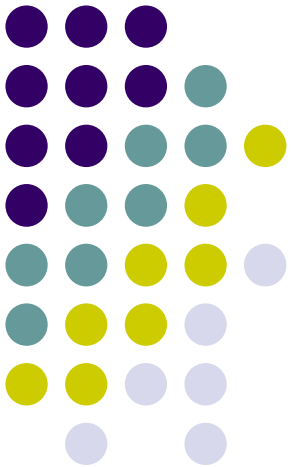
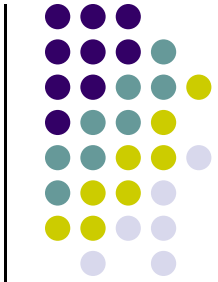
ECE/ME/EMA/CS 759
High Performance Computing for Engineering Applications

Parallel Computing via MPI

November 11, 2015
Lecture 25



Quote of the Day

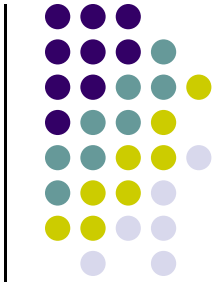


“Do what you can, with what you have, where you are.”

-- Theodore Roosevelt, US President

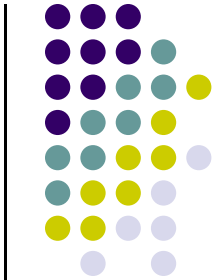
1958-1919

Before We Get Started

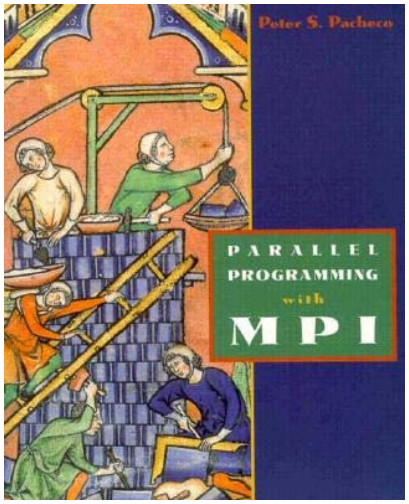


- Issues covered last time:
  - SSE and AVX quick overview
  - Parallel computing w/ MPI
- Today's topics
  - Examples, MPI-enabled parallel computing
  - Point-to-point message passing
- Other issues:
  - HW08, due on Th, Nov. 12, at 11:59 PM
  - New assignment: HW09, due on Wd, Nov. 18, at 11:59 PM. Posted online today.
  - Final Project proposal due on 11/13 in Learn@UW
  - Second and last exam: coming up on 11/23 at 7:15 PM (Room TBA)
    - Review during regular lecture hours, on 11/23

MPI: A Second Example Application



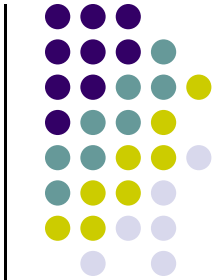
- Example out of Pacheco's book:
  - "Parallel Programming with MPI"
  - Good book, newer edition available




```
/* greetings.c -- greetings program
 *
 * Send a message from all processes with rank != 0 to process 0.
 *    Process 0 prints the messages received.
 *
 * Input: none.
 * Output: contents of messages received by process 0.
 *
 * See Chapter 3, pp. 41 & ff in PPMPI.
 */
```

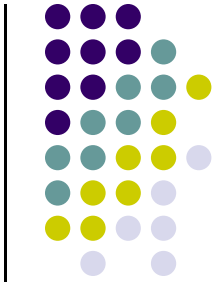
MPI: A Second Example Application

[Cntd.]



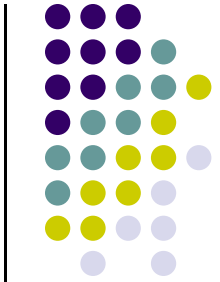
```c
#include "mpi.h"
#include <stdio.h>
#include <string.h>

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

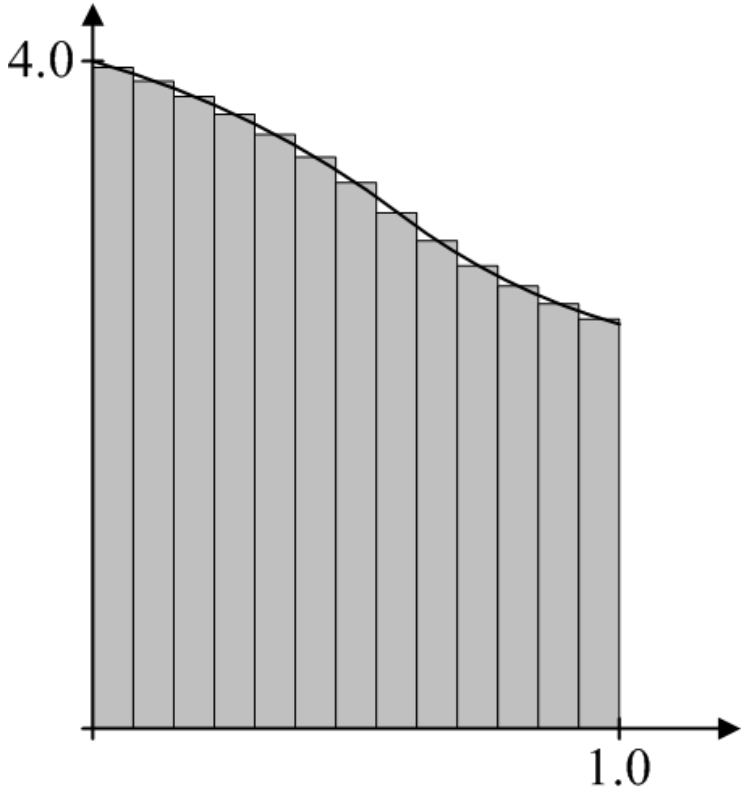


```
[negrut@euler CodeBits]$ mpiexec -np 8 ./greetingsMPI.exe
Greetings from process 1!
Greetings from process 2!
Greetings from process 3!
Greetings from process 4!
Greetings from process 5!
Greetings from process 6!
Greetings from process 7!
[negrut@euler CodeBits]$
```

MPI, a Third Example: Approximating π



$$\int_0^1 \frac{4}{1+x^2} = 4 \cdot \tan^{-1}\left(1\right) = \pi$$

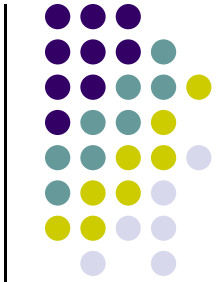


Numerical Integration: Midpoint rule

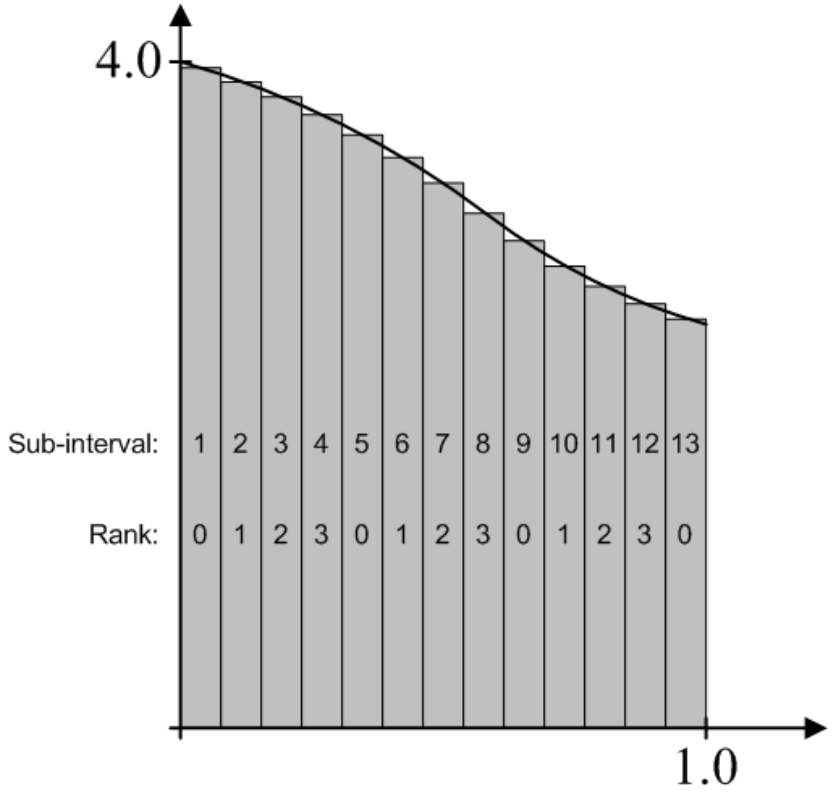
$$\int_0^1 \frac{4}{1+x^2} \approx \sum_{i=1}^{n} \frac{1}{n} f\left((i-0.5)\cdot h\right)$$

[T. Heyn]→

MPI, a Third Example: Approximating π

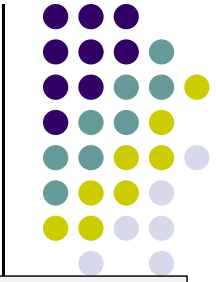


- Use 4 MPI processes (rank 0 through 3)
- In the picture, n=13
- Sub-intervals are assigned to ranks in a round-robin manner
  - Rank 0: 1,5,9,13
  - Rank 1: 2,6,10
  - Rank 2: 3,7,11
  - Rank 3: 4,8,12
- Each rank computes the area in its associated sub-intervals
- `MPIReduce` is used to sum the areas computed by each rank yielding final approximation to π



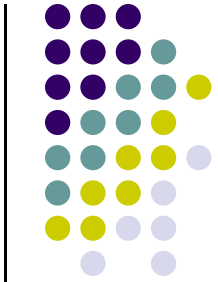
[T. Heyn]→

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 = 3.14159265358979323846264 3;
    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 * (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

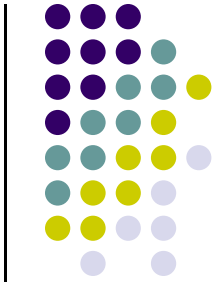
How many instances of this data type are moved around

Partial contribution of "this" process

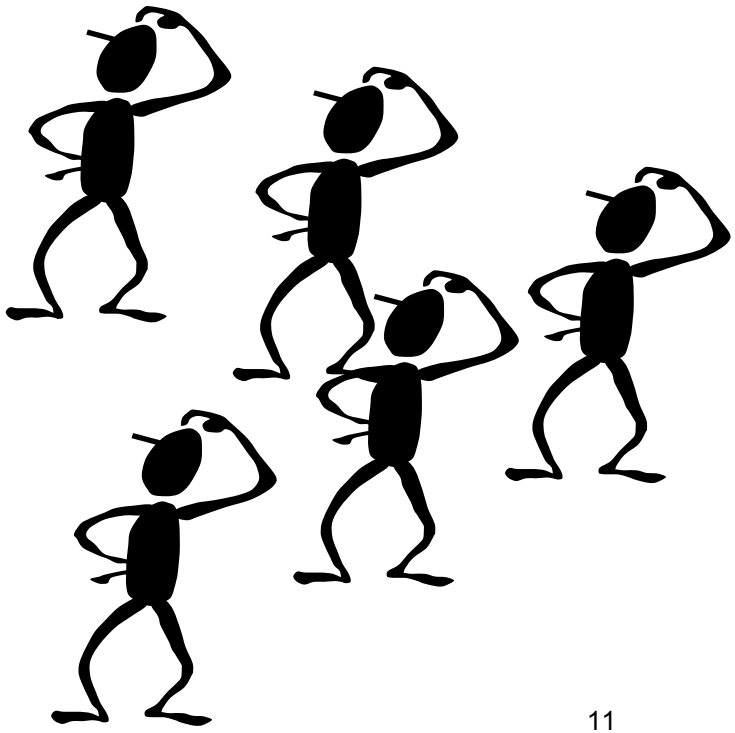
Where the reduce operation stores the result

Broadcast

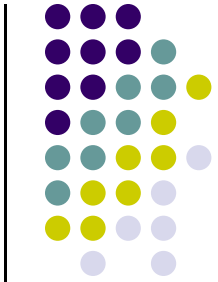
[MPI function used in Example]



- A one-to-many communication.



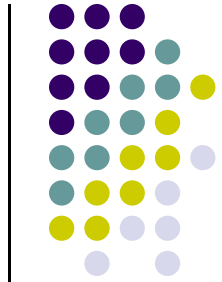
Collective Communications



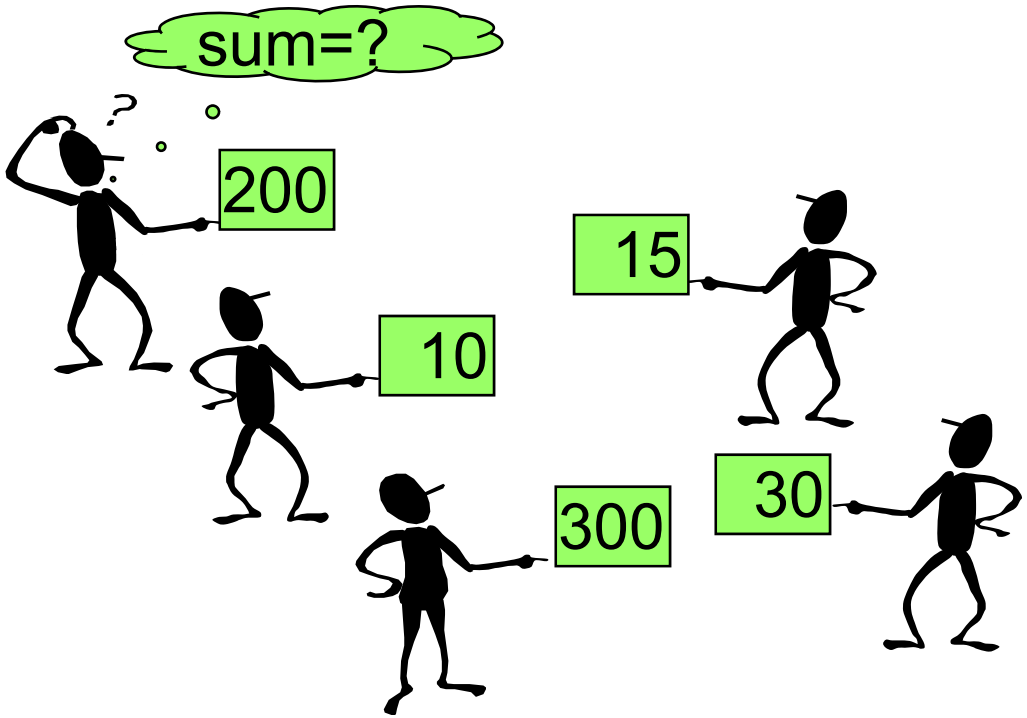
- Collective communication routines are higher level routines
- Several processes are involved at a time
- May allow **optimized internal** implementations, e.g., tree based algorithms
  - Require O(log(N)) time as opposed to O(N) for naïve implementation

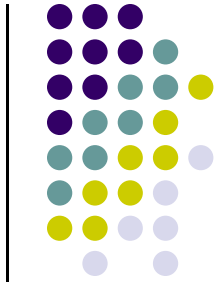
Reduction Operations

[MPI function used in Example]



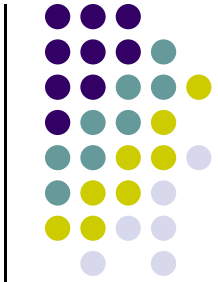
- Combine data from several processes to produce a single result





MPI, Practicalities

MPI on Euler
[Selecting MPI Distribution]



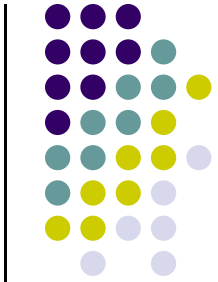
- What's available: OpenMPI, MVAPICH, MVAPICH2
- OpenMPI is default on Euler

- To load OpenMPI environment variables:
  - Typically not needed, should be done automatically for you

```
$ module load openmpi
```


[Colin]→

MPI on Euler:
[Compiling MPI Code by Hand]

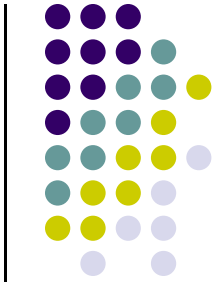


- Most MPI distributions provide wrapper scripts named `mpicc` or `mpicxx`
  - Adds in `-L`, `-l`, `-I`, etc. flags for MPI
  - Passes any options to your native compiler (`gcc`)
  - Very similar to what `nvcc` did for CUDA – it's a compile driver…

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


[Colin]→

Running MPI Code on Euler



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

Number of processors. Inside SLURM, this is handled automatically.

List of hostnames to use. Inside SLURM, this is handled automatically.

Your program and its arguments

- **`-np`** will be set automatically by SLURM. Do not use it.
- **`-machinefile`** will be set automatically by SLURM. Do not use it.
- See the **`mpirun`** manpage for more options

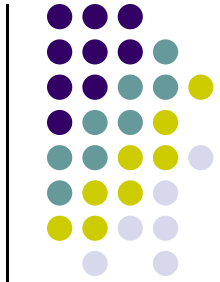
[Colin]→

Example

```
### BEGINNING OF submit_mpi.sh SCRIPT ###

#!/bin/bash
#SBATCH -t 0-5:0:0
#SBATCH -o output.txt

cd $SLURM_SUBMIT_DIR
mpirun ./integrate_mpi

### END OF SCRIPT ###
```

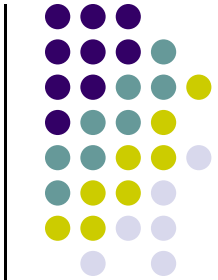
```
euler $ sbatch -N 2 -n 4 submit_mpi.sh
euler $ cat output.txt
8 32.121040666358297 in 2.171963s

euler $ sbatch -N 2 -n 2 submit_mpi.sh
euler $ cat output.txt
4 32.121040666358297 in 4.600204s

euler $ sbatch -N 1 -n 1
euler $ cat output.txt
1 32.121040666358297 in 15.163330s
```


[Colin]→



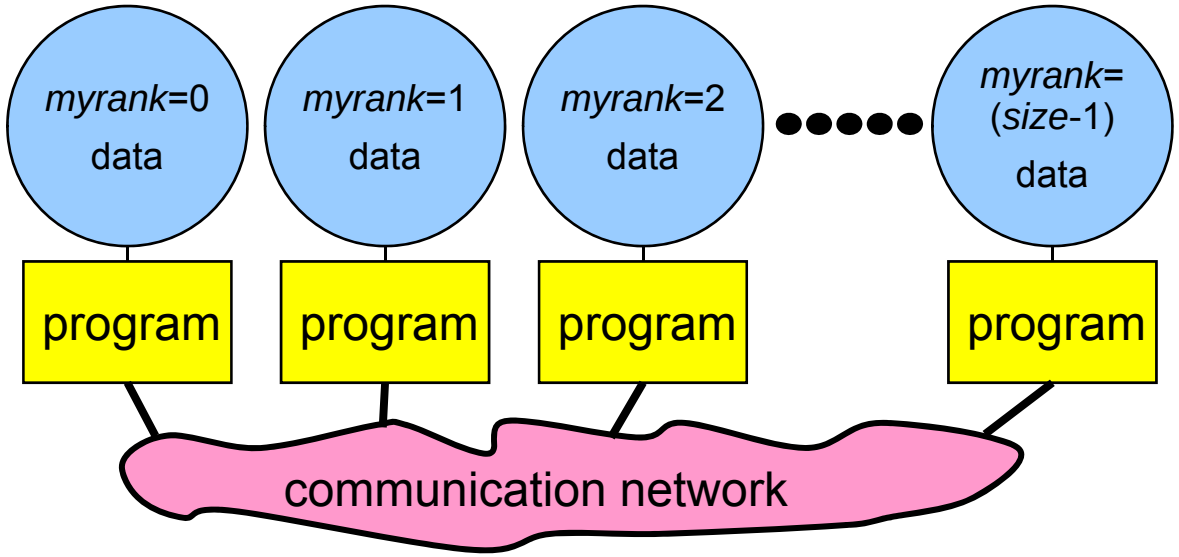
MPI Nuts and Bolts

The Rank & The Communicator
[As Facilitators for Data and Work Distribution]

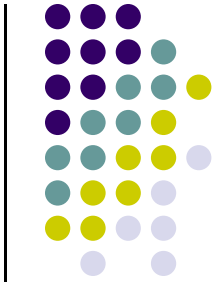


- To communicate with each other MPI processes need identifiers: **rank = identifying number**

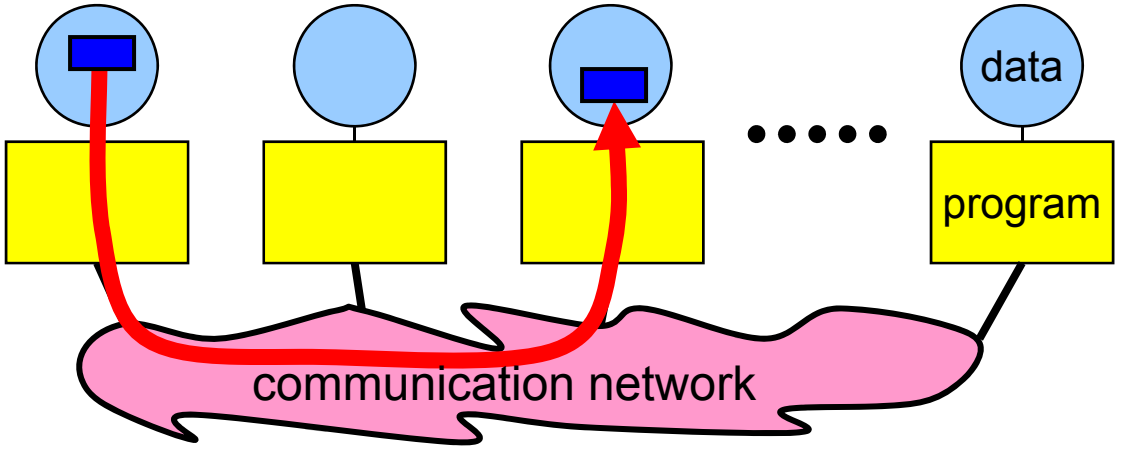
- Work distribution decisions are based on the ***rank***
  - Helps establish which process works on which data
  - Just like we had thread and block indices in CUDA



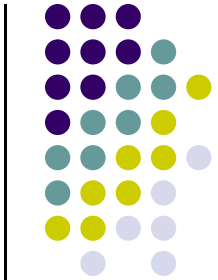
Message Passing



- 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

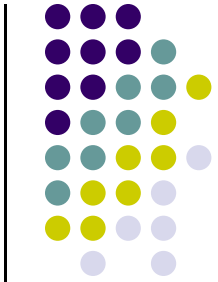


MPI: Revisiting Previous Example



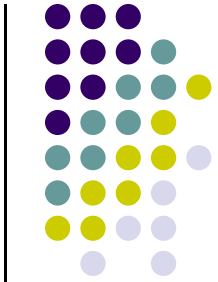
```c
#include "mpi.h"
#include <stdio.h>
#include <string.h>

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

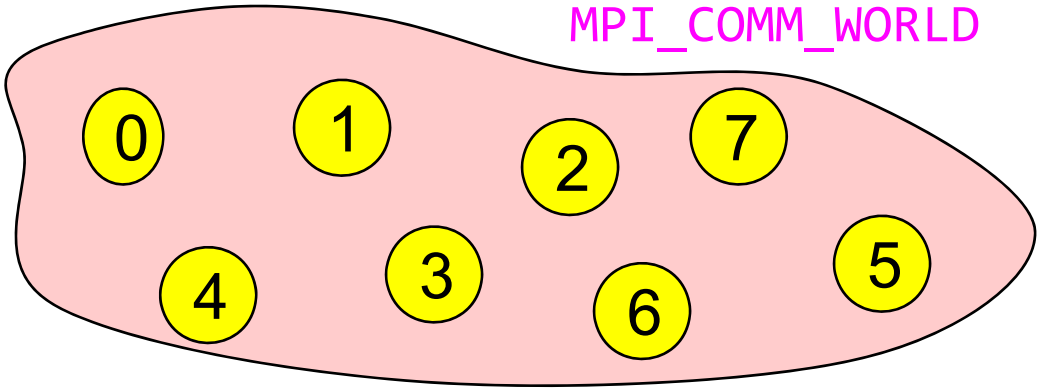


```
[negrut@euler CodeBits]$ mpiexec -np 8 ./greetingsMPI.exe
Greetings from process 1!
Greetings from process 2!
Greetings from process 3!
Greetings from process 4!
Greetings from process 5!
Greetings from process 6!
Greetings from process 7!
[negrut@euler CodeBits]$
```

Communicator MPI_COMM_WORLD



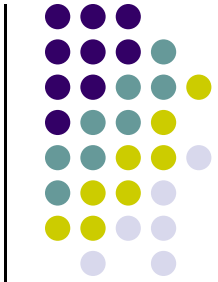
- All processes of an MPI program are members of the default communicator `MPI_COMM_WORLD`
- `MPI_COMM_WORLD` is a predefined **handle** in **`mpi.h`**
- Each process has its own **rank** in a given communicator:
  - starting with 0
  - ending with (size-1)



- 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);
```

MPI_Comm_create



- Synopsis

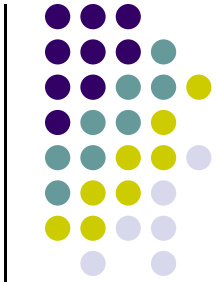
```
int MPI_Comm_create(MPI_Comm comm, MPI_Group group, MPI_Comm *newcomm);
```

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

- Output Parameter
  - newcomm - new communicator (handle)

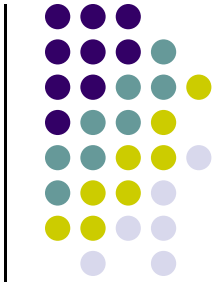
[New Topic]

Point-to-Point Communication

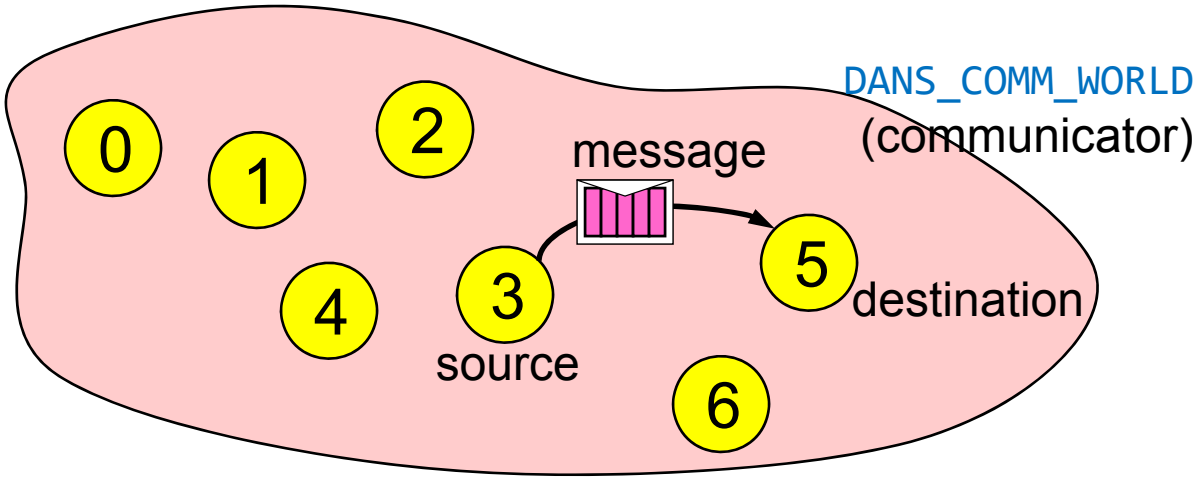


- Simplest form of message passing
- One process sends a message to another process
  - `MPI_Send`
  - `MPI_Recv`
- Sends and receives can be
  - Blocking
  - Non-blocking
  - More on this shortly

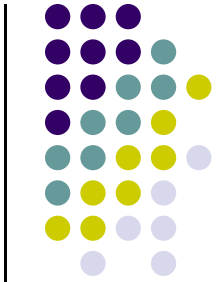
Point-to-Point Communication



- 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



The Data Type

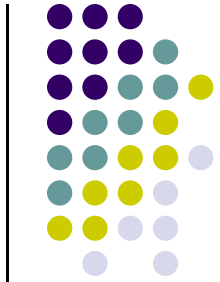


- A message contains a number of elements of some particular data type
- MPI data types:
  - Basic data type
  - Derived data types – more on this later
- Data type handles are used to describe the type of the data moved around

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:

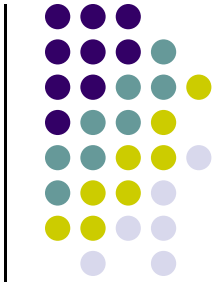
2345	654	96574	-12	7676

count=5

datatype=MPI_INT

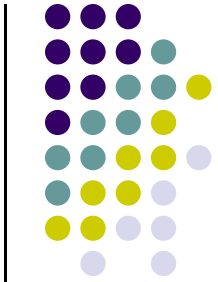
int arr[5]

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 runtime (daemon) can buffer the content and actually carry out the transaction later on when the receiving process asks for data
    - Can’t play though this trick if you attempt to move around a huge chunk of data

MPI_Send & MPI_Recv: The Eager and Rendezvous Flavors

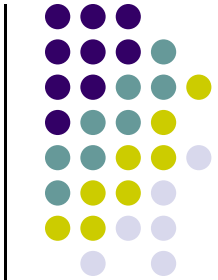


- NOTE: Each implementation of MPI has a default value (which might change at run time) beyond which a larger `MPI_Send` stops acting "eager"
  - The MPI standard doesn't provide specifics
  - You don't know how large is too large…

- Does it matter if it's Eager or Rendezvous?
  - In fact it does, sometimes the code can hang – example to come

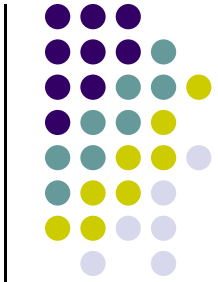
- Remark: In the message-passing paradigm for parallel programming you'll always have to deal with the fact that the data that you send needs to "live" somewhere during the send-receive transaction

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 collection 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
A blocking alternative: MPI_Send

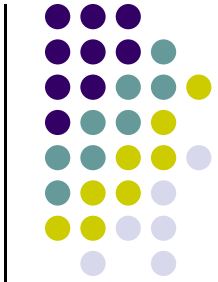


- Several other blocking flavors exist, to be discussed later

- 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

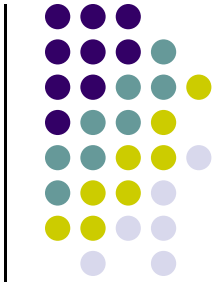
Example: Send & Receive
A non-blocking alternative: MPI_Isend



- If non-blocking, the data "lives" in your array – 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 a *blocking* version that comes pretty close to `MPI_Isend` in terms of performance
  - Called `MPI_Bsend`
    - "B" stands for "buffered"
  - *You* need to provide an additional staging buffer that stages the data transfer
    - Interesting question: how large should *that* staging buffer be?
  - Adding another twist to the story: if you keep posting `MPI_Bsend` sends that are not matched by corresponding "`MPI_Recv`" operations, you are going to overflow this staging buffer

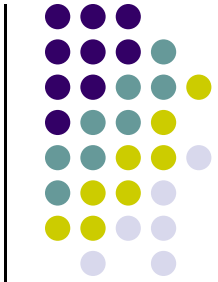
The Mechanics of P2P Communication: Sending a Message



```
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 information, additionally transferred with the message
  - The `tag` can be used to distinguish between different messages
  - Rarely used

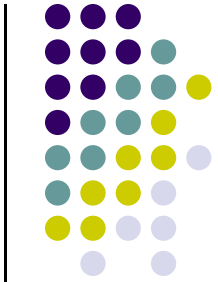
The Mechanics of P2P Communication: Receiving a Message



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

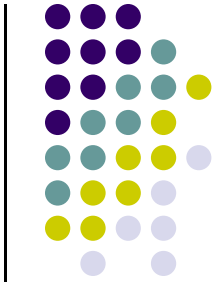
- `buf`/`count`/`datatype` describe the receive buffer
- Receiving the message sent by process with rank `source` in `comm`
- Only messages with matching `tag` are received
- Envelope information is returned in the `MPI_Status` object `status`

MPI_Recv:
The Need for an MPI_Status Argument



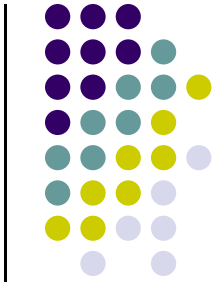
- The `MPI_Status` object returned by the call settles a series of questions:
  - The receive call does not specify the size of an incoming message, but only an upper bound
  - The source or tag of a received message may not be known if wildcard values were used in a receive operation

The Mechanics of P2P Communication: Wildcarding

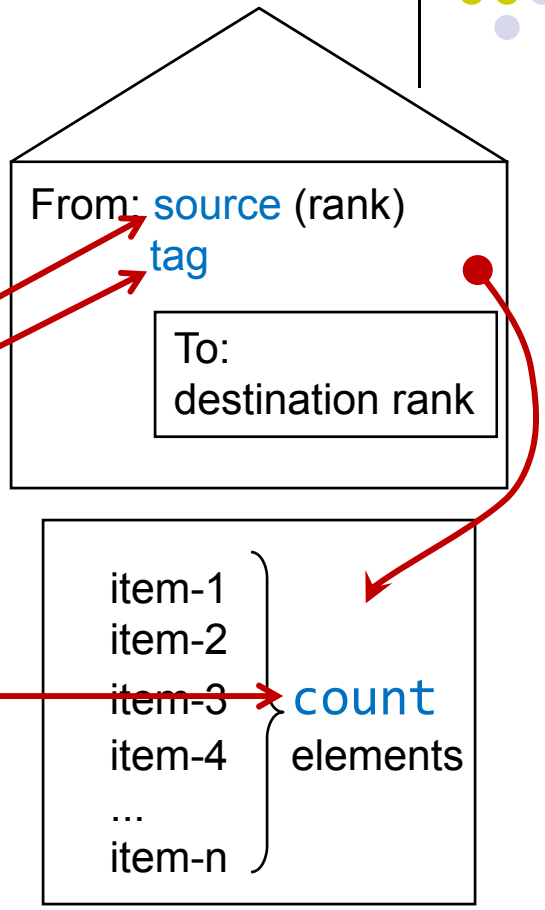


- Receiver can wildcard
  - To receive from any source – `source` = `MPI_ANY_SOURCE`
  - To receive from any tag – `tag` = `MPI_ANY_TAG`
  - Actual source and tag returned in receiver's `status` argument

The Mechanics of P2P Communication: Communication Envelope

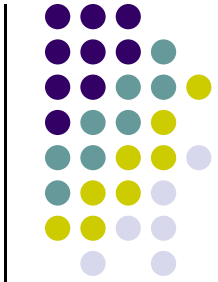


- Envelope information is returned from MPI_RECV in `status`.
- `status.MPI_SOURCE`
  `status.MPI_TAG`
  `count` via `MPI_Get_count()`




```
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 complete fine:

- 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