CSC 447: Parallel Programming for Multi-Core and Cluster Systems

Message Passing with MPI

Instructor: Haidar M. Harmanani

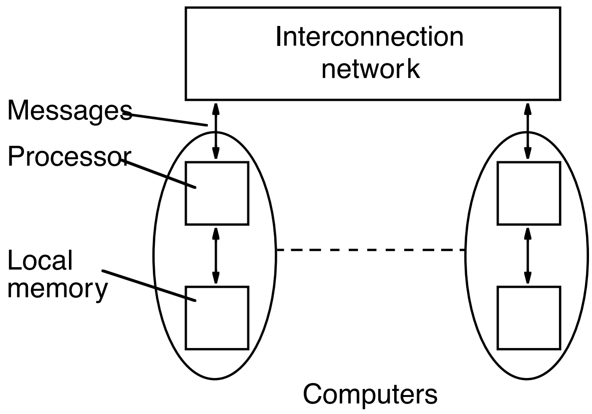
Spring 2017

Outline

- Message-passing model
- Message Passing Interface (MPI)
- Coding MPI programs
- Compiling MPI programs
- Running MPI programs
- Benchmarking MPI programs
- Mixing MPI and Pthreads

Message-Passing Multicomputer

- Complete computers connected through an interconnection network:



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.
- We will be looking at the Message Passing Interface
  – MPI

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

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

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 MPI C

- **`mpi.h`** must be **`#included`**
- MPI functions return error codes or **`MPI_SUCCESS`**
- 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
- `mpirun -np <p> <exec> <args>`

Execution on 3 CPUs

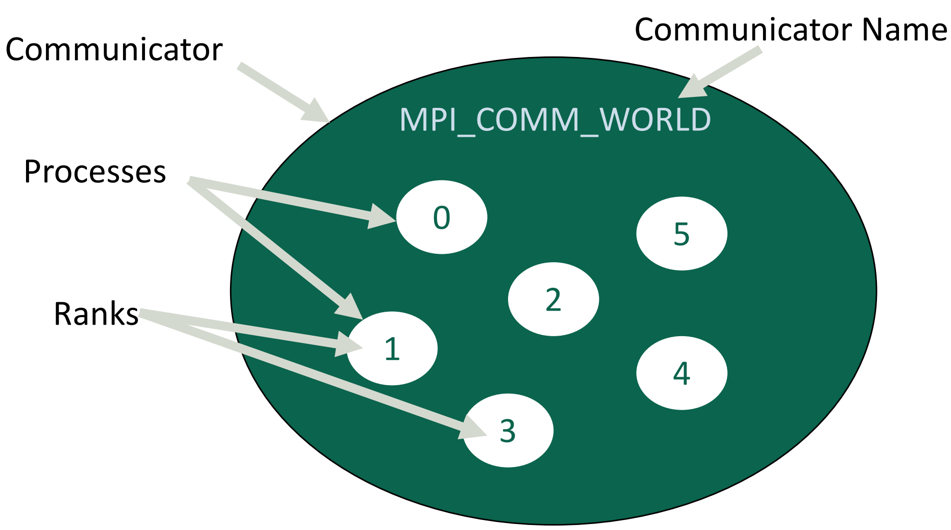
- `% mpirun -np 3 sat`

- `0) 0110111110011001`
- `0) 1110111111011001`
- `2) 1010111110011001`
- `1) 1110111110011001`
- `1) 1010111111011001`
- `1) 0110111110111001`
- `0) 1010111110111001`
- `2) 0110111111011001`
- `2) 1110111110111001`
- `Process 1 is done`
- `Process 2 is done`
- `Process 0 is done`

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

Communicator



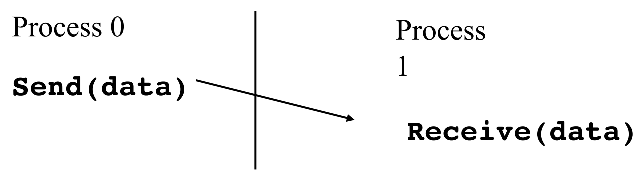
Better Hello (C)

```
#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

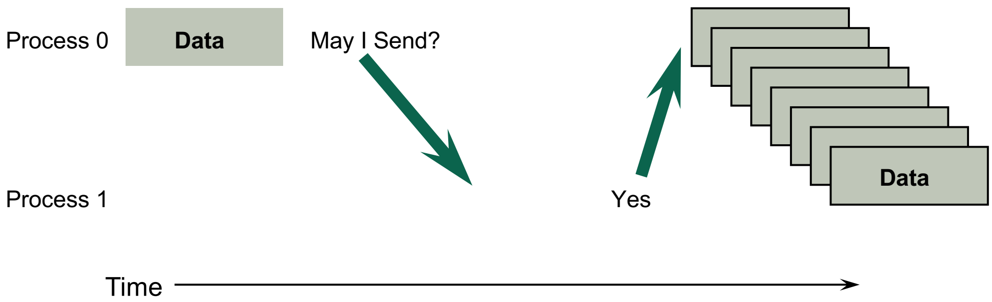
- We need to fill in the details in



- 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`**.

Using SPMD Computational Model

```
main (int argc, char *argv[])
{
MPI_Init(&argc, &argv);
        .
        .
/*find process rank */
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);

if (myrank == 0)
        master();
else
        slave();
        .
        .
MPI_Finalize();
}
```

where master() and slave() are to be executed by master process and slave process, respectively.

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.

Example

To send an integer x from process 0 to process 1,

```
MPI_Comm_rank(MPI_COMM_WORLD,&myrank); /* find rank */

if (myrank == 0) {
  int x;
  MPI_Send(&x, 1, MPI_INT, 1, msgtag, MPI_COMM_WORLD);
} else if (myrank == 1) {
  int x;
  MPI_Recv(&x, 1, MPI_INT,0,msgtag,MPI_COMM_WORLD,status);
}
```

Retrieving Further Information

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

```
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 );
```


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

```
#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 (Continued)

```
    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;
}
```


Example 2:

```
#include "mpi.h"
#include <stdio.h>
#include <math.h>
#define MAXSIZE 1000
void main(int argc, char *argv)
{
  int myid, numprocs;
  int data[MAXSIZE], i, x, low, high, myresult, result;
  char fn[255];
  char *fp;
  MPI_Init(&argc,&argv);
  MPI_Comm_size(MPI_COMM_WORLD,&numprocs);
  MPI_Comm_rank(MPI_COMM_WORLD,&myid);
```

(Continued)

```
if (myid == 0) {  /* Open input file and initialize data */
          strcpy(fn,getenv("HOME"));
          strcat(fn,"/MPI/rand_data.txt");
          if ((fp = fopen(fn,"r")) == NULL) {
                    printf("Can't open the input file: %s\n\n", fn);
                    exit(1);
          }
          for(i = 0; i < MAXSIZE; i++) fscanf(fp,"%d", &data[i]);
}
MPI_Bcast(data, MAXSIZE, MPI_INT, 0, MPI_COMM_WORLD); /* broadcast data */
x = n/nproc; /* Add my portion Of data */
low = myid * x;
high = low + x;
for(i = low; i < high; i++)
    myresult += data[i];
printf("I got %d from %d\n", myresult, myid); /* Compute global sum */
MPI_Reduce(&myresult, &result, 1, MPI_INT, MPI_SUM, 0, MPI_COMM_WORLD);
if (myid == 0) printf("The sum is %d.\n", result);
MPI_Finalize();
}
```


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

When to use MPI

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

Benchmarking MPI Programs

- **`MPI_Barrier`** — barrier synchronization
- **`MPI_Wtick`** — timer resolution
- **`MPI_Wtime`** — current time

Benchmarking MPI Programs

- ```
  double elapsed_time;
  …
  ```
- ```
  MPI_Init (&argc, &argv);
  MPI_Barrier (MPI_COMM_WORLD);
  elapsed_time = - MPI_Wtime();
  …
  ```
- ```
  MPI_Reduce (…);
  elapsed_time += MPI_Wtime();
  ```


When *not* to use MPI

- Regular computation matches HPF
  – But see PETSc/HPF comparison (ICASE 97-72)
- Solution (e.g., library) already exists
  – http://www.mcs.anl.gov/mpi/libraries.html
- Require Fault Tolerance
  – Sockets
- Distributed Computing
  – CORBA, DCOM, etc.
  ```

Mixing MPI with Pthreads

- Each MPI process typically creates and then manages **N** threads, where **N** makes the best use of the available cores/node.
- Finding the best value for **N** will vary with the platform and your application's characteristics.
- In general, there may be problems if multiple threads make MPI calls.
  - The program may fail or behave unexpectedly.
- If MPI calls must be made from within a thread, they should be made only by one thread.

Mixing MPI with Pthreads: `dotprod`

```
void *dotprod(void *arg)
{
   int i, start, end, len, numthrds, myid;
   long mythrd;
   double mysum, *x, *y;

   mythrd = (long)arg;
   MPI_Comm_rank (MPI_COMM_WORLD, &myid);

   numthrds = dotstr.numthrds;
   len = dotstr.veclen;
   start = myid*numthrds*len + mythrd*len;
   end   = start + len;
   x = dotstr.a;
   y = dotstr.b;
```

Continued

Mixing MPI with Pthreads: `dotprod`

```
/* Perform the dot product and assign result to the appropriate variable in the
structure. */

mysum = 0;
for (i=start; i<end ; i++)
 {
   mysum += (x[i] * y[i]);
 }

/* Lock a mutex prior to updating the value in the structure, and unlock it
upon updating.*/

pthread_mutex_lock (&mutexsum);
printf("Task %d thread %ld adding partial sum of %f to node sum of %f\n",
        myid, mythrd, mysum, dotstr.sum);
dotstr.sum += mysum;
pthread_mutex_unlock (&mutexsum);

pthread_exit((void*)0);
}
```

End dotprod()

Mixing MPI with Pthreads: `main`

```
int main(int argc, char* argv[])
{
int len=VECLEN, myid, numprocs;
long i;
int nump1, numthrds;
double *a, *b;
double nodesum, allsum;
void *status;
pthread_attr_t attr;

/* MPI Initialization */
MPI_Init (&argc, &argv);
MPI_Comm_size (MPI_COMM_WORLD, &numprocs);
MPI_Comm_rank (MPI_COMM_WORLD, &myid);

/* Assign storage and initialize values */
numthrds=MAXTHRDS;
a = (double*) malloc (numprocs*numthrds*len*sizeof(double));
b = (double*) malloc (numprocs*numthrds*len*sizeof(double));
...
```

Continued

Mixing MPI with Pthreads: `main`

```
a = (double*) malloc (numprocs*numthrds*len*sizeof(double));
b = (double*) malloc (numprocs*numthrds*len*sizeof(double));

for (i=0; i<len*numprocs*numthrds; i++) {
  a[i]=1;
  b[i]=a[i];
  }

dotstr.veclen = len;
dotstr.a = a;
dotstr.b = b;
dotstr.sum=0;
dotstr.numthrds=MAXTHRDS;

/* Create thread attribute to specify that the main thread needs
to join with the threads it creates. */

pthread_attr_init(&attr );
pthread_attr_setdetachstate(&attr, PTHREAD_CREATE_JOINABLE);
```

Continued

Mixing MPI with Pthreads: `main`

```
/* Create a mutex */
pthread_mutex_init (&mutexsum, NULL);

/* Create threads within this node to perform the dotproduct  */
for(i=0;i<numthrds;i++) {
  pthread_create( &callThd[i], &attr, dotprod, (void *)i);
  }

/* Release the thread attribute handle as it is no longer needed */
pthread_attr_destroy(&attr );

/* Wait on the other threads within this node */
for(i=0;i<numthrds;i++) {
  pthread_join( callThd[i], &status);
  }

nodesum = dotstr.sum;
printf("Task %d node sum is %f\n",myid, nodesum);
```

Continued

Mixing MPI with Pthreads: `main`

```
/* After the dot product, perform a summation of results on each node */
MPI_Reduce (&nodesum, &allsum, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);

if (myid == 0)
printf ("Done. MPI with threads version: sum  =  %f \n", allsum);
MPI_Finalize();
free (a);
free (b);
pthread_mutex_destroy(&mutexsum);
exit (0);
}
```

End main()

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.