ME759
High Performance Computing for Engineering Applications

Parallel Computing with the Message Passing Interface (MPI)

November 1, 2013

"As a rule, software systems do not work well until they have been used, and have failed repeatedly, in real applications."
Dave Parnas

Before We Get Started…

- Last time: Started the MPI segment of the course
  - Basic concepts related to computing on clusters of CPUs
  - Getting started on the Message Passing Interface (MPI) standard
- Today:
  - MPI practicalities
  - Point-to-point communication in MPI
- Miscellaneous
  - I provided feedback to all students who uploaded a project proposal
    - Email me if you uploaded a proposal yet haven't heard from me
  - Choose your Final Project presentation time slot - see post http://sbel.wisc.edu/Forum/viewtopic.php?f=15&t=508

Code for Approximating π

```
// MPI_PI.cpp : Defines the entry point for the console application.
//

#include "mpi.h"
#include <math.h>
#include <iostream>

using namespace std;

int main(int argc, char *argv[])
{
    int n, rank, size, i;
    double PI25DT = 3.141592653589793238462643;
    double mypi, pi, h, sum, x;
    char processor_name[MPI_MAX_PROCESSOR_NAME];
    int namelen;


    MPI_Init(&argc,&argv);
    MPI_Comm_size(MPI_COMM_WORLD,&size);
    MPI_Comm_rank(MPI_COMM_WORLD,&rank);
    MPI_Get_processor_name(processor_name, &namelen);

    cout << "Hello from process " << rank << " of " << size << " on " << processor_name << endl;
```

Code [Cntd.]

```
    if (rank == 0) {
    //cout << "Enter the number of intervals: (0 quits) ";
    //cin >> n;
        if (argc<2 || argc>2)
            n=0;
        else
            n=atoi(argv[1]);
    }

    MPI_Bcast(&n, 1, MPI_INT, 0, MPI_COMM_WORLD);
    if (n>0) {
        h = 1.0 / (double) n;
        sum = 0.0;
        for (i = rank + 1; i <= n; i += size) {
            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 (rank == 0)
            cout << "pi is approximately " << pi << ", Error is " << fabs(pi - PI25DT) << endl;
    }

    MPI_Finalize();
    return 0;
}
```

Data type we are moving around

Reduce through a "sum" operation

Root process, it ends up storing the result

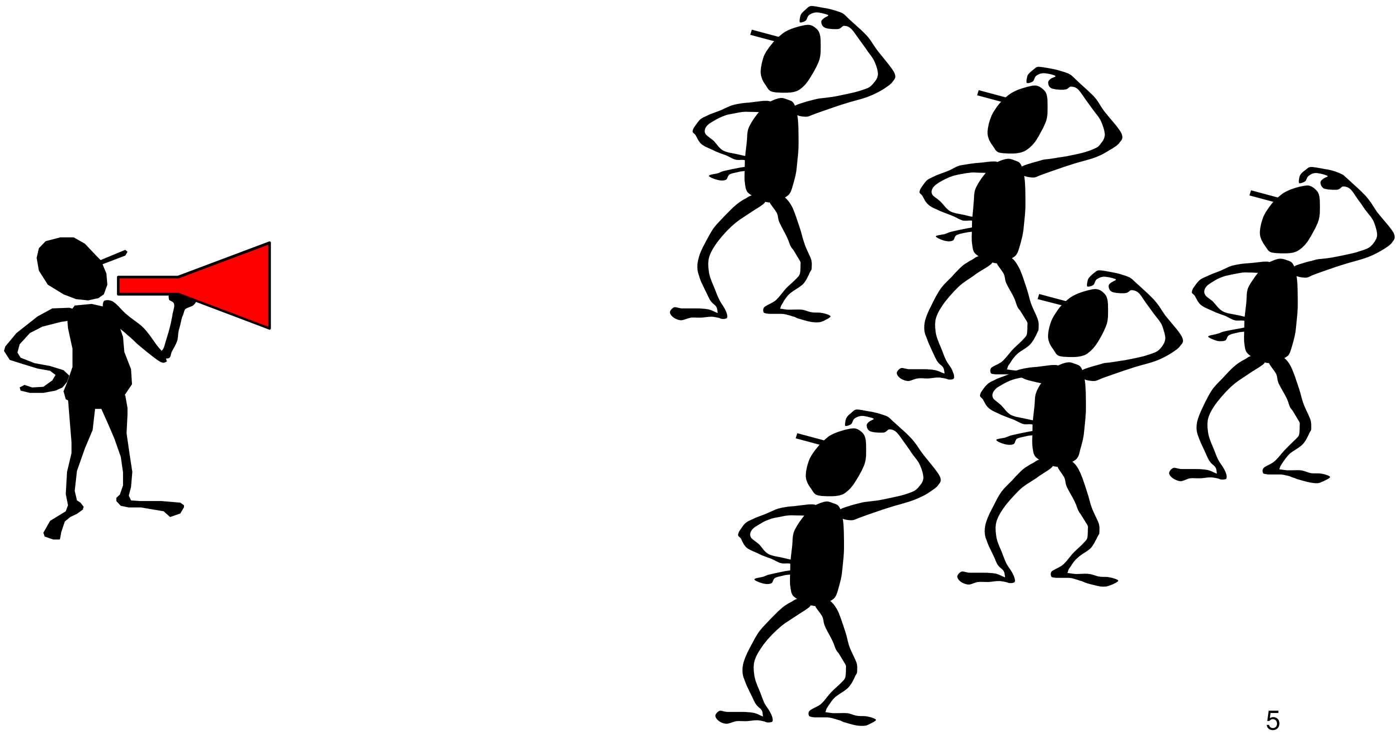
How many instances of this data type are moved around

Where the reduce operation stores the result

Partial contribution of "this" process

Broadcast
[MPI function used in Example]

- A one-to-many communication.

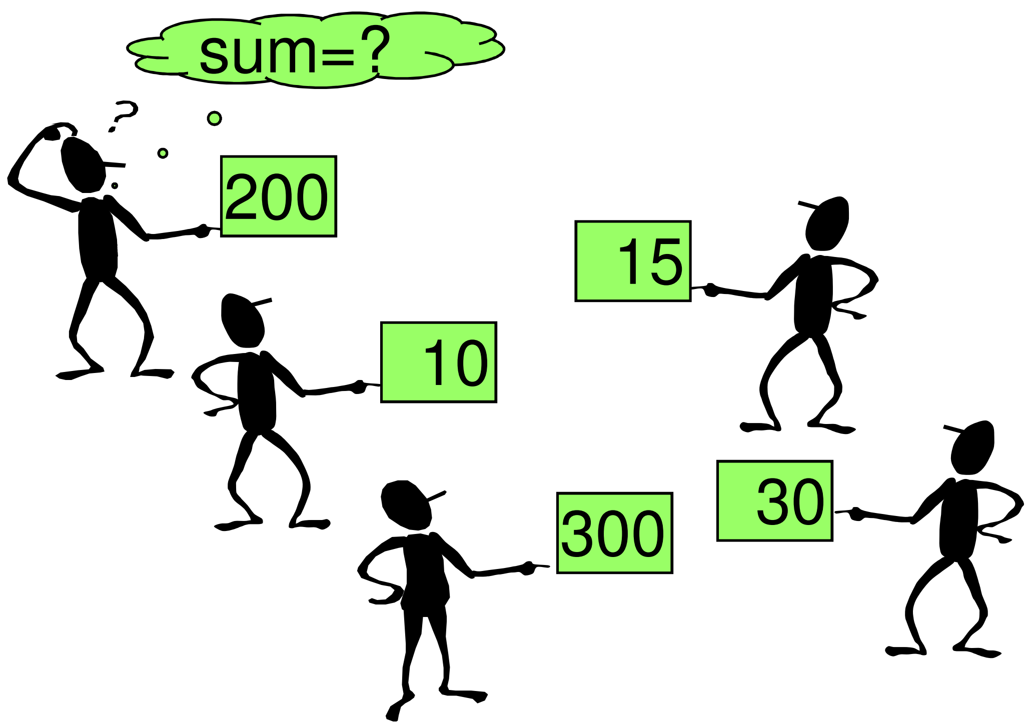


Collective Communications

- Collective communication routines are higher level routines
- Several processes are involved at a time
- May allow **optimized internal** implementations, e.g., tree based algorithms
  - Require O(log(N)) time as opposed to O(N) for naïve implementation

Reduction Operations
[MPI function used in Example]

- Combine data from several processes to produce a single result



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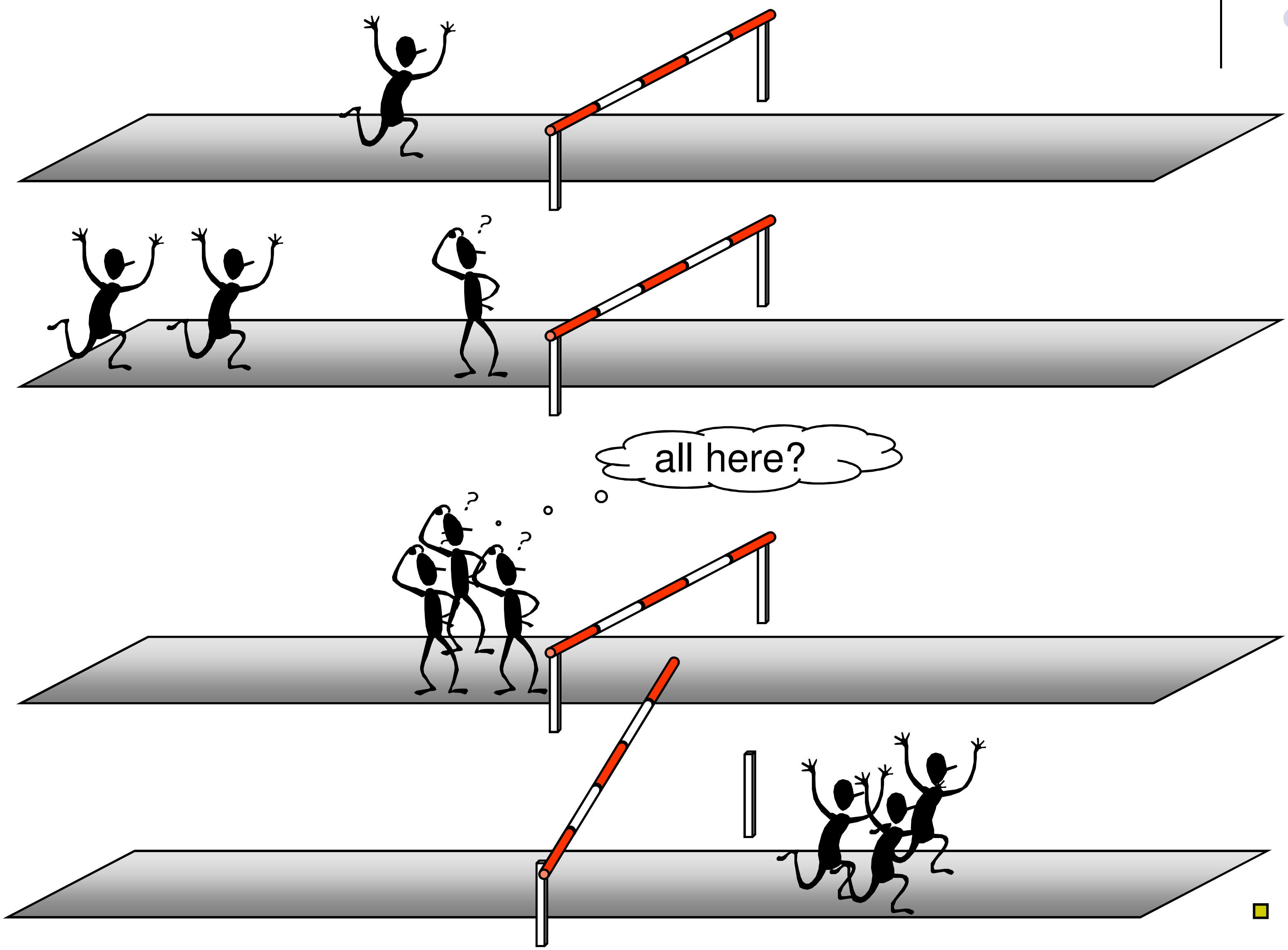
Barriers

- Used implicitly or explicitly to synchronize processes



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MPI, Practicalities

MPI on Euler
[Selecting MPI Distribution]

- What's available: OpenMPI, MVAPICH, MVAPICH2
- OpenMPI is default on Euler
  - This is the only one we'll support in ME759

- To load OpenMPI environment variables:
  - (This should have been done automatically)

```
$ module load mpi/gcc/openmpi
```


[A. Seidl]→

MPI on Euler:
[Compiling MPI Code via Cmake]

```
# Minimum version of CMake required.
cmake_minimum_required(VERSION 2.8)

# Set the name of your project
project(ME964-mpi)

# Include macros from the SBEL utils library
Include(ParallelUtils.cmake)

# Example MPI program
enable_mpi_support()
add_executable(integrate_mpi integrate_mpi.cpp)
target_link_libraries(integrate_mpi ${MPI_CXX_LIBRARIES})
```

With the template

```
find_package("MPI" REQUIRED)

list(APPEND CMAKE_C_COMPILE_FLAGS ${MPI_C_COMPILE_FLAGS})
list(APPEND CMAKE_C_LINK_FLAGS ${MPI_C_LINK_FLAGS})
include_directories(${MPI_C_INCLUDE_PATH})

list(APPEND CMAKE_CXX_COMPILE_FLAGS ${MPI_CXX_COMPILE_FLAGS})
list(APPEND CMAKE_CXX_LINK_FLAGS ${MPI_CXX_LINK_FLAGS})
include_directories(${MPI_CXX_INCLUDE_PATH})
```

Without the template

Replaces include(SBELUtils.cmake) and enable_mpi_support() above

[A. Seidl]→

MPI on Euler:
[Compiling MPI Code by Hand]

- Most MPI distributions provide wrapper scripts named **`mpicc`** or **`mpicxx`**
  - Adds in **`-L`**, **`-l`**, **`-I`**, etc. flags for MPI
  - Passes any options to your native compiler (**`gcc`**)
  - Very similar to what **`nvcc`** did for CUDA – it's a compile driver…

```
$ mpicxx -o integrate_mpi integrate_mpi.cpp
```


[A. Seidl]→

Running MPI Code on Euler

```
mpiexec [-np #] [-machinefile file] <program> [<args>]
```

- `-np #`: Number of processors. Optional if using a machinefile
- `-machinefile file`: List of hostnames to use. Inside Torque, this file is at $PBS_NODEFILE
- `<program> [<args>]`: Your program and its arguments

- The machinefile/nodefile is required for multi-node jobs with the version of OpenMPI on Euler
- **`-np`** will be set automatically from the machinefile; can select lower, but not higher
- See the **`mpiexec`** manpage for more options

[A. Seidl]→

Example

```
euler $ qsub -I -l nodes=8:ppn=4:amd,walltime=5:00
qsub: waiting for job 15246.euler to start
qsub: job 15246.euler ready

euler07 $ cd $PBS_O_WORKDIR
euler07 $ mpiexec -machinefile $PBS_NODEFILE ./integrate_mpi
32 32.121040666358297 in 0.998202s

euler07 $ mpiexec -np 16 -machinefile $PBS_NODEFILE ./integrate_mpi
16 32.121040666359455 in 1.524001s

euler07 $ mpiexec -np 8 -machinefile $PBS_NODEFILE ./integrate_mpi
8 32.121040666359136 in 2.171963s

euler07 $ mpiexec -np 4 -machinefile $PBS_NODEFILE ./integrate_mpi
4 32.121040666360585 in 4.600204s

euler07 $ mpiexec -np 2 -machinefile $PBS_NODEFILE ./integrate_mpi
2 32.121040666366788 in 7.615060s

euler07 $ ./integrate_mpi
1 32.121040666353437 in 15.163330s
```


[A. Seidl]→

Compiling MPI Code, Known Issue…

- Why do I get a compilation error "**`catastrophic error: #error directive: SEEK_SET is #defined but must not be for the C++ binding of MPI`**" when I compile C++ application?
  - Define the `MPICH_IGNORE_CXX_SEEK` macro at compilation stage to avoid this issue. For instance,

    ```
    $ mpicc -DMPICH_IGNORE_CXX_SEEK
    ```

- Why?
  - There are name-space clashes between **`stdio.h`** and the MPI C++ binding. MPI standard requires **`SEEK_SET`**, **`SEEK_CUR`**, and **`SEEK_END`** names in the MPI namespace, but **`stdio.h`** defines them to integer values. To avoid this conflict make sure your application includes the **`mpi.h`** header file before **`stdio.h`** or **`iostream.h`** or undefine **`SEEK_SET`**, **`SEEK_CUR`**, and **`SEEK_END`** names before including **`mpi.h`**.

MPI Nuts and Bolts

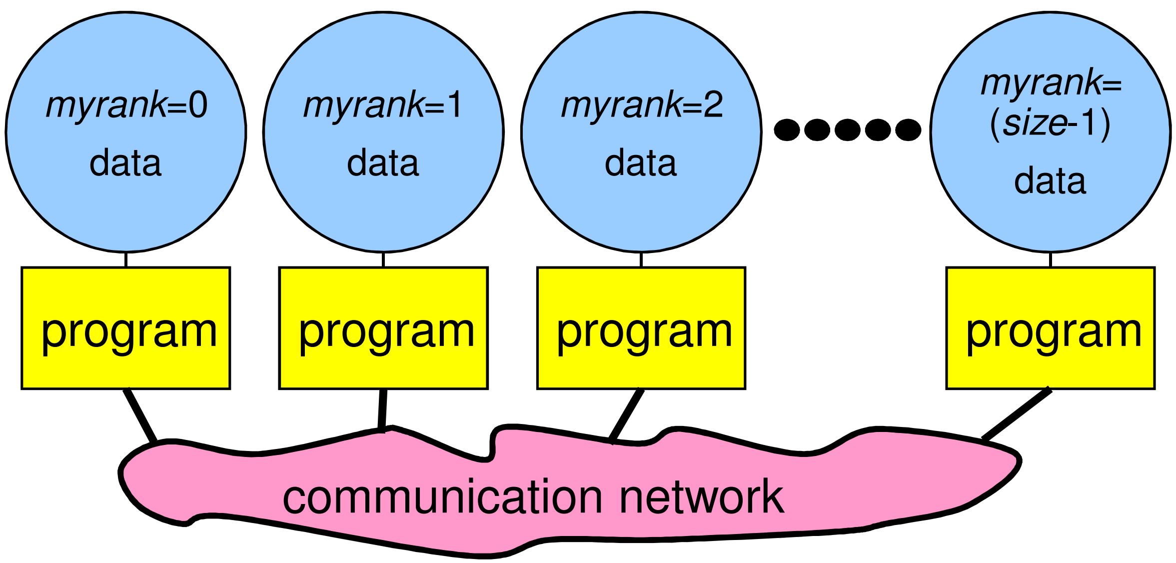
Goals/Philosophy of MPI

- MPI's prime goals
  - Provide a message-passing interface for parallel computing
  - Make source-code portability a reality
  - Provide a set of services (building blocks) that increase developer's productivity

- The philosophy behind MPI:
  - Specify a standard and give vendors the freedom to go about its implementation
  - Standard should be hardware platform & OS agnostic – key for code portability

The Rank, as a Facilitator for Data and Work Distribution

- To communicate together MPI processes need identifiers: **rank = identifying number**
- Work distribution decisions are based on the ***rank***
  - Helps establish which process works on which data
  - Just like we had thread and block indices in CUDA



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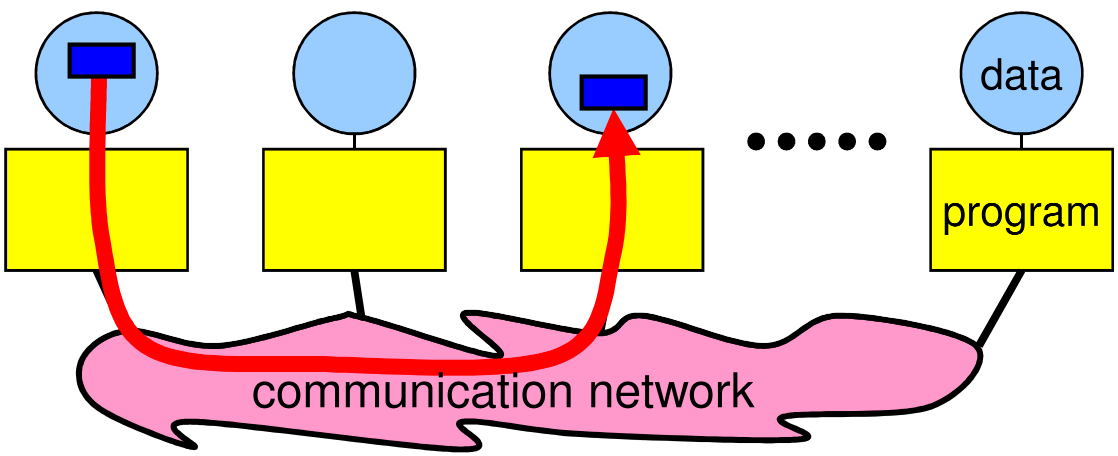
Message Passing

- Messages are packets of data moving between different processes
- Necessary information for the message passing system:
  - sending process + receiving process } i.e., the two “ranks”
  - source location + destination location
  - source data type + destination data type
  - source data size + destination buffer size



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MPI: An Example Application

[From previous lecture]

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

int main(int argc, char* argv[]) {
    int         my_rank;       /* rank of process      */
    int         p;             /* number of processes  */
    int         source;        /* rank of sender       */
    int         dest;          /* rank of receiver     */
    int         tag = 0;       /* tag for messages     */
    char        message[100];  /* storage for message  */
    MPI_Status  status;        /* return status for receive  */

    MPI_Init(&argc, &argv); // Start up MPI
    MPI_Comm_rank(MPI_COMM_WORLD, &my_rank); // Find out process rank
    MPI_Comm_size(MPI_COMM_WORLD, &p); // Find out number of processes

    if (my_rank != 0) {
        /* Create message */
        sprintf(message, "Greetings from process %d!", my_rank);
        dest = 0;
        /* Use strlen+1 so that '\0' gets transmitted */
        MPI_Send(message, strlen(message)+1, MPI_CHAR, dest, tag, MPI_COMM_WORLD);
    }
    else { /* my_rank == 0 */
        for (source = 1; source < p; source++) {
            MPI_Recv(message, 100, MPI_CHAR, source, tag, MPI_COMM_WORLD, &status);
            printf("%s\n", message);
        }
    }

    MPI_Finalize(); // Shut down MPI
    return 0;
} /* main */
```

Program Output

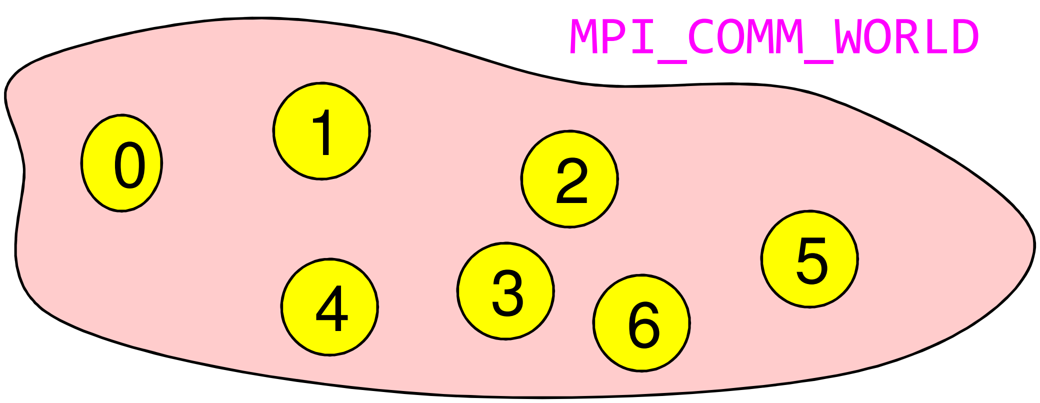
```
[negrut@euler CodeBits]$ mpiexec -np 8 ./greetingsMPI.exe
Greetings from process 1!
Greetings from process 2!
Greetings from process 3!
Greetings from process 4!
Greetings from process 5!
Greetings from process 6!
Greetings from process 7!
[negrut@euler CodeBits]$
```

Communicator MPI_COMM_WORLD

- All processes of an MPI program are members of the default communicator MPI_COMM_WORLD

- MPI_COMM_WORLD is a predefined **handle** in **`mpi.h`**

- Each process has its own **rank** in a given communicator:
  - starting with 0
  - ending with (size-1)



- You can define a new communicator in case you find it useful
  - Use MPI_Comm_create call. Example creates the communicator DANS_COMM_WORLD

```
MPI_Comm_create(MPI_COMM_WORLD, new_group, &DANS_COMM_WORLD);
```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MPI_Comm_create

- Synopsis

```
int MPI_Comm_create(MPI_Comm comm, MPI_Group group, MPI_Comm *newcomm);
```

- Input Parameters
  - `comm` - communicator (handle)
  - `group` - subset of the family of processes making up the `comm` (handle)

- Output Parameter
  - `comm_out` - new communicator (handle)

Point-to-Point Communication

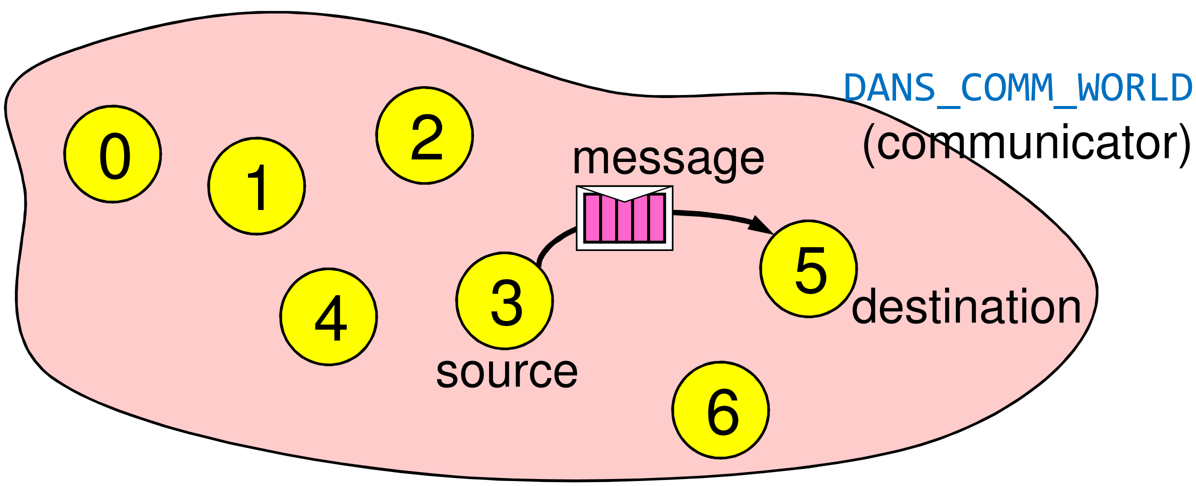
- Simplest form of message passing

- One process sends a message to another process
  - `MPI_Send`
  - `MPI_Recv`

- Sends and receives can be
    - Blocking
    - Non-blocking
  - More on this shortly

Point-to-Point Communication

- Communication between two processes
- Source process sends message to destination process
- Communication takes place within a communicator, e.g., `DANS_COMM_WORLD`
- Processes are identified by their ranks in the communicator



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The Data Type

- A message contains a number of elements of some particular data type
- MPI data types:
  - Basic data type
  - Derived data types – more on this later
- Data type handles are used to describe the type of the data moved around

Example: message with 5 integers

2345	654	96574	-12	7676

MPI Datatype	C datatype
MPI_CHAR	signed char
MPI_SHORT	signed short int
MPI_INT	signed int
MPI_LONG	signed long int
MPI_UNSIGNED_CHAR	unsigned char
MPI_UNSIGNED_SHORT	unsigned short int
MPI_UNSIGNED	unsigned int
MPI_UNSIGNED_LONG	unsigned long int
MPI_FLOAT	float
MPI_DOUBLE	double
MPI_LONG_DOUBLE	long double
MPI_BYTE	
MPI_PACKED	

Example:

2345	654	96574	-12	7676

count=5
datatype=MPI_INT

int arr[5]

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MPI_Send & MPI_Recv: The Eager and Rendezvous Flavors

- If you send small messages, the content of the buffer is sent to the receiving partner immediately
  - Operation happens in “eager mode”

- If you send a large amount of data, the sender function waits for the receiver to post a receive before sending the actual data of the message

- Why this eager-rendezvous dichotomy?
  - Because of the size of the data and the desire to have a safe implementation
  - If you send a small amount of data, the MPI implementation can buffer the content and actually carry out the transaction later on when the receiving process asks for data
    - Can’t play this trick if you attempt to move around a huge chunk of data though

MPI_Send & MPI_Recv: The Eager and Rendezvous Flavors

- NOTE: Each implementation of MPI has a default value (which might change at run time) beyond which a larger `MPI_Send` stops acting "eager"
  - The MPI standard doesn't provide specifics
  - You don't know how large is too large…
- Does it matter if it's Eager or Rendezvous?
  - In fact it does, sometimes the code can hang – example to come
- Remark: In the message-passing paradigm for parallel programming you'll always have to deal with the fact that the data that you send needs to "live" somewhere during the send-receive transaction

MPI_Send & MPI_Recv: Blocking vs. Non-blocking

- Moving away from the Eager vs. Rendezvous modes → they only concern the MPI_Send and MPI_Recv pair

- Messages can be sent with other vehicles than plain vanilla MPI_Send

- The class of send-receive operations can be classified based on whether they are blocking or non-blocking
  - Blocking send: upon return from a send operation, you can modify the content of the buffer in which you stored data to be sent since a copy of the data has been sent
  - Non-blocking: the send call returns immediately and there is no guarantee that the data has actually been transmitted upon return from send call
    - Take home message: before you modify the content of the buffer you better make sure (through a MPI status call) that the send actually completed

Example: Send & Receive
Non-blocking Alternative: MPI_Isend

- If non-blocking, the data "lives" in your buffer – that's why it's not safe to change it since you don't know when transaction was closed
  - This typically realized through a `MPI_Isend`
    - "I" stands for "immediate"

- NOTE: there is another way for providing a buffer region but this alternative is blocking
  - Realized through `MPI_Bsend`
    - "B" stands for "buffered"
  - The problem here is that *you* need to provide this additional buffer that stages the transfer
    - Interesting question: how large should *that* staging buffer be?
  - Adding another twist to the story: if you keep posting non-blocking sends that are not matched by corresponding "`MPI_Recv`" operations, you are going to overflow this staging buffer

Example: Send & Receive
<u>Blocking</u> Options (several of them)

- The plain vanilla MPI_Send & MPI_Recieve pair is blocking
  - It’s safe to modify the data buffer upon return

- The problem with plain vanilla:
  - 1: when sending large messages, there is no overlap of compute & data movement
    - This is what we strived for when using “streams” in CUDA
  - 2: if not done properly, the processes executing the MPI code can hang

- There are several other flavors of send/receive operations, to be discussed later, that can help with concerns 1 and 2 above

The Mechanics of P2P Communication: Sending a Message

```
int MPI_Send(void *buf, int count, MPI_Datatype datatype, int dest, int tag, MPI_Comm comm)
```

- `buf` is the starting point of the message with `count` elements, each described with `datatype`
- `dest` is the rank of the destination process within the communicator `comm`
- `tag` is an additional nonnegative integer piggyback information, additionally transferred with the message
  - The `tag` can be used to distinguish between different messages
  - Rarely used

The Mechanics of P2P Communication: Receiving a Message

```
int MPI_Recv(void *buf, int count, MPI_Datatype datatype, int source, int tag,
                MPI_Comm comm, MPI_Status *status)
```

- `buf`/`count`/`datatype` describe the receive buffer
- Receiving the message sent by process with rank `source` in `comm`
- Only messages with matching `tag` are received
- Envelope information is returned in the `MPI_Status` object `status`

MPI_Recv:
The Need for an MPI_Status Argument

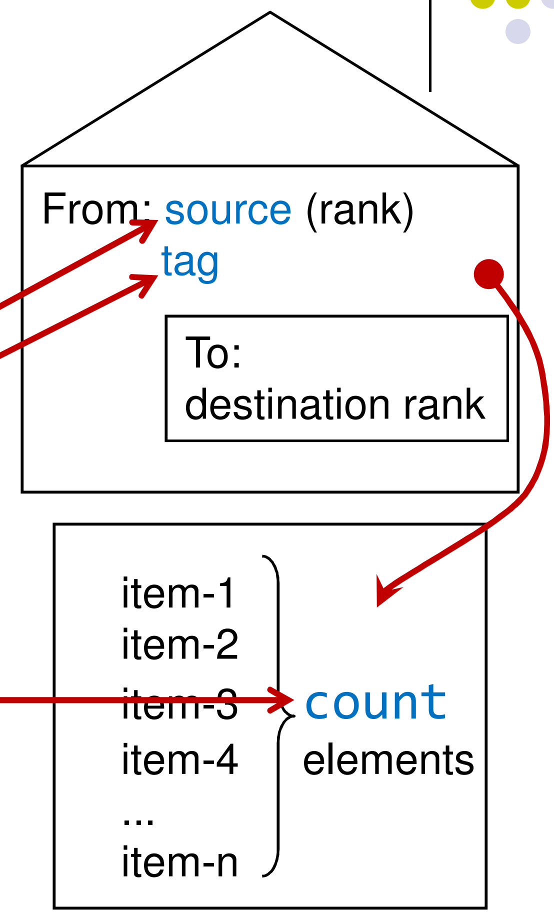
- The `MPI_Status` object returned by the call settles a series of questions:
  - The receive call does not specify the size of an incoming message, but only an upper bound
  - If multiple requests are completed by a single MPI function, a distinct error code may need to be returned for each request
  - The source or tag of a received message may not be known if wildcard values were used in a receive operation

The Mechanics of P2P Communication: Wildcarding

- Receiver can wildcard
  - To receive from any source – `source` = `MPI_ANY_SOURCE`
  - To receive from any tag – `tag` = `MPI_ANY_TAG`
  - Actual source and tag returned in receiver's `status` argument

The Mechanics of P2P Communication: Communication Envelope

- Envelope information is returned from MPI_RECV in `status`.
- `status.MPI_SOURCE`
  `status.MPI_TAG`
  `count` via `MPI_Get_count()`




```
int MPI_Get_count(MPI_Status *status, MPI_Datatype datatype, int *count);
```

The Mechanics of P2P Communication: Some Rules of Engagement

For a communication to succeed:

- Sender must specify a valid destination rank
- Receiver must specify a valid source rank
- The communicator must be the same
- Tags must match
- Message data types must match
- Receiver's buffer must be large enough

Blocking Type: Communication Modes

- Send communication modes:
  - Synchronous send → MPI_SSEND
  - Buffered [asynchronous] send → MPI_BSEND
  - Standard send → MPI_SEND
  - Ready send → MPI_RSEND
- Receiving all modes → MPI_RECV

Cheat Sheet, Blocking Options

Sender modes	Definition	Notes
Synchronous send **MPI_SSEND**	Only completes when the receive has started	
Buffered send **MPI_BSEND**	Always completes (unless an error occurs), irrespective of receiver	needs application-defined buffer to be declared with MPI_BUFFER_ATTACH
Synchronous **MPI_SEND**	Standard send	
Ready send **MPI_RSEND**	May be started **only** if the matching receive is already posted!	avoid, might cause unforeseen problems...
Receive **MPI_RECV**	Completes when a the message (data) has arrived	

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