An Introduction to MPI

Parallel Programming with the Message Passing Interface

Outline

- Background
  - The message-passing model
  - Origins of MPI and current status
  - Sources of further MPI information
- Basics of MPI message passing
  - Hello, World!
  - Fundamental concepts
  - Simple examples in Fortran and C
- Extended point-to-point operations
  - non-blocking communication
  - modes

Outline (continued)

- Advanced MPI topics
  - Collective operations
  - More on MPI datatypes
  - Application topologies
  - The profiling interface
- Toward a portable MPI environment

The Message-Passing Model

- A *process* is (traditionally) a program counter and address space.
- Processes may have multiple *threads* (program counters and associated stacks) sharing a single address space. MPI is for communication among processes, which have separate address spaces.
- Interprocess communication consists of
  – Synchronization
  – Movement of data from one process's address space to another's.

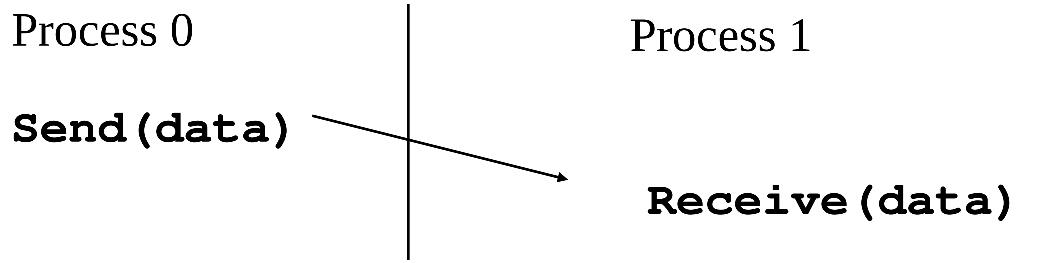
Types of Parallel Computing Models

- Data Parallel - the same instructions are carried out simultaneously on multiple data items (SIMD)
- Task Parallel - different instructions on different data (MIMD)
- SPMD (single program, multiple data) not synchronized at individual operation level
- SPMD is equivalent to MIMD since each MIMD program can be made SPMD (similarly for SIMD, but not in practical sense.)

Message passing (and MPI) is for MIMD/SPMD parallelism. HPF is an example of an SIMD interface.

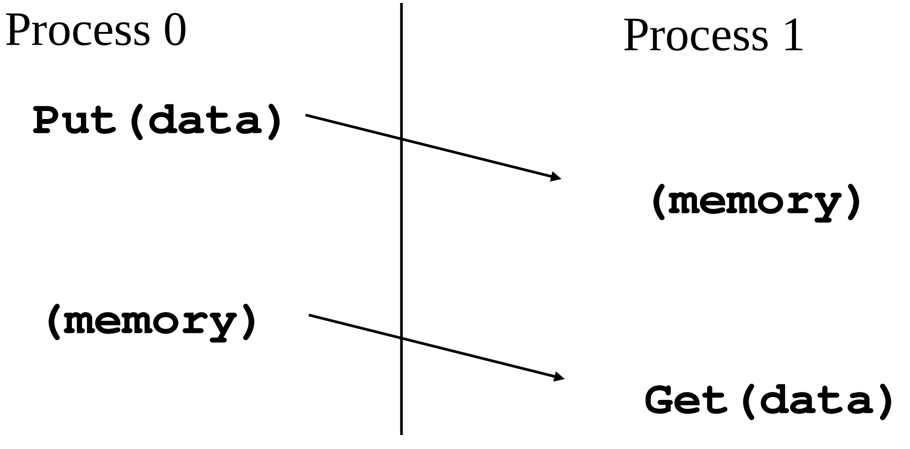
Cooperative Operations for Communication

- The message-passing approach makes the exchange of data *cooperative*.
- Data is explicitly *sent* by one process and *received* by another.
- An advantage is that any change in the receiving process's memory is made with the receiver's explicit participation.
- Communication and synchronization are combined.



One-Sided Operations for Communication

- One-sided operations between processes include remote memory reads and writes
- Only one process needs to explicitly participate.
- An advantage is that communication and synchronization are decoupled
- One-sided operations are part of MPI-2.



What is MPI?

- A *message-passing library specification*
  - extended message-passing model
  - not a language or compiler specification
  - not a specific implementation or product
- For parallel computers, clusters, and heterogeneous networks
- Full-featured
- Designed to provide access to advanced parallel hardware for
  - end users
  - library writers
  - tool developers

MPI Sources

- The Standard itself:
  - at http://www.mpi-forum.org
  - All MPI official releases, in both postscript and HTML
- Books:
  - *Using MPI: Portable Parallel Programming with the Message-Passing Interface*, by Gropp, Lusk, and Skjellum, MIT Press, 1994.
  - *MPI: The Complete Reference,* by Snir, Otto, Huss-Lederman, Walker, and Dongarra, MIT Press, 1996.
  - *Designing and Building Parallel Programs*, by Ian Foster, Addison-Wesley, 1995.
  - *Parallel Programming with MPI*, by Peter Pacheco, Morgan-Kaufmann, 1997.
  - *MPI: The Complete Reference Vol 1 and 2,*MIT Press, 1998(Fall).
- Other information on Web:
  - at http://www.mcs.anl.gov/mpi
  - pointers to lots of stuff, including other talks and tutorials, a FAQ, other MPI pages

Why Use MPI?

- MPI provides a powerful, efficient, and *portable* way to express parallel programs
- MPI was explicitly designed to enable libraries…
- … which may eliminate the need for many users to learn (much of) MPI

A Minimal MPI Program (C)

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

int main( int argc, char *argv[] )
{
    MPI_Init( &argc, &argv );
    printf( "Hello, world!\n" );
    MPI_Finalize();
    return 0;
}
```

Notes on C and Fortran

- C and Fortran bindings correspond closely
- In C:
  - mpi.h must be #included
  - MPI functions return error codes or **`MPI_SUCCESS`**
- In Fortran:
  - mpif.h must be included, or use MPI module (MPI-2)
  - All MPI calls are to subroutines, with a place for the return code in the last argument.
- C++ bindings, and Fortran-90 issues, are part of MPI-2.

Error Handling

- By default, an error causes all processes to abort.
- The user can cause routines to return (with an error code) instead.
  - In C++, exceptions are thrown (MPI-2)
- A user can also write and install custom error handlers.
- Libraries might want to handle errors differently from applications.

Running MPI Programs

- The MPI-1 Standard does not specify how to run an MPI program, just as the Fortran standard does not specify how to run a Fortran program.
- In general, starting an MPI program is dependent on the implementation of MPI you are using, and might require various scripts, program arguments, and/or environment variables.
- **`mpiexec <args>`** is part of MPI-2, as a recommendation, but not a requirement
  - You can use mpiexec for MPICH and mpirun for SGI's MPI in this class

Finding Out About the Environment

- Two important questions that arise early in a parallel program are:
  - How many processes are participating in this computation?
  - Which one am I?
- MPI provides functions to answer these questions:
  - **`MPI_Comm_size`** reports the number of processes.
  - **`MPI_Comm_rank`** reports the *rank*, a number between 0 and size-1, identifying the calling process

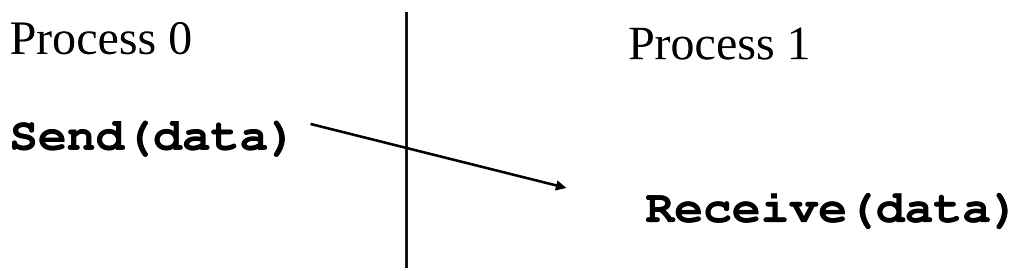
Better Hello (C)

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

int main( int argc, char *argv[] )
{
    int rank, size;
    MPI_Init( &argc, &argv );
    MPI_Comm_rank( MPI_COMM_WORLD, &rank );
    MPI_Comm_size( MPI_COMM_WORLD, &size );
    printf( "I am %d of %d\n", rank, size );
    MPI_Finalize();
    return 0;
}
```

MPI Basic Send/Receive

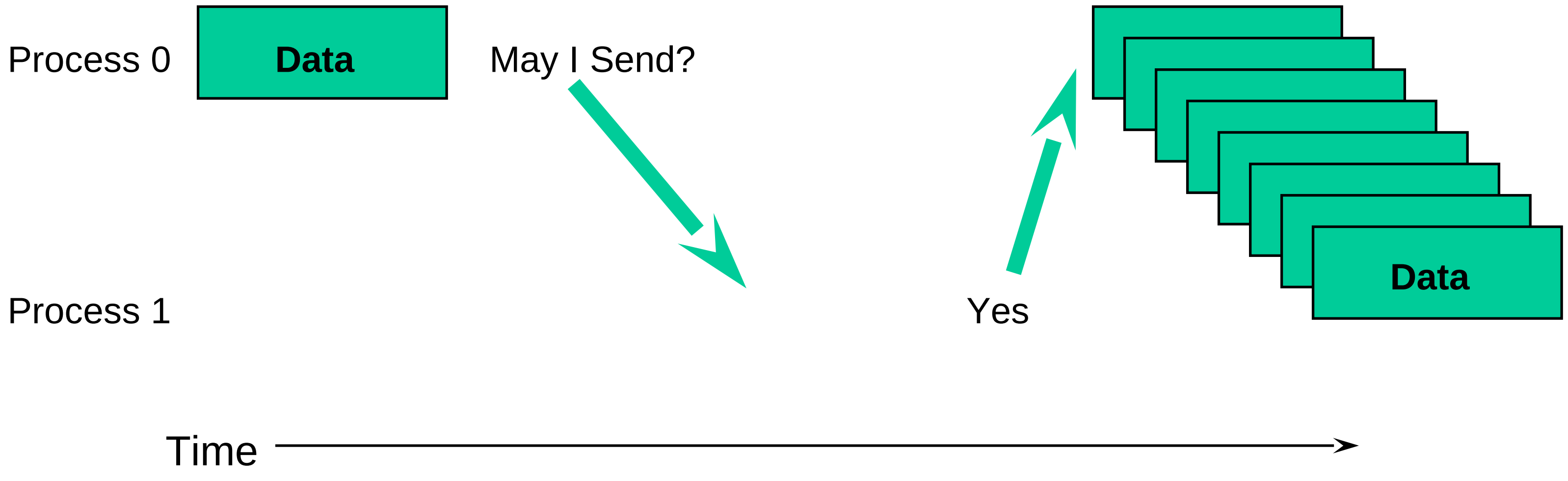
- We need to fill in the details in



- Things that need specifying:
  - How will “data” be described?
  - How will processes be identified?
  - How will the receiver recognize/screen messages?
  - What will it mean for these operations to complete?

What is message passing?

- Data transfer plus synchronization



- Requires cooperation of sender and receiver
- Cooperation not always apparent in code

Some Basic Concepts

- Processes can be collected into *groups*.
- Each message is sent in a *context*, and must be received in the same context.
- A group and context together form a *communicator*.
- A process is identified by its *rank* in the group associated with a communicator.
- There is a default communicator whose group contains all initial processes, called **`MPI_COMM_WORLD`**.

MPI Datatypes

- The data in a message to sent or received is described by a triple (address, count, datatype), where
- An MPI *datatype* is recursively defined as:
  – predefined, corresponding to a data type from the language (e.g., MPI_INT, MPI_DOUBLE_PRECISION)
  – a contiguous array of MPI datatypes
  – a strided block of datatypes
  – an indexed array of blocks of datatypes
  – an arbitrary structure of datatypes
- There are MPI functions to construct custom datatypes, such an array of (int, float) pairs, or a row of a matrix stored columnwise.

MPI Tags

- Messages are sent with an accompanying user-defined integer *tag*, to assist the receiving process in identifying the message.
- Messages can be screened at the receiving end by specifying a specific tag, or not screened by specifying **`MPI_ANY_TAG`** as the tag in a receive.
- Some non-MPI message-passing systems have called tags “message types”. MPI calls them tags to avoid confusion with datatypes.

MPI Basic (Blocking) Send

MPI_SEND (start, count, datatype, dest, tag, comm)

- The message buffer is described by (**`start, count, datatype`**).
- The target process is specified by **`dest`**, which is the rank of the target process in the communicator specified by **`comm`**.
- When this function returns, the data has been delivered to the system and the buffer can be reused. The message may not have been received by the target process.

MPI Basic (Blocking) Receive

MPI_RECV(start, count, datatype, source, tag, comm, status)

- Waits until a matching (on **`source`** and **`tag`**) message is received from the system, and the buffer can be used.
- **`source`** is rank in communicator specified by **`comm`**, or **`MPI_ANY_SOURCE`**.
- **`status`** contains further information
- Receiving fewer than **`count`** occurrences of **`datatype`** is OK, but receiving more is an error.

Retrieving Further Information

- **`Status`** is a data structure allocated in the user's program.
- In C:

```
int recvd_tag, recvd_from, recvd_count;
MPI_Status status;
MPI_Recv(..., MPI_ANY_SOURCE, MPI_ANY_TAG, ..., &status )
recvd_tag  = status.MPI_TAG;
recvd_from = status.MPI_SOURCE;
MPI_Get_count( &status, datatype, &recvd_count );
```

- In Fortran:

```
integer recvd_tag, recvd_from, recvd_count
integer status(MPI_STATUS_SIZE)
call MPI_RECV(..., MPI_ANY_SOURCE, MPI_ANY_TAG, .. status, ierr)
tag_recvd  = status(MPI_TAG)
recvd_from = status(MPI_SOURCE)
call MPI_GET_COUNT(status, datatype, recvd_count, ierr)
```

Why Datatypes?

- Since all data is labeled by type, an MPI implementation can support communication between processes on machines with very different memory representations and lengths of elementary datatypes (heterogeneous communication).
- Specifying application-oriented layout of data in memory
  - reduces memory-to-memory copies in the implementation
  - allows the use of special hardware (scatter/gather) when available

Tags and Contexts

- Separation of messages used to be accomplished by use of tags, but
  - this requires libraries to be aware of tags used by other libraries.
  - this can be defeated by use of “wild card” tags.
- Contexts are different from tags
  - no wild cards allowed
  - allocated dynamically by the system when a library sets up a communicator for its own use.
- User-defined tags still provided in MPI for user convenience in organizing application
- Use MPI_Comm_split to create new communicators

MPI is Simple

- Many parallel programs can be written using just these six functions, only two of which are non-trivial:
  - **`MPI_INIT`**
  - **`MPI_FINALIZE`**
  - **`MPI_COMM_SIZE`**
  - **`MPI_COMM_RANK`**
  - **`MPI_SEND`**
  - **`MPI_RECV`**
- Point-to-point (send/recv) isn’t the only way...

Introduction to Collective Operations in MPI

- Collective operations are called by all processes in a communicator.
- **`MPI_BCAST`** distributes data from one process (the root) to all others in a communicator.
- **`MPI_REDUCE`** combines data from all processes in communicator and returns it to one process.
- In many numerical algorithms, **`SEND/RECEIVE`** can be replaced by **`BCAST/REDUCE`**, improving both simplicity and efficiency.

Example: PI in C -1

```
#include "mpi.h"
#include <math.h>
int main(int argc, char *argv[])
{
   int done = 0, n, myid, numprocs, i, rc;
   double PI25DT = 3.141592653589793238462643;
   double mypi, pi, h, sum, x, a;
   MPI_Init(&argc,&argv);
   MPI_Comm_size(MPI_COMM_WORLD,&numprocs);
   MPI_Comm_rank(MPI_COMM_WORLD,&myid);
   while (!done)  {
     if (myid == 0) {
       printf("Enter the number of intervals: (0 quits) ");
       scanf("%d",&n);
     }
     MPI_Bcast(&n, 1, MPI_INT, 0, MPI_COMM_WORLD);
     if (n == 0) break;
```

Example: PI in C - 2

```
    h   = 1.0 / (double) n;
     sum = 0.0;
     for (i = myid + 1; i <= n; i += numprocs) {
       x = h * ((double)i - 0.5);
       sum += 4.0 / (1.0 + x*x);
     }
     mypi = h * sum;
     MPI_Reduce(&mypi, &pi, 1, MPI_DOUBLE, MPI_SUM, 0,
                MPI_COMM_WORLD);
     if (myid == 0)
       printf("pi is approximately %.16f, Error is %.16f\n",
               pi, fabs(pi - PI25DT));
   }
   MPI_Finalize();
  return 0;
}
```

Alternative set of 6 Functions for Simplified MPI

  - **MPI_INIT**
  - **MPI_FINALIZE**
  - **MPI_COMM_SIZE**
  - **MPI_COMM_RANK**
  - **MPI_BCAST**
  - **MPI_REDUCE**
- What else is needed (and why)?

Sources of Deadlocks

- Send a large message from process 0 to process 1
  - If there is insufficient storage at the destination, the send must wait for the user to provide the memory space (through a receive)
- What happens with

Process 0	Process 1
`Send(1)`	**`Send(0)`**
`Recv(1)`	**`Recv(0)`**

- This is called "unsafe" because it depends on the availability of system buffers

Some Solutions to the “unsafe” Problem

- Order the operations more carefully:

Process 0	Process 1
`Send(1)`	**`Recv(0)`**
`Recv(1)`	**`Send(0)`**

- Use non-blocking operations:

Process 0	Process 1
`Isend(1)`	**`Isend(0)`**
`Irecv(1)`	**`Irecv(0)`**
`Waitall`	**`Waitall`**

Toward a Portable MPI Environment

- MPICH is a high-performance portable implementation of MPI (1).
- It runs on MPP's, clusters, and heterogeneous networks of workstations.
- In a wide variety of environments, one can do:

```
configure
make
mpicc -mpitrace myprog.c
mpirun -np 10 myprog
upshot myprog.log
```

to build, compile, run, and analyze performance.

Extending the Message-Passing Interface

- Dynamic Process Management
  - Dynamic process startup
  - Dynamic establishment of connections
- One-sided communication
  - Put/get
  - Other operations
- Parallel I/O
- Other MPI-2 features
  - Generalized requests
  - Bindings for C++/ Fortran-90; interlanguage issues

Some Simple Exercises

- Compile and run the **`hello`** and **`pi`** programs.
- Modify the **`pi`** program to use send/receive instead of bcast/reduce.
- Write a program that sends a message around a ring. That is, process 0 reads a line from the terminal and sends it to process 1, who sends it to process 2, etc. The last process sends it back to process 0, who prints it.
- Time programs with **`MPI_WTIME`**. (Find it.)

When to use MPI

- Portability and Performance
- Irregular Data Structures
- Building Tools for Others
  - Libraries
- Need to Manage memory on a per processor basis

Summary

- The parallel computing community has cooperated on the development of a standard for message-passing libraries.
- There are many implementations, on nearly all platforms.
- MPI subsets are easy to learn and use.
- Lots of MPI material is available.