - 1 + size) % size)) {
    errs++;
    printf( "dest for shift -1 is %d\n", dest ):fflush(stdout):
```