CSE 6220
Introduction to High Performance Computing
Introduction to MPI

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Thanks to Patrick Flick and Jaroslaw Zola for the slides.

What is MPI?

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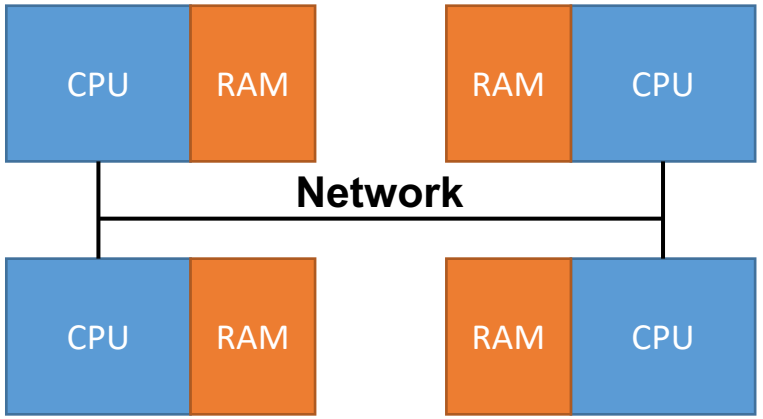
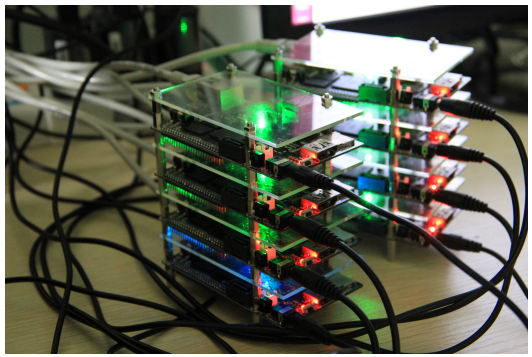
Message **P**assing **I**nterface

- **Standard** for parallel programming via message passing
- For parallel computers and distributed memory systems
  - Computing clusters
  - Supercomputers
  - Heterogeneous systems
  - Multi-core/processor systems
- Designed to be portable, flexible, and efficient

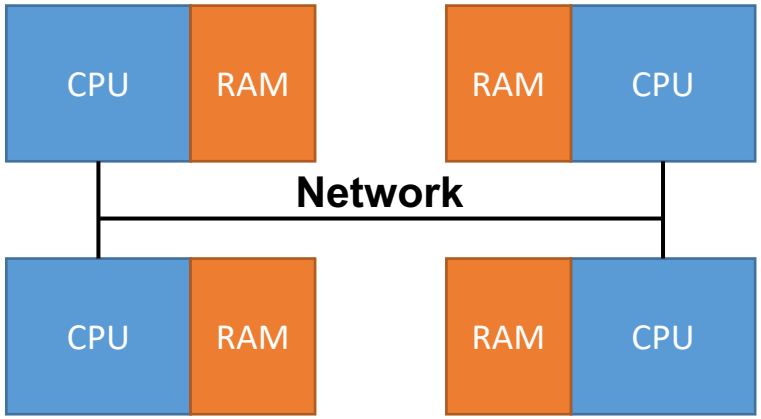




What is MPI?

Message **P**assing **I**nterface

- **Standard** for parallel programming via message passing
- Not a library or software package
- Specifies API for C/C++ and Fortran
- Many Implementations:
  - **OpenMPI**
  - MPICH
  - MVAPICH (MPI via Infiniband)
  - Proprietary vendor specific implementations
    - Intel, Cray, IBM, Microsoft, Oracle
  - E.g. On the IBM Blue Gene, many MPI calls are implemented in Hardware



MPI Implementation

Every MPI implementation must provide three components (we consider only C/C++):

1. MPI library with `mpi.h` header
2. Compiler wrapper: `mpicc` or `mpicxx`
3. Runtime system with `mpirun` tool (sometimes `mpiexec`)

All three are essential:

- MPI library to write parallel programs
- Compiler wrapper (e.g. `mpicc`) to compile MPI programs
- `mpirun` to run parallel MPI programs

Structure of an MPI program

p1.cpp:

```
#include <mpi.h>

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

    // ...

    // finished with MPI
    MPI_Finalize();
    return 0;
}
```

Every MPI program **must** include `mpi.h`

Every MPI program **must call** `MPI_Init` once, before any other MPI calls

All MPI calls must be within an initialized MPI program

Every MPI program **must call** `MPI_Finalize` once, before exiting the application

Structure of an MPI program

p1.cpp:

```
#include <mpi.h>

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

    // ...

    // finished with MPI
    MPI_Finalize();
    return 0;
}
```

Compiling and running:

```
$ mpicxx p1.cpp -o p1

$ mpiexec -np 4 ./p1
```

Communicators

Key concept in MPI: **Communicators**

- ***Communicator:*** group of MPI processes
- In a communicator, each process has a unique rank
- Ranks are integers from *0* to *(p − 1)*, where *p* is the total number of processes in the communicator
- Special Communicators:
  - `MPI_COMM_WORLD` (all processes)
  - `MPI_COMM_SELF`
- Operations:
  - **`MPI_Comm_size`**
  - **`MPI_Comm_rank`**
  - `MPI_Comm_split`
  - `MPI_Comm_create`
  - `MPI_Comm_free`
  - …

Communicators: Example

p2.cpp:

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

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

    // get communicator size and ranks
    MPI_Comm comm = MPI_COMM_WORLD;
    int rank, size;
    MPI_Comm_size(comm, &size);
    MPI_Comm_rank(comm, &rank);

    // print rank and size
    printf("Hello from rank %d/%d.\n", rank, size);

    // finished with MPI
    MPI_Finalize();
    return 0;
}
```

```
int MPI_Comm_size(MPI_Comm comm, int* size);
int MPI_Comm_rank(MPI_Comm comm, int* rank);
```

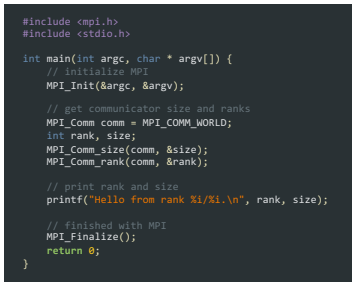
MPI_Comm object initialized to contain all processes (WORLD)

Get total number of processes in communicator, and the current process' rank

Communicators: Example

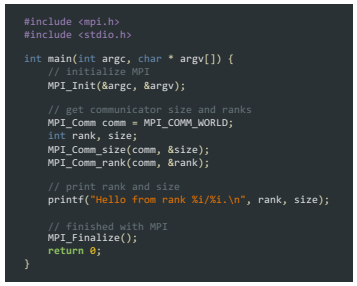
```
mpiexec -np 4 ./p2
```

Process 0



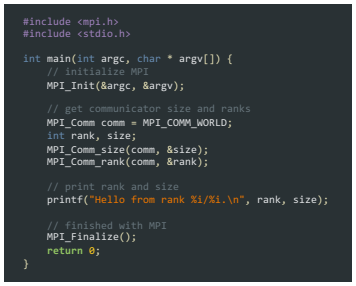
```
size = 4
rank = 0
```

Process 1



```
size = 4
rank = 1
```

Process 2



```
size = 4
rank = 2
```

Process 3

```
size = 4
rank = 3
```

```
Hello from rank 1/4.
```

```
Hello from rank 0/4.
```

```
Hello from rank 3/4.
```

```
Hello from rank 2/4.
```

Point-to-Point Communication

Point to point communication

- Sending messages from one process to another
- Always involves both processes (***source*** and ***destination***)


```
MPI_Send(Message, dest=Y, comm)
```

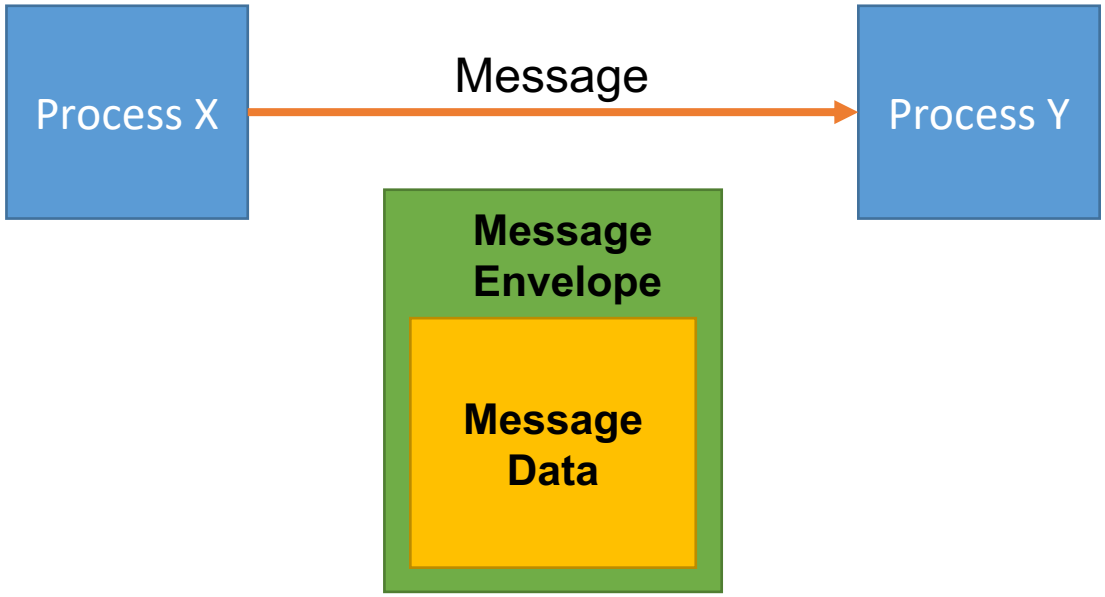
```
MPI_Receive(Message, src=X, comm)
```

Source and **destination** ranks are always with respect to the given communicator ***comm***

(NOTE: These are not the actual APIs of MPI_Send/MPI_Receive)

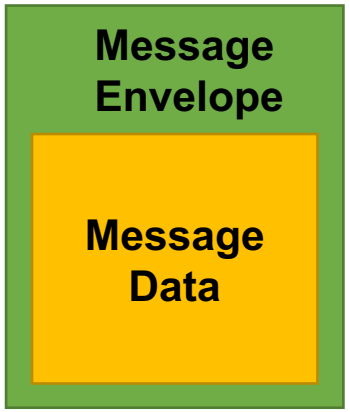
Point to point communication

- Sending messages from one process to another
- Always involves both processes (***source*** and ***destination***)



- Every message consists of a *Message Envelope* and the *Message Data*

Message Data

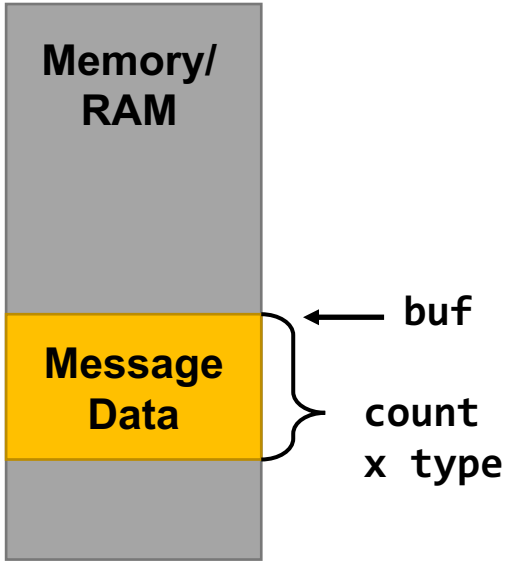


The ***Message Data*** for each message is described by:

1. Memory buffer storing data: `void* buf,`
2. Number of objects in the buffer: `int count,`
3. Data type of the data in the buffer: `MPI_Datatype type`

- MPI defines **`MPI_Datatype`** for all built-in C/C++ types
  - `MPI_CHAR, MPI_INT, MPI_UNSIGNED, MPI_FLOAT, MPI_DOUBLE,…`
  - `See the standard for complete list`

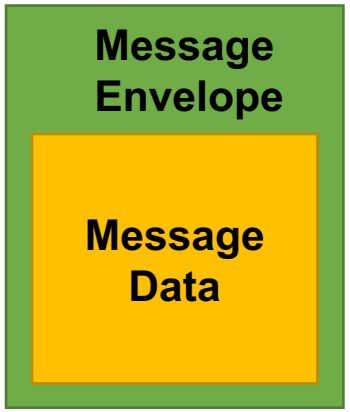
- Effectively, the Message Data is described as a block of memory:
  - **`buf`** is a pointer to where the data lies in memory
  - **`count`** and **`type`** define how large the memory block is (e.g. 8 x MPI_INT = 32 bytes)



Message Envelope

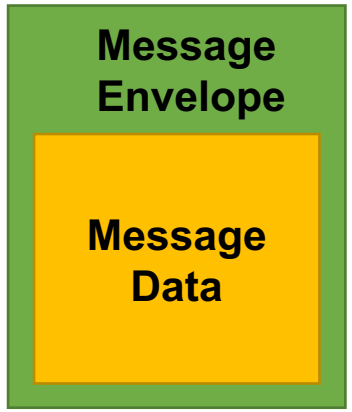
The ***Message Envelope*** contains:

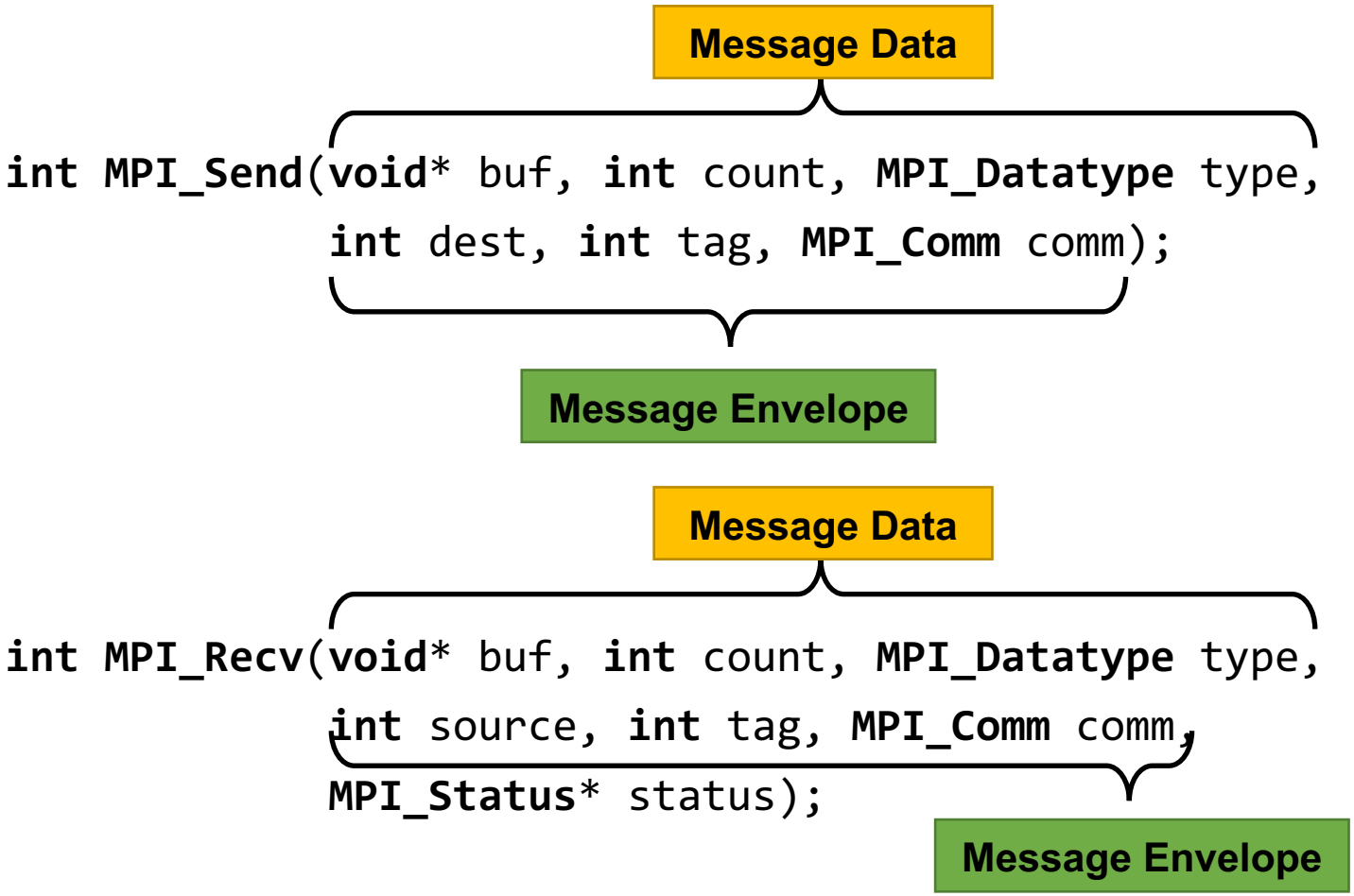
- **source rank:** `int src,`
- **destination rank:** `int dest,`
- **tag**: integer used to distinguish messages `int tag,`
- **Communicator:** universe of communication `MPI_Comm comm`



MPI_Send/MPI_Recv

Function signatures for `MPI_Send` and `MPI_Recv`:





Example Send/Recv

p3.cpp:

```
#include <mpi.h>
#include <iostream>

int main(int argc , char* argv []) {
    int rank;
    MPI_Init (&argc , &argv);
    MPI_Comm_rank (MPI_COMM_WORLD , &rank );
    const int N = 32;
    int tab[N];
    if (rank == 0) {
        tab[N - 1] = 13;
        MPI_Send(tab, N, MPI_INT,
                 1, 111, MPI_COMM_WORLD);
    } else if (rank == 1) {
        MPI_Status stat;
        MPI_Recv(tab, N, MPI_INT,
                 0, 111, MPI_COMM_WORLD, &stat);
        std::cout << tab[N - 1] << std::endl;
    }
    return MPI_Finalize();
}
```

Send N integers from rank 0 to rank 1.
Blocks till everything is sent.

Receive N integers.
Blocks till everything is received.

```
Output: 13
```

Message Matching

- Each send operation **must be matched** by a corresponding receive operation
- Messages are matched via their **envelope:**
  - communicator
  - source rank
  - tag
  - **NOT** by type or size
- Thus: for a receive to succeed, a message needs to match the communicator, tag, and rank

Blocking:

- An `MPI_Recv` operation **blocks** until a matching message is received
- An `MPI_Send` operation **may block** until the message has been received by the destination process

Examples: Message Matching

p4.cpp

```
#include <mpi.h>

int main(int argc , char* argv []) {
    int rank;
    MPI_Init(&argc , &argv);
    MPI_Comm_rank(MPI_COMM_WORLD , &rank);
    int x;
    if (rank == 0) {
        x = 13;
        MPI_Send(&x, 1, MPI_INT,
                 1, 111, MPI_COMM_WORLD);
    } else if (rank == 1) {
        MPI_Status stat;
        MPI_Recv(&x, 1, MPI_INT,
                 0, 222, MPI_COMM_WORLD, &stat);
    }
    return MPI_Finalize();
}
```

What's wrong?

Tags are not matching
111 != 222

MPI program will deadlock!

Examples: Message Matching

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```
#include <mpi.h>
int main(int argc, char* argv[]) {
    int rank;
    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    int x[16];
    float y[16];
    if (rank == 0) {
        x[13] = 13;
        y[13] = 0.13f;
        MPI_Send(x, 16, MPI_INT,
                 1, 111, MPI_COMM_WORLD);
        MPI_Send(y, 16, MPI_FLOAT,
                 1, 222, MPI_COMM_WORLD);
    } else if (rank == 1) {
        MPI_Status stat;
        MPI_Recv(y, 16, MPI_FLOAT,
                 0, 222, MPI_COMM_WORLD, &stat);
        MPI_Recv(x, 16, MPI_INT,
                 0, 111, MPI_COMM_WORLD, &stat);
    }
    return MPI_Finalize();
}
```

What's wrong?

Blocks until message with tag 111 is received.

Blocks until message with tag 222 is sent.

MPI program will deadlock!

Examples: Message Matching

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Correct!

```
#include <mpi.h>
int main(int argc , char* argv []) {
    int rank;
    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    int x, y;
    if (rank == 0) {
        x = 13;
        MPI_Send (&x, 1, MPI_INT,
                  1, 111, MPI_COMM_WORLD);
        x = 113;
        MPI_Send (&x, 1, MPI_INT,
                  1, 111, MPI_COMM_WORLD);
    } else if (rank == 1) {
        MPI_Status stat;
        MPI_Recv (&x, 1, MPI_INT,
                  0, 111, MPI_COMM_WORLD, &stat);
        MPI_Recv (&y, 1, MPI_INT,
                  0, 111, MPI_COMM_WORLD, &stat);
    }
    return MPI_Finalize();
}
```

x = 13
y = 113

ANY

- Useful trick:
  - We can use any combination of **`tag = MPI_ANY_TAG`** and/or **`source = MPI_ANY_SOURCE`** in **`MPI_Recv`** to receive any message from any processor
  - We can use the **`MPI_Status`** structure to check envelope of the received message

- Example:

```
int x;
MPI_Status stat;
MPI_Recv(&x, 1, MPI_INT,
         MPI_ANY_SOURCE, MPI_ANY_TAG, MPI_COMM_WORLD, &stat);
int source = stat.MPI_SOURCE;
int tag = stat.MPI_TAG;
```

Example: any tag, any src

```
#include <mpi.h>
#include <iostream>

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 );
    int x;
    if (rank == 0) {
        MPI_Status stat;
        for (int i = 1; i < size; ++i) {
            MPI_Recv(&x, 1, MPI_INT,
                     MPI_ANY_SOURCE, MPI_ANY_TAG, MPI_COMM_WORLD,
                     &stat);
            std::cout << "From: " << stat.MPI_SOURCE << " "
            << "Tag: " << stat.MPI_TAG << std::endl;
        }
    } else {
        x = rank;
        MPI_Send(&x, 1, MPI_INT,
                 0, size - rank, MPI_COMM_WORLD);
    }
    return MPI_Finalize();
}
```

Receives any one of the messages. No order guaranteed.

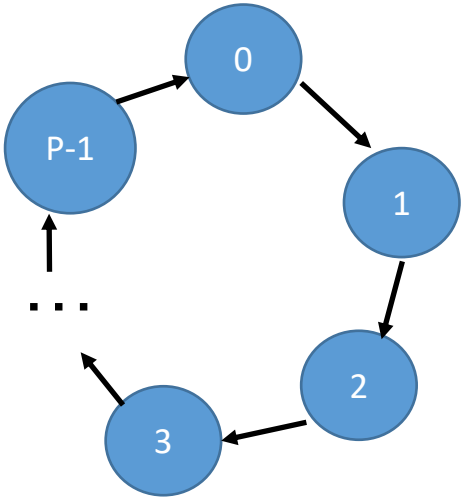
Message Ordering

The **MPI** standard defines the order in which messages will be received, when ANY_TAG or ANY_SRC is used:

- If messages originate from **different processors**, the order in which they are received is **arbitrary**
- If messages have **different tags**, the order in which they are received is **arbitrary**
- Only if two or more messages have the **same source AND** the **same tag**, their **order is preserved**
  - This means: they are received in the same order in which they were sent

Cyclic dependencies

- Let's say we want to send messages in a cyclic dependency:
  - Processor `i` sends a message to `(i+1) mod p`



Example:

```
MPI_Send(&x, 1, MPI_INT,
         (rank+1) % size, 13, MPI_COMM_WORLD);
MPI_Recv(&y, 1, MPI_INT,
         MPI_ANY_SOURCE, 13, MPI_COMM_WORLD, &stat);
```

What's wrong?

May block till message is received, MPI_Recv never called

Reverse?

```
MPI_Recv(&y, 1, MPI_INT,
         MPI_ANY_SOURCE, 13, MPI_COMM_WORLD, &stat);
MPI_Send(&x, 1, MPI_INT,
         (rank+1) % size, 13, MPI_COMM_WORLD);
```

Same problem.

Non-blocking Communication

- Enter: Non-blocking Communication
  - **`MPI_Isend`** and **`MPI_Irecv`** will initiate transfers but **not block** until they succeed
  - Enables:
    - Dead-lock avoidance
    - Hiding latency by overlapping computation and communication
  - Same parameters as `MPI_Send`, `MPI_Recv` but additional output parameter:

```
int MPI_Isend(void* buf, int count, MPI_Datatype type,
              int dest, int tag, MPI_Comm comm,
              MPI_Request* req);

int MPI_Irecv(void* buf, int count, MPI_Datatype type,
              int source, int tag, MPI_Comm comm,
              MPI_Request* req);
```

Non-blocking Communication

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Communication Completion

- Two functions can be used to check for communication status:

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

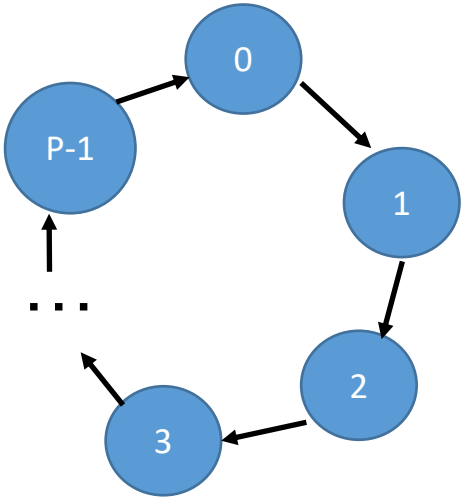
- `MPI_Wait` will block till the send/receive operation is completed.
- `MPI_Test` returns a flag of either 0 or 1 depending on whether the send/receive operation is completed

```
MPI_Status stat;
MPI_Request req;
MPI_Isend(..., &req);
MPI_Wait(&req, &stat);
```

```
MPI_Send(... );
```

Cyclic dependencies

- Let's say we want to send messages in a cyclic dependency:
  - Processor `i` sends a message to `(i+1) mod p`



Example:

```
MPI_Send(&x, 1, MPI_INT,
         (rank+1) % size, 13, MPI_COMM_WORLD);
MPI_Recv(&y, 1, MPI_INT,
         MPI_ANY_SOURCE, 13, MPI_COMM_WORLD, &stat);
```

What's wrong?

May block till message is received, MPI_Recv never called

Using Non-blocking receive:

```
MPI_Request req;
MPI_Irecv(&y, 1, MPI_INT,
         MPI_ANY_SOURCE, 13, MPI_COMM_WORLD, &req);
MPI_Send(&x, 1, MPI_INT,
         (rank+1) % size, 13, MPI_COMM_WORLD);
MPI_Wait(&req, &stat);
```

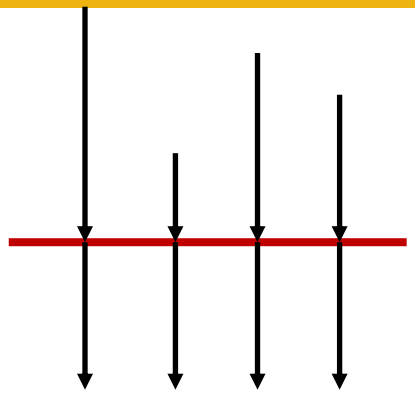
Correct!

Collective Communication

Collective Communication

- All processes within a communicator must participate
- All collective operations are **blocking**
- Except of `MPI_Barrier`, no synchronization can be assumed
- All collective operations are guaranteed to not interfere with point-to-point messages
- Collective operations can be implemented using only point-to-point calls
- In practice, they are optimized to use various hardware (interconnect) properties

Barrier



- Block until all processes called the barrier:

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

- Establishes full synchronization

Side Note: Measuring Time

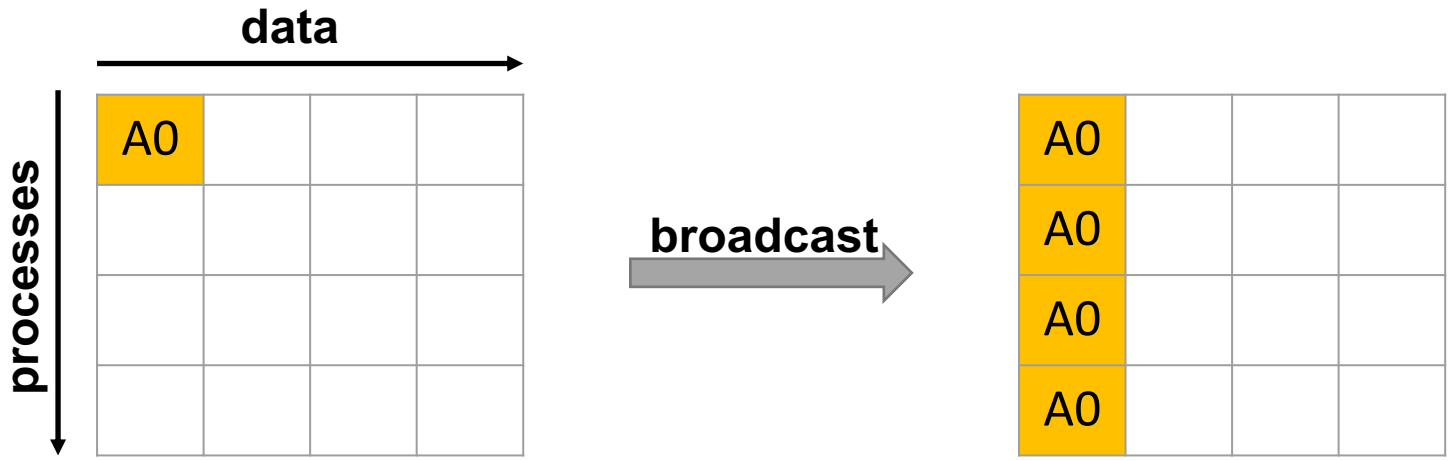
MPI provides a function to check execution time:

```
double MPI_Wtime();
```

It returns time elapsed since “some point” in the past.

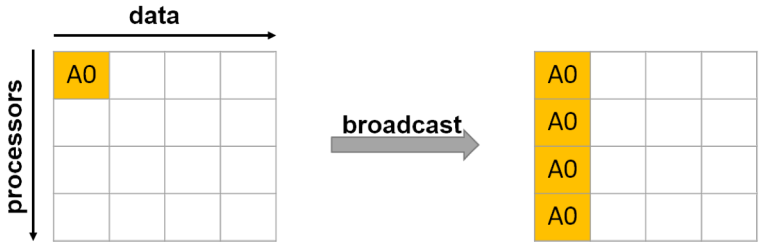
```
#include <mpi.h>
#include <iostream>

int main(int argc, char* argv[]) {
    MPI_Init(&argc, &argv);
    double t0 = MPI_Wtime();
    // ...
    MPI_Barrier(MPI_COMM_WORLD);
    double t1 = MPI_Wtime();
    std::cout << (t1 - t0) << std::endl;
    return MPI_Finalize();
}
```

Broadcast



Broadcast

Broadcast a message from one process(=root) to all other processes




```
int MPI_Bcast(void* buf, int count, MPI_Datatype type,
              int root, MPI_Comm comm);
```

Example:

```
#include <mpi.h>
#include <iostream>
int main(int argc , char* argv []) {
    int rank;
    MPI_Init(&argc, &argv);
    MPI_Comm_rank (MPI_COMM_WORLD, &rank);
    double x = 0.0;
    if (rank == 0) x = -13.13;
    MPI_Bcast(&x, 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
    std::cout << x << std::endl;
    return MPI_Finalize ();
}
```

Prints -13.13 on every process.

MPI Programming Assignments

Programming Assignments

- During the semester, there will be multiple programming assignments
- Each one will test different aspects of MPI programming
- C/C++ programming is required

- You will run your programs on instructional HPC resources
  - Information regarding how to use the cluster and few others can be found in Canvas under “Files/Additional Material/MPI”

Getting Set Up

- Before running your programs on one of the Georgia Tech clusters, you should make sure it works locally (on your desktop/laptop).
- We are going to use **OpenMPI (or mvapich)** in this class
  - Can easily be installed on Debian/Ubuntu via *`apt-get`* or on Mac via *`homebrew`*
  - You could install Ubuntu (or your favorite Linux distribution) on either your machine or inside a virtual machine/virtual box
  - All clusters are running Linux
  - MPI support is best on Linux based systems

- **Preparation** for the programming assignments:
  - (Install Ubuntu/Linux)
  - Install OpenMPI
  - Compile and run some of the small sample programs from before
  - Play around with MPI and C/C++ a little

Additional Documentation

Additional Documentation

- A good MPI tutorial: https://computing.llnl.gov/tutorials/mpi/
- Official MPI Standard Documents: http://www.mpi-forum.org/docs/
- MPICH web-based MPI reference: http://www.mpich.org/documentation/guides/
- PACE Training: http://www.pace.gatech.edu/training

C++ and MPI

- MPI used to include C++ bindings, but these are **deprecated** as of MPI 2.2
- Don't use the C++ bindings!

- Caveats when using C++:
  - The buffer argument in MPI calls expects a void pointer to the raw, contiguous data.
  - Only contiguous containers can be sent via MPI: **std::vector** (can't easily send std::map, std::list, std::deque, etc).
  - Sending a `std::vector`:

```
MPI_Send(&vec[0], vec.size(), …)
```

  - Space has to be allocated prior to receiving, i.e., you have to know how many elements you will receive

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Sending and Receiving std::vector

- Assuming the receiving end does not yet know the total size of the vector
- First send the size, then the data:

```
// sending a vector (send size first)
std::vector<int> vec(some_size);
int send_size = vec.size();
MPI_Send(&send_size, 1, MPI_INT, dest, 1234, MPI_COMM_WORLD);
MPI_Send(&vec[0], send_size, MPI_INT, dest, 1234, MPI_COMM_WORLD);
```

- On the receiving side:

```
// receiving a vector (receive size first)
MPI_Status stat;
std::vector<int> recv_buf;
int recv_size;
MPI_Recv(&recv_size, 1, MPI_INT, src, 1234, MPI_COMM_WORLD, &stat);
recv_buf.resize(recv_size);
MPI_Recv(&recv_buf[0], recv_size, MPI_INT, src, 1234, MPI_COMM_WORLD, &stat);
```

Questions?