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Recitation: Introduction to MPI

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Based on slides by Greg Kesden

Based on earlier slides by William Gropp, Ewing Lusk of Argonne National Laboratory

Today we’ll learn…

- Message Passing Interface (MPI)
  - Basics
    - Communicators
    - Datatypes
  - How to build & run MPI programs
  - Send / Receive messages
    - Blocking
    - Non-blocking
  - Broadcast / Reduce
  - Debug / Profile

The Message-Passing Model

- A *process* is (traditionally) a program counter and address space.
- Processes may have multiple *threads* (program counters and associated stacks), which share a single address space.
- **MPI is for communication among processes**
  - Synchronization + data movement between address spaces

Flynn Parallelism Taxonomy

- SIMD (data-parallel): Vector
- SPMD (loosely sync'd data-parallel): GPU / **MPI?**
- MIMD (task-parallel): Pthreads / **MPI**
- MISD: streaming ???

MPI is Simple

- Many parallel programs can be written using just these six functions:
  - **`MPI_INIT`**
  - **`MPI_FINALIZE`**
  - **`MPI_COMM_SIZE`**
  - **`MPI_COMM_RANK`**
  - **`MPI_SEND`**
  - **`MPI_RECV`**

Setup / teardown (`MPI_INIT`, `MPI_FINALIZE`)

Who am I? (`MPI_COMM_SIZE`, `MPI_COMM_RANK`)

Message passing (`MPI_SEND`, `MPI_RECV`)

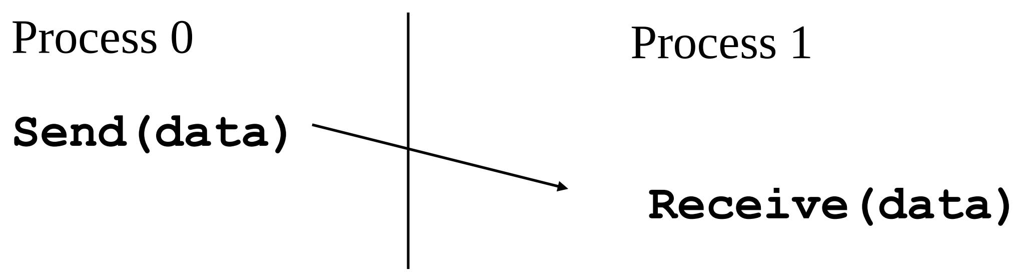
…But often painful

- In OpenMP, only needed a few #pragmas to make sequential code parallel
  - Easy because hardware takes care of data movement **implicitly** + guarantees coherence
  - ➔ Threads get the data they need when they need it automatically

- MPI requires **explicit** data movement
- ➔ Programmer (that's **you!**) must say exactly what data goes where and when

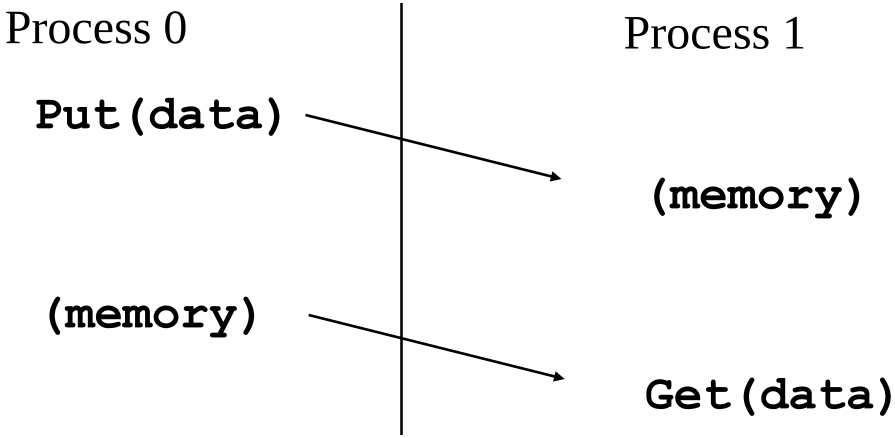
Cooperative Operations for Communication

- 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 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



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
- Designed to provide access to advanced parallel hardware for
  - end users
  - library writers
  - tool developers

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;
}
```

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

- MPI does not specify how to run an MPI program
  - Just as the C/C++ standard does not specify how to run a C/C++ program
- **`mpirun <args>`** is a recommendation, but not a requirement

Building MPI programs on GHC machines

- Setup your environment:
  - export PATH=$PATH:/usr/lib64/openmpi/bin
- Compile with MPIC++ / MPICC:
  - $ mpic++ -o hello hello.cpp
- Run via mpirun:
  - $ mpirun -c <NPROCS> hello

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)

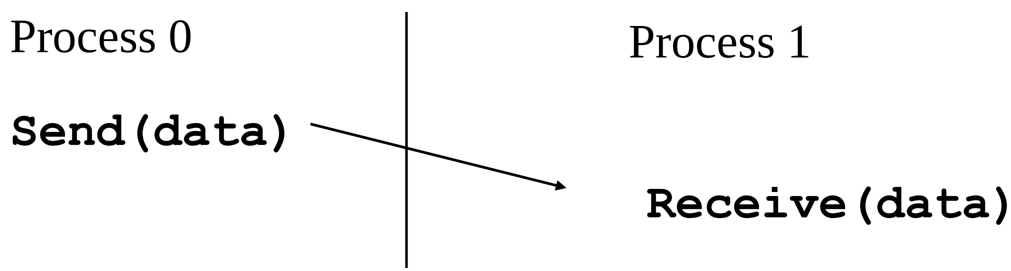
```
#include "mpi.h"
#include <stdio.h>

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;
}
```

Better Hello

- Note that in MPI each process is identical
- There is no “main thread” where execution begins

MPI Basic Send/Receive

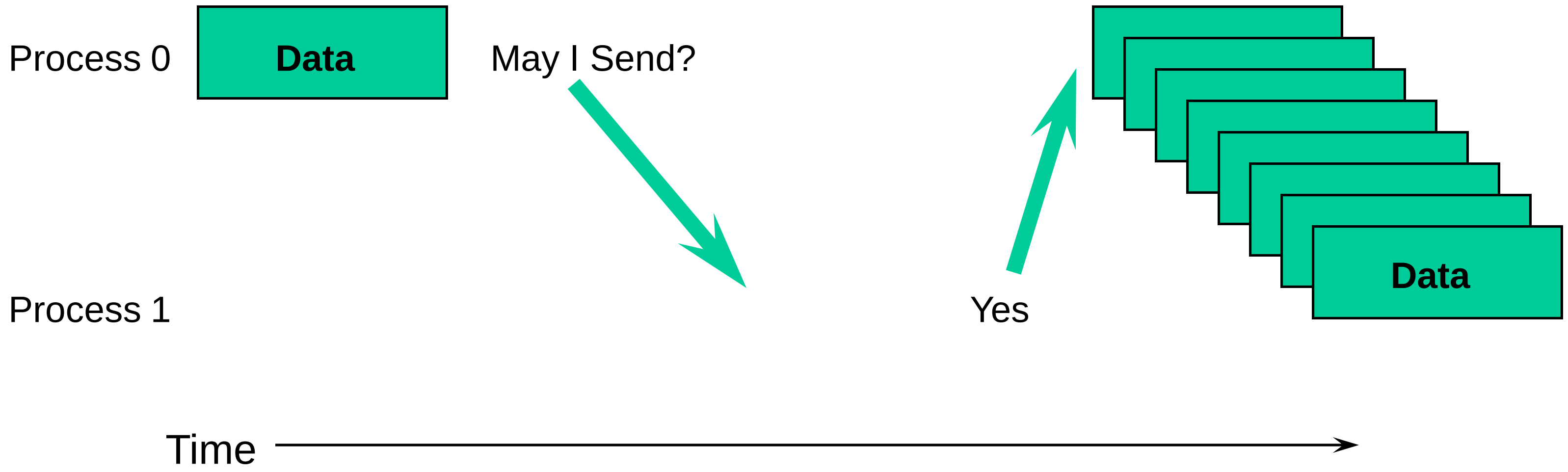
- We need to fill in the details in



- 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.
- Group + context ➔ *communicator*.

- There is a default communicator whose group contains all initial processes, called **`MPI_COMM_WORLD`**.

MPI Datatypes

- Messages are 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.

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 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.
  – Beware: 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.

MPI_Status

```
typedef struct _MPI_Status {
  int count;
  int cancelled;
  int MPI_SOURCE;
  int MPI_TAG;
  int MPI_ERROR;
} MPI_Status, *PMPI_Status;
```

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 );
```

Send & Receive Example (non-MPI version)

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

int main(int argc, char* argv[]) {
  int N = 32;
  double fibs[N+2];
  fibs[0] = 1; fibs[1] = 1;
  for (int i = 2; i < N; i++) {
    fibs[i] = fibs[i-1] + fibs[i-2];
    printf("The %dth Fibonacci number is %g.\n", i, fibs[i]);
  }
  return 0;
}
```

Send & Receive Example

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

int main(int argc, char* argv[]) {
  MPI_Init(&argc, &argv);

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

  MPI_Status status;
  double msg[2] = {1,1};

  if (rank > 0) {
    double fibs[2];

    do {
      MPI_Recv(fibs, 2, MPI_DOUBLE,
               MPI_ANY_SOURCE, /*tag*/ 0,
               MPI_COMM_WORLD, &status);
    }
    while (status.MPI_ERROR);
    double next = fibs[0] + fibs[1];
    msg[0] = fibs[1]; msg[1] = next;

    printf("The %dth Fibonacci number is
%g.\n",
           rank+2, next);
  }

  if (rank+1 < size) {
    int ret;
    ret = MPI_Send(msg, 2, MPI_DOUBLE,
                   /*dest*/ rank + 1,
                   /*tag*/ 0, MPI_COMM_WORLD);
    assert(ret == MPI_SUCCESS);
  }

  MPI_Finalize();
  return 0;
}
```

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

Deadlock example

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

int main(int argc, char* argv[]) {
  MPI_Init(&argc, &argv);

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

  MPI_Status status;

  int msg = 1;

  MPI_Recv(&msg, 1, MPI_INTEGER, (rank-1) % size, 0, MPI_COMM_WORLD, NULL);
  MPI_Send(&msg, 1, MPI_INTEGER, (rank+1) % size, 0, MPI_COMM_WORLD);

  printf("Process %d done.\n", rank);

  MPI_Finalize();
  return 0;
}
```

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`**

(Fixed?) Deadlock example

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

int main(int argc, char* argv[]) {
  MPI_Init(&argc, &argv);

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

  MPI_Status status;

  int msg = 1;

  MPI_Send(&msg, 1, MPI_INTEGER, (rank+1) % size, 0, MPI_COMM_WORLD);
  MPI_Recv(&msg, 1, MPI_INTEGER, (rank-1) % size, 0, MPI_COMM_WORLD, NULL);

  printf("Process %d done.\n", rank);

  MPI_Finalize();
  return 0;
}
```

Will (probably) work in this case only because message is small - not reliable!!!

Non-Blocking Receive and Send

- int MPI_Isend(const void *buf,
  int count,
  MPI_Datatype datatype,
  int dest, int tag,
  MPI_Comm comm,
  MPI_Request *request)

- int MPI_Irecv(void *buf,
  int count,
  MPI_Datatype datatype,
  int source,
  int tag,
  MPI_Comm comm,
  MPI_Request *request)

Waiting for a Non-Blocking Send and Receive to Complete

- Isend/Irecv return a MPI_Request* handle

- int MPI_Wait(MPI_Request *request,
  MPI_Status *status)
  - Blocks for a previously non-blocking receive

- int MPI_Test(MPI_Request *request,
  int *flag,
  MPI_Status *status)
  - Test determines if done
    - C/C++ Convention: True/0, False/Non-Zero otherwise

Fixed deadlock example #1

```
…
int main(int argc, char* argv[]) {
  MPI_Init(&argc, &argv);

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

  int sendmsg = 1, recvmsg;
  MPI_Request request;

  MPI_Irecv(&recvmsg, 1, MPI_INTEGER, (rank-1)%size, 0, MPI_COMM_WORLD, &request);
  MPI_Send(&sendmsg, 1, MPI_INTEGER, (rank+1)%size, 0, MPI_COMM_WORLD);
  MPI_Wait(&request, MPI_STATUS_IGNORE);

  printf("Process %d done.\n", rank, recvmsg, 0);
  assert(recvmsg == 1);

  MPI_Finalize();
  return 0;
}
```

MPI_Probe

- int MPI_Probe(int source,
  int tag,
  MPI_Comm comm,
  MPI_Status *status)

- Like a MPI_Recv, but just gets status

Probe example

```
… if (rank == 0) {
    int msglen = rand() % 1024; /* send a message of dynamic size */
    int *msg = new int[msglen];
    for (int i = 0; i < msglen; i++) {
      msg[i] = rand();
    }
    MPI_Send(msg, msglen, MPI_INTEGER, 1, 0, MPI_COMM_WORLD);
    delete [] msg;

  } else if (rank == 1) {
    MPI_Status status; /* figure out how big the message is before recving */
    MPI_Probe(MPI_ANY_SOURCE, 0, MPI_COMM_WORLD, &status);
    int msglen;
    MPI_Get_count(&status, MPI_INTEGER, &msglen);
    int* msg = new int[msglen];
    MPI_Recv(msg, msglen, MPI_INTEGER, MPI_ANY_SOURCE, 0, MPI_COMM_WORLD,
             MPI_STATUS_IGNORE);
    delete [] msg;
  }
…
```

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.

Bcast/reduce example:

```
int main(int argc, char *argv[])
{
    int done = 0, n;
    double PI25DT = 3.141592653589793238462643;
    double mypi, pi, h, sum, x, a;
    while (!done)  {
      printf("Enter the number of intervals: (0 quits) ");
      scanf("%d",&n);
      if (n == 0) break;
      h = 1.0 / (double) n;
      sum = 0.0;
      for (int i = 1; i <= n; i++) {
        x = h * ((double)i - 0.5);
        sum += 4.0 / (1.0 + x*x);
      }
      mypi = h * sum;
      if (myid == 0)
      printf("pi is approximately %.16f, Error is %.16f\n",
                pi, fabs(pi - PI25DT));
    }
    return 0;
}
```

Bcast/reduce example (OpenMP):

```
int main(int argc, char *argv[])
{
    int done = 0, n;
    double PI25DT = 3.141592653589793238462643;
    double mypi, pi, h, sum, x, a;
    while (!done)  {
      printf("Enter the number of intervals: (0 quits) ");
      scanf("%d",&n);
      if (n == 0) break;
      h = 1.0 / (double) n;
      sum = 0.0;
      # pragma omp parallel for schedule(static)
      for (int i = 1; i <= n; i++) {
        x = h * ((double)i - 0.5);
        sum += 4.0 / (1.0 + x*x);
      }
      mypi = h * sum;
      if (myid == 0)
      printf("pi is approximately %.16f, Error is %.16f\n",
              pi, fabs(pi - PI25DT));
    }
    return 0;
}
```

Bcast/reduce example (MPI):

```
#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;
}
```

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.)

Debugging MPI programs

- Don't neglect your old friend printf
  - `#define checkpoint() do { fprintf(stderr, "%s:%d\n", __FILE__, __LINE__) } while(0)`
- Attaching gdb to MPI processes
  - https://www.open-mpi.org/faq/?category=debugging
  - `#define wait_for_gdb() do { int __wait_for_gdb = 0; while(__wait_for_gdb == 0) { sleep(1); }; } while(0)`
  - Run gdb and attach at runtime, then manually set __wait_for_gdb
- There are more powerful tools…
  - https://portal.tacc.utexas.edu/software/ddt

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

Companion Material

- Online examples available at http://www.mcs.anl.gov/mpi/tutorials/perf
- ftp://ftp.mcs.anl.gov/mpi/mpiexmpl.tar.gz contains source code and run scripts that allows you to evaluate your own MPI implementation

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.