CS267
MPI

Bill Saphir

Berkeley Lab/NERSC

Phone: 510-486-4373

wcsaphir@lbl.gov

What is Message Passing?

- Message passing is a model for programming distributed memory parallel computers
  - Every processor executes an independent process
  - Disjoint address spaces, no shared data
  - All communication between processes is done cooperatively, through subroutine calls

- SPMD: single program, multiple data
  - Every processes is the “same” (e.g. a.out); may act on different data
- MPMD: multiple program, multiple data
  - Not all processes are the “same” (e.g. a.out, b.out, c.out)

What is the Message Passing Interface?

MPI is the de facto standard for scientific programming on distributed memory parallel computers.

- MPI is a library of routines that enable message passing applications
- MPI is an interface specification, not a specific implementation
- Almost all high performance scientific applications run at NERSC and other supercomputer centers use MPI

The message passing model is

- A painful experience for many application programmers
- Old technology – "assembly language for parallel programming"

Message passing has succeeded because

- It maps well to a wide range of hardware
- Parallelism is explicit and communication is explicit
    - Forces the programmer to tackle parallelization from the beginning.
- Parallelizing compilers are very hard
- MPI makes programs portable

MPI History

- Before MPI: different library for each type of computer:
  - CMMD (Thinking Machines CM5)
  - NX (Intel iPSC/860, Paragon)
  - MPL (SP2)
  - and many more
- PVM: tried to be a standard, but not high performance, not carefully specified
- MPI was developed by the **MPI Forum**: voluntary organization representing industry, government labs, academia
  - 1994 MPI-1 – codified existing practice
  - 1997 MPI-2 – research project
  - Both MPI-1 and MPI-2 were designed by committee. There is a core of good stuff but just because it’s in the standard doesn’t mean you should use it.

What’s in MPI

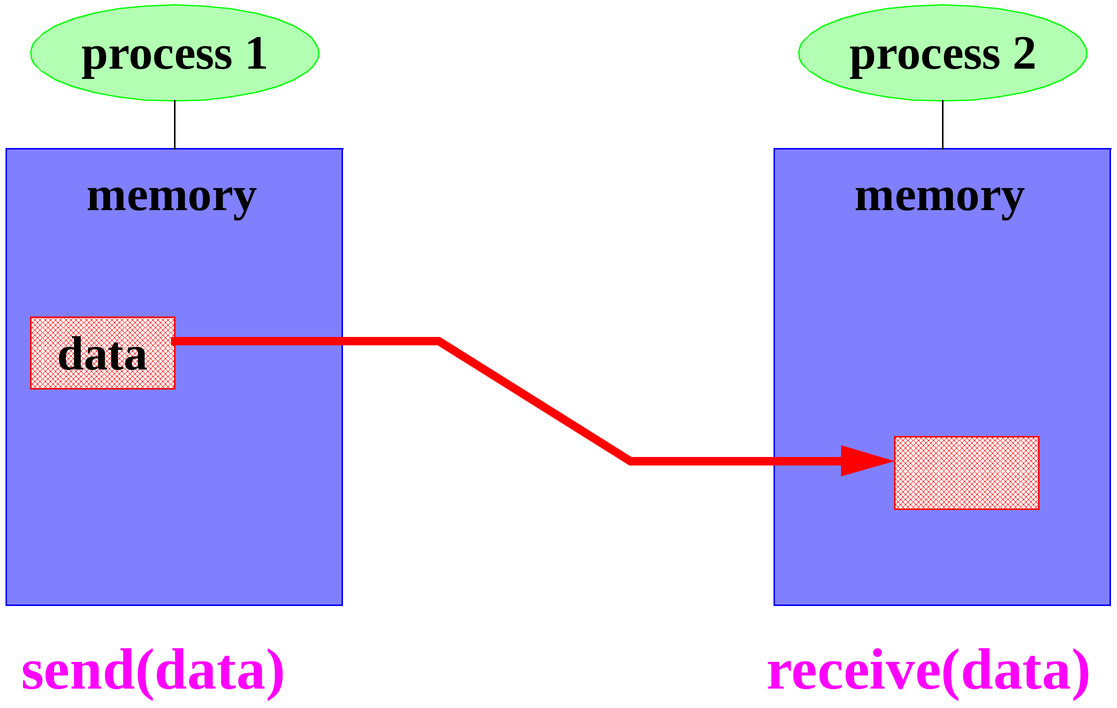
- MPI-1
  - Utilities: “who am I?”, “how many processes are there”
  - Send/recv communication
  - Collective communication e.g. broadcast, reduction, all-to-all
  - Lots of other stuff (for the longer version of this talk)

- MPI-2
  - Parallel I/O
  - C++/Fortran 90
  - One-sided communication – get/put
  - More stuff that is rarely used

Most of this talk will be about how to exchange data using MPI

Cooperative Data Transfer

Send operation in process 1 is matched by **receive** operation in process 2:



Models related to message passing

Active messages

- Message contains address of handler that processes incoming data
- No receive operations
- Separate bulk transfer mechanism

Remote memory operations (get/put, 1-sided communication)

- Process may directly access memory of another process with **get** and **put** operations
- Other synchronization mechanisms to coordinate access

Common features

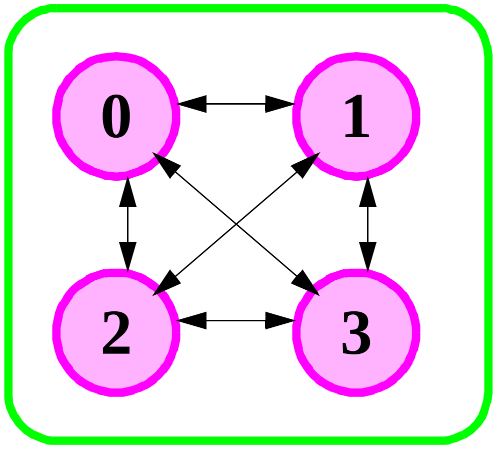
- Separate processes
- Separate address spaces (distributed memory model)
- Processes execute independently and concurrently

What’s in MPI

- MPI-1
  - Utilities: “who am I?”, “how many processes are there”
  - Send/receive communication
  - Collective communication e.g. broadcast, reduction, all-to-all
  - Many other things
- MPI-2
  - Parallel I/O
  - C++/Fortran 90
  - One-sided communication – get/put
  - Many other things
- Not in MPI
  - Process startup, environment, standard input/output
  - Fault tolerance

An MPI Application

An MPI application



The elements of the application are:

- **4 processes**, numbered zero through three
- **Communication paths** between them

The set of processes plus the communication channels is called "**`MPI_COMM_WORLD`**". More on the name later.

“Hello World” — C

```
#include <mpi.h>
main(int argc, char *argv[])
{
    int me, nprocs
    MPI_Init(&argc, &argv)
    MPI_Comm_size(MPI_COMM_WORLD, &nprocs)
    MPI_Comm_rank(MPI_COMM_WORLD, &me)

    printf(“Hi from node %d of %d\n”, me, nprocs)

    MPI_Finalize()
}
```

Compiling and Running

Different on every machine.

Compile:

```
mpicc -o hello hello.c
mpif77 -o hello hello.c
```

Start four processes (somewhere):

```
mpirun -np 4 ./hello
```

“Hello world” output

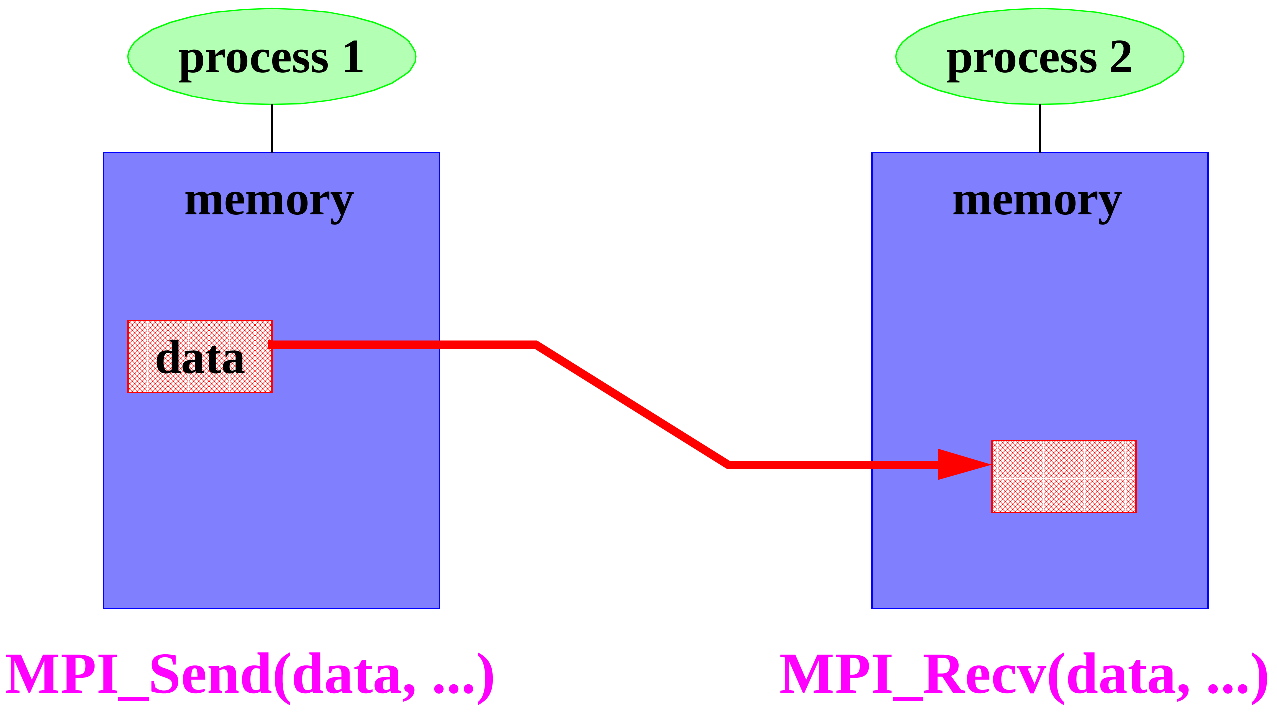
Run with 4 processes:

```
Hi from node 2 of 4
Hi from node 1 of 4
Hi from node 3 of 4
Hi from node 0 of 4
```

Note:

- Order of output is not specified by MPI
- Ability to use **`stdout`** is not even guaranteed by MPI!

Point-to-point communication in MPI



Point-to-point Example

Process 0 sends array “A” to process 1 which receives it as “B”

1:

```
#define TAG 123
double A[10];
MPI_Send(A, 10, MPI_DOUBLE, 1, TAG, MPI_COMM_WORLD)
```

2:

```
#define TAG 123
double B[10];
MPI_Recv(B, 10, MPI_DOUBLE, 0, TAG,
          MPI_COMM_WORLD, &status)
```

or

```
MPI_Recv(B, 10, MPI_DOUBLE, MPI_ANY_SOURCE,
      MPI_ANY_TAG, MPI_COMM_WORLD, &status)
```

Some Predefined datatypes

C:

```
MPI_INT
MPI_FLOAT
MPI_DOUBLE
MPI_CHAR
MPI_LONG
MPI_UNSIGNED
```

Fortran:

```
MPI_INTEGER
MPI_REAL
MPI_DOUBLE_PRECISION
MPI_CHARACTER
MPI_COMPLEX
MPI_LOGICAL
```

Language-independent

```
MPI_BYTE
```

Source/Destination/Tag

`src/dest`

`dest`

- Rank of process message is being sent to (destination)
- Must be a valid rank (0...N-1) in communicator

`src`

- Rank of process message is being received from (source)
- “Wildcard” **`MPI_ANY_SOURCE`** matches any source

`tag`

- On the sending side, specifies a label for a message
- On the receiving side, must match incoming message
- On receiving side, **`MPI_ANY_TAG`** matches any tag

Status argument

In C: MPI_Status is a structure

- **`status.MPI_TAG`** is tag of incoming message (useful if **`MPI_ANY_TAG`** was specified)
- **`status.MPI_SOURCE`** is source of incoming message (useful if **`MPI_ANY_SOURCE`** was specified)
- How many elements of given datatype were received

```
MPI_Get_count(IN status, IN datatype, OUT count)
```

In Fortran: status is an array of integer

```
integer status(MPI_STATUS_SIZE)
status(MPI_SOURCE)
status(MPI_TAG)
```

In MPI-2: Will be able to specify **`MPI_STATUS_IGNORE`**

Guidelines for using wildcards

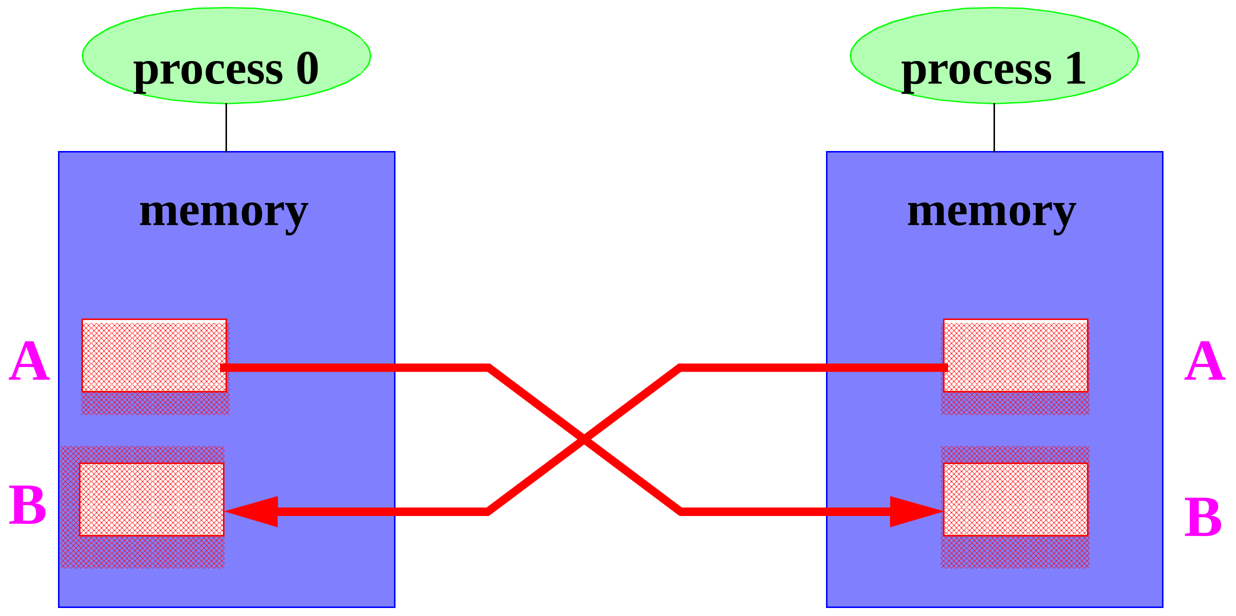
Unless there is a good reason to do so, do not use wildcards

Good reasons to use wildcards:

- Receiving messages from several sources into the same buffer but don't care about the order (use **`MPI_ANY_SOURCE`**)
- Receiving several messages from the same source into the same buffer, and don't care about the order (use **`MPI_ANY_TAG`**)

Exchanging Data

- Example with two processes: 0 and 1
- General data exchange is very similar



MPI_Send(A, ...)
MPI_Recv(B, ...)

MPI_Send(A, ...)
MPI_Recv(B, ...)

Requires Buffering to succeed!

Deadlock

The MPI specification is wishy-washy about deadlock.

- A **safe** program does not rely on system buffering.
- An **unsafe** program may rely on buffering but is not as portable.

Ignore this. MPI is all about writing portable programs.

Better:

- A **correct** program does not rely on buffering
- A program that relies on buffering to avoid deadlock is **incorrect**.

In other words, it is your fault it your program deadlocks.

Non-blocking operations

Split communication operations into two parts.

- First part initiates the operation. It does not block.
- Second part waits for the operation to complete.

```
MPI_Request request;

MPI_Recv(buf, count, type, dest, tag, comm, status)
   =
MPI_Irecv(buf, count, type, dest, tag, comm, &request)
   +
MPI_Wait(&request, &status)

MPI_Send(buf, count, type, dest, tag, comm)
   =
MPI_Isend(buf, count, type, dest, tag, comm, &request)
   +
MPI_Wait(&request, &status)
```

Using non-blocking operations

```
#define MYTAG 123
#define WORLD MPI_COMM_WORLD
MPI_Request request;
MPI_Status status;
```

Process 0:

```
MPI_Irecv(B, 100, MPI_DOUBLE, 1, MYTAG, WORLD, &request)
MPI_Send(A, 100, MPI_DOUBLE, 1, MYTAG, WORLD)
MPI_Wait(&request, &status)
```

Process 1:

```
MPI_Irecv(B, 100, MPI_DOUBLE, 0, MYTAG, WORLD, &request)
MPI_Send(A, 100, MPI_DOUBLE, 0, MYTAG, WORLD)
MPI_Wait(&request, &status)
```

- No deadlock
- Data may be transferred concurrently

Using non-blocking operations (II)

Also possible to use nonblocking send:

```
#define MYTAG 123
#define WORLD MPI_COMM_WORLD
MPI_Request request;
MPI_Status status;
p=1-me; /* calculates partner in 2 process exchange */
```

Process 0 and 1:

```
MPI_Isend(A, 100, MPI_DOUBLE, p, MYTAG, WORLD, &request)
MPI_Recv(B, 100, MPI_DOUBLE, p, MYTAG, WORLD, &status)
MPI_Wait(&request, &status)
```

- No deadlock
- "status" argument to **`MPI_Wait`** doesn't return useful info here.
- Better to use **`Irecv`** instead of **`Isend`** if only using one.

Overlapping communication and computation

On some computers it may be possible to do useful work while data is being transferred.

```
MPI_Request requests[2];
MPI_Status statuses[2];

MPI_Irecv(B, 100, MPI_DOUBLE, p, 0, WORLD, &request[1])
MPI_Isend(A, 100, MPI_DOUBLE, p, 0, WORLD, &request[0])

.... do some useful work here ....

MPI_Waitall(2, requests, statuses)
```

- **`Irecv`**/**`Isend`** initiate communication
- Communication proceeds “behind the scenes” while processor is doing useful work
- Need both **`Isend`** and **`Irecv`** for real overlap (not just one)
- Hardware support necessary for true overlap
- This is why “o” in “LogP” is interesting.

Operations on MPI_Request

`MPI_Wait(INOUT request, OUT status)`

- Waits for operation to complete
- Returns information (if applicable) in status
- Frees request object (and sets to MPI_REQUEST_NULL)

`MPI_Test(INOUT request, OUT flag, OUT status)`

- Tests to see if operation is complete
- Returns information in status if complete
- Frees request object if complete

`MPI_Request_free(INOUT request)`

- Frees request object but does not wait for operation to complete

`MPI_Waitall(..., INOUT array_of_requests, ...)`
`MPI_Testall(..., INOUT array_of_requests, ...)`
`MPI_Waitany`/`MPI_Testany`/`MPI_Waitsome`/`MPI_Testsome`

`MPI_Cancel` cancels or completes a request. Problematic.

Non-blocking communication gotchas

Obvious caveats:

1. You may not modify the buffer between **`Isend()`** and the corresponding **`Wait()`**. Results are undefined.

2. You may not look at or modify the buffer between **`Irecv()`** and the corresponding **`Wait()`**. Results are undefined.

3. You may not have two pending **`Irecv()`**s for the same buffer.

Less obvious gotchas:

4. You may not *look* at the buffer between **`Isend()`** and the corresponding **`Wait()`**.

5. You may not have two pending I**`send()`**s for the same buffer.

MPI_Send semantics

Most important:

- Buffer may be reused after MPI_Send() returns
- May or may not block until a matching receive is called (non-local)

Others:

- Messages are non-overtaking
- Progress happens
- Fairness not guaranteed

MPI_Send does not require a particular implementation, as long as it obeys these semantics.

Point-to-point Performance (review)

How do you model and measure point-to-point communication performance?

```
    data transfer time = f(message size)
```

Often a linear model is a good approximation

```
    data transfer time = latency + message size / bandwidth
```

- **latency** is startup time, independent of message size
- **bandwidth** is number of bytes per second

- linear is often a good approximation
- piecewise linear is sometimes better
- the latency/bandwidth model helps understand performance issues

Latency and bandwidth

- for **short messages**, **latency dominates** transfer time
- for **long messages**, the **bandwidth** term **dominates** transfer time

What are short and long?

```
    latency term = bandwidth term
```
when
```
    latency = message_size/bandwidth
```

Critical message size = **`latency * bandwidth`**

Example: **`50 us * 50 MB/s = 2500 bytes`**

- messages longer than 2500 bytes are bandwidth dominated
- messages shorter than 2500 bytes are latency dominated

Effect of buffering on performance

Copying to/from a buffer is like sending a message

```
    copy time = copy latency + message_size / copy bandwidth
```

For a single-buffered message:

```
    total time    = buffer copy time + network transfer time
                  = copy latency + network latency
                      + message_size *
                (1/copy bandwidth + 1/network bandwidth)
```

Copy latency is sometimes trivial compared to effective network latency

```
    1/effective bandwidth = 1/copy_bandwidth +
                           1/network_bandwidth
```

Lesson: **Buffering hurts bandwidth**

Mixing protocols for high performance of MPI_Send

Description

- **Eager** for short messages
- **Rendezvous** for long messages
- Switch protocols near latency-bandwidth product

Features

- Low latency for latency-dominated (short) messages
- High bandwidth for bandwidth-dominated (long) messages
- Reasonable memory management (upper limit on size of message that may be buffered)
- Non-ideal performance for some messages near critical size

Send Modes

Standard

- Send may not complete until matching receive is posted
- **`MPI_Send`**, **`MPI_Isend`**

Synchronous

- Send does not complete until matching receive is posted
- **`MPI_Ssend`**, **`MPI_Issend`**

Ready

- Matching receive must already have been posted
- **`MPI_Rsend`**, **`MPI_Irsend`**

Buffered

- Buffers data in user-supplied buffer
- **`MPI_Bsend`**, **`MPI_Ibsend`**

Don't use these.

They exist because MPI was designed by committee and they offer little benefit.

Communicators

- MPI_COMM_WORLD is a communicator

- A communicator is an object that represents
  - A set of processes
  - Private communication channels between those processes

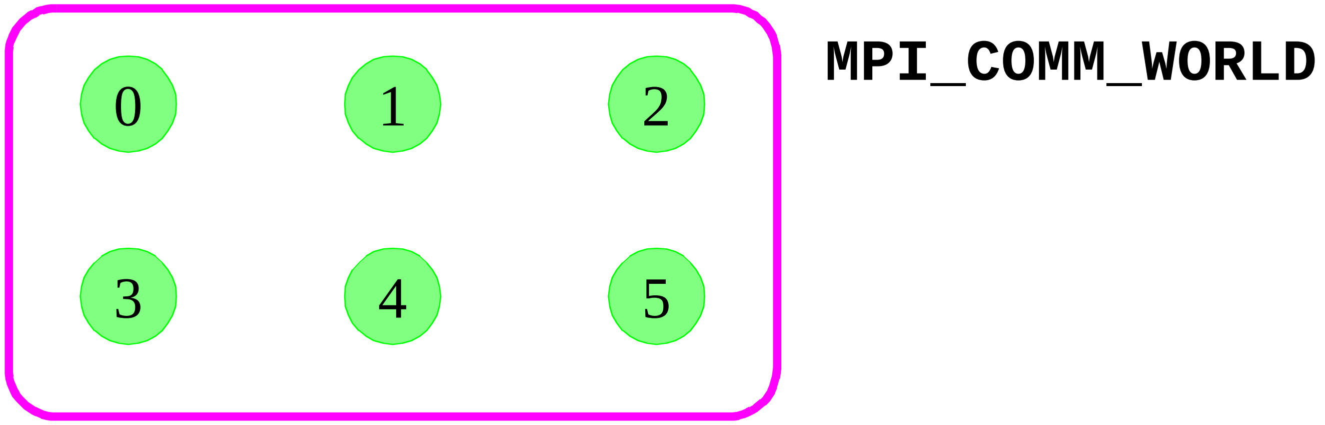
- Uses of communicators
  - Scope for collective operations
  - Writing safe libraries

```
isend(); irecv();
library_call_with_internal_communication();
MPI_Wait();
```

MPI_COMM_WORLD

`MPI_COMM_WORLD` is

- A group of all initial MPI processes
- Communication channels between them



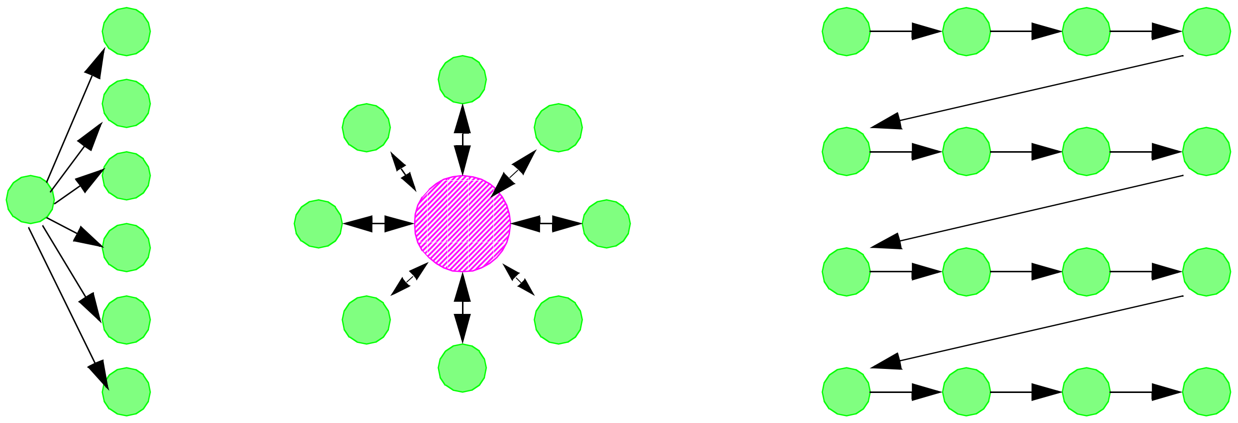
```
MPI_Send(buf, len, type, dest, tag, MPI_COMM_WORLD)
```

`dest` is a rank in **`MPI_COMM_WORLD`**

Collective Operations

Collective communication is communication among a group of processes:

- Broadcast
- Synchronization (barrier)
- Global operations (reductions)
- Scatter/gather
- Parallel prefix (scan)



Barrier

```
MPI_Barrier(communicator)
```

No process leaves the barrier until all processes have entered it.

Model for collective communication:

- All processes in communicator must participate
- Process might not finish until have all have started.

Broadcast

```
MPI_Bcast(buf, len, type, root, comm)
```

- Process with rank = root is source of data (in buf)
- Other processes receive data

```
MPI_Comm_rank(MPI_COMM_WORLD, &myid);
if (myid == 0) {
   /* read data from file */
}
MPI_Bcast(data, len, type, 0, MPI_COMM_WORLD);
```

Note:

- All processes must participate
- MPI has no “multicast” that is matched by a receive

Reduction

Combine elements in input buffer from each process, placing result in output buffer.

```
MPI_Reduce(indata, outdata, count, type, op, root, comm)
MPI_Allreduce(indata, outdata, count, type, op, comm)
```

- Reduce: output appears only in buffer on root
- Allreduce: output appears on all processes

operation types:

- **`MPI_SUM`**
- **`MPI_PROD`**
- **`MPI_MAX`**
- **`MPI_MIN`**
- **`MPI_BAND`**
- arbitrary user-defined operations on arbitrary user-defined datatypes

Reduction example: dot product

```
/* distribute two vectors over all processes such that
   processor 0 has elements 0...99
   processor 1 has elements 100...199
   processor 2 has elements 200...299
   etc.
*/

double dotprod(double a[100], double b[100])
{
   double gresult = lresult = 0.0;
   integer i;
   /* compute local dot product */
   for (i = 0; i < 100; i++) lresult += a[i]*b[i];
   MPI_Allreduce(lresult, gresult, 1, MPI_DOUBLE,
      MPI_SUM, MPI_COMM_WORLD);
   return(gresult);
}
```

Data movement: all-to-all

All processes send and receive data from all other processes.

```
    MPI_Alltoall(sendbuf, sendcount, sendtype,
                 recvbuf, recvcount, recvtype,
                 comm)
```

For a communicator with N processes:

- `sendbuf` contains N blocks of `sendcount` elements each
- `recvbuf` receives N blocks of `recvcount` elements each
- Each process sends block `i` of `sendbuf` to process `i`
- Each process receives block `i` of `recvbuf` from process `i`

Example: multidimensional FFT (matrix transpose)

Other collective operations

There are many more collective operations provided by MPI:

`MPI_Gather`/`Gatherv`/`Allgather`/`Allgatherv`

- each process contributes local data that is gathered into a larger array

`MPI_Scatter`/`Scatterv`

- subparts of a single large array are distributed to processes

`MPI_Reduce_scatter`

- same as Reduce + Scatter

`Scan`

- prefix reduction

The “v” versions allow processes to contribute different amounts of data

Semantics of collective operations

For all collective operations:

- Must be called by all processes in a communicator

Some collective operations also have the “barrier” property:

- Will not return until all processes have started the operation
- **`MPI_Barrier`**, **`MPI_Allreduce`**, **`MPI_Alltoall`**, etc.

Others have the weaker property:

- May not return until all processes have started the operation
- **`MPI_Bcast`**, **`MPI_Reduce`**, **`MPI_Comm_dup`**, etc.

Performance of collective operations

Consider the following implementation if **`MPI_Bcast`**:

```
if (me == root) {
    for (i = 0; i < N; i++) {
        if (i != me) MPI_Send(buf, ..., dest=i, ...);
    }
} else {
    MPI_Recv(buf, ..., src=i, ...);
}
```

Non-scalable: time to execute grows linearly with number of processes.

High-quality implementations of collective operations use algorithms with better scaling properties *if* the network supports multiple simultaneous data transfers.

- Algorithm may depend on size of data
- Algorithm may depend on topology of network

Timing

Double precision wallclock time, in seconds.

```
double t1, t2;
t1 = MPI_Wtime();

.... do some work ...

t2 = MPI_Wtime();
printf("Elapsed time is %f seconds\n", t2-t1);
```

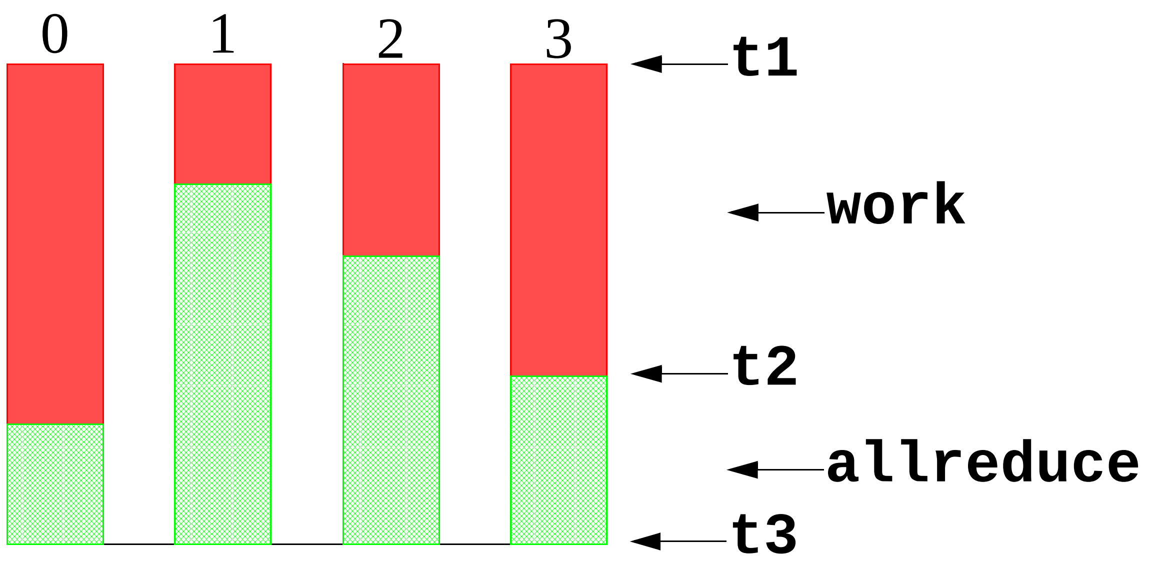
Notes:

- Time starts at some arbitrary point in the past
- Note times not synchronized unless **MPI_WTIME_IS_GLOBAL**

Accurate timing is not simple -

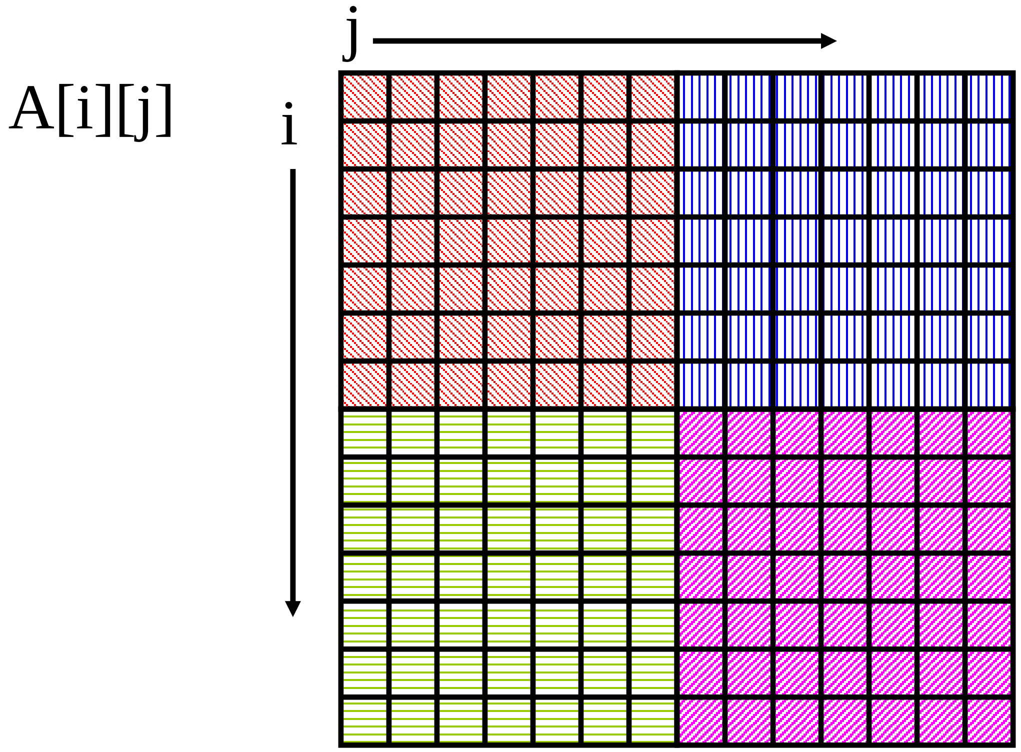
Three standard problems

- Processes are unsynchronized to start
- Load imbalance shows up in collective and point-to-point operations
- Extra synchronization to avoid problems 1+2 causes network contention



Motivation for MPI-2 I/O

- Consider 2D array, row-major order, to be stored in single file, partitioned among 4 processors
- **Each processor writes many small non-contiguous blocks**



C++

- **MPI needs a C++ interface**
  - Key question: closely related to C interface or full-blown OO?
  - Decision: C++ interface is close to C/Fortran interface.

- General principles:
  - MPI handles (**`MPI_Comm`**, etc.) become C++ objects.
  - MPI functions become methods on C++ classes.
  - Do what C++ programmers expect where possible but
  - Don't stray too far from MPI principles.

More C++ principles

- Shallow copies

- Constructors create **`MPI_XXX_NULL`**. Destructors do not free.
  - User must generally use **`create`** and **`free`**
  - Reasons
    - Variables going in and out of scope could be collective operations
    - Automatic destruction violates shallow copy semantics

Fortran 90 support

Fortran 90 has many "modern" features.

- User-defined types
- Function overloading
- Parameterized types
- Mechanisms for strict type checking (interface blocks)
- First class arrays

Can MPI take advantage of these? Mostly **no**.

Fortran 90 vs. MPI

Fortran 90 and MPI are not completely compatible

- **MPI has choice arguments**
  - F90 argument checking is strict
  - Derived types require argument checking

- **MPI assumes flat address space**
  - F90 does not require sequence association

Advanced topics for followup reading

- **Creation and manipulation of communicators**
  - Useful if you need to do collective operations over subsets of processes
- **Topologies**
  - Allow applications with simple communication topology to be well-mapped to network topology. Can be important on machines with mesh networks (Red Storm, X1, Blue Gene)
- **Profiling interface**
  - Makes it easy and transparent to application to wrap MPI routines with profiling routines
- **User Defined Datatypes**
  - Difficult to use, and can result in poor performance
- **Persistent communication**
- **One-sided communication – get/put**
  - MPI is not the standard interface. Cray shmem library is still the standard)
- **Dynamic process management** (a solution in search of a problem)
- And a large number of other features.

Where to get more information

Home pages

- `http://www.mpi-forum.org`
- `http://www.mcs.anl.gov/mpi`

Newsgroups

- comp.parallel.mpi

Books

- **Using MPI**, by Gropp, Lusk, Skjellum. The MIT Press
- **MPI: The Complete Reference**, by Snir, Otto, Huss-Lederman, Walker, Dongarra. The MIT Press
- **MPI: The Complete Reference, Volume 2**, by Gropp, Lederman, Lusk, Nitzberg, Saphir, Snir. The MIT Press
- **Parallel Programming with MPI**, by Pacheco. Morgan Kauffman