Parallel Programming with MPI

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a passion for discovery



Plan of the Tutorial

Morning

- 9:00 -10:30 Introduction to MPI
 - Example 1: Hello World
 - Exercise 1: Running your first MPI program
- 10:45 -12:00 Point-to-Point Communications
 - Example 2: Greetings
 - Exercise 2: Trapezoidal rule

Afternoon

- 13:00 15:30 Collective Communications
 - Example 3: Vector dot product
 - Exercise 3: Rewrite Trapezoidal rule
 - Example 4: Matrix Vector multiplication
 - Exercise 4: Matrix Matrix multiplication
- 15:45 17:00 Other Topics in MPI



Disclaimer

- This is not a parallel algorithm course.
 - I will not talk about the best way to parallelize the problems.
- This is not a programming language course.
 - I will not talk about the best way to write the C programs.
- All the examples and exercises are for demonstration purposes only.
 - They do not necessarily use the most efficient implementations.
- I will focus on the basic MPI functions and how to use them in parallel programming.



Introduction to MPI



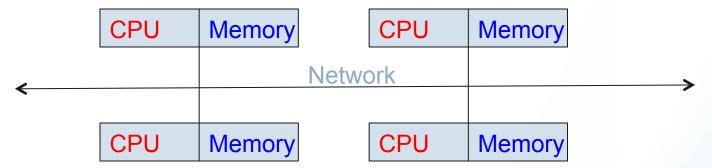
What is MPI?

- MPI = Message Passing Interface
 - It is a standard for implementing communication between compute nodes/processes in parallel programming.
 - It defines the syntax and semantics of a core of library routines.
- MPI is NOT a new programming language.
 - It merely consists of a library of definitions and functions that can be used in C (or Fortran, Python, ...)
- MPI is designed to be efficient, flexible, practical and portable.
- The reports of the MPI standard can be found on MPI Forum: http://www.mpi-forum.org/

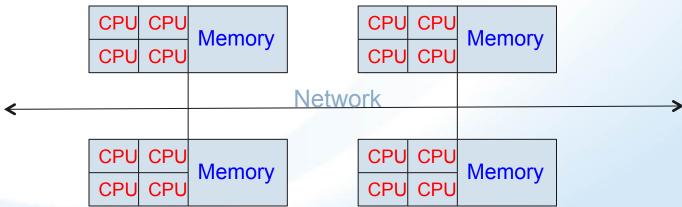


Parallel Systems

Distributed-memory architectures.



Shared-memory/distributed-memory hybrid systems.



MPI in Shared-Memory and Hybrid Systems

- On shared-memory systems, MPI provides the internode message passing routines, e.g., one MPI process per node.
- On hybrid systems, there are two ways to configure MPI:
 - Use MPI for both inter-node and intra-node communications, e.g. one MPI process per core.
 - ✓ Use MPI for inter-node communication, and use OpenMP for the intra-node work-sharing. In this case, we will run one MPI process per node. (MPI/OpenMP hybrid programming.)
 - ✓ Most current HPC systems are hybrid systems.



Evolution of MPI

MPI-1.x:

- The goal was to develop a widely used standard for writing messagepassing programs.
- Initially over 40 organizations participated in the discussion.
- The final report of Version 1.0 was completed in 1994.

MPI-2.x:

- Contains corrections and extensions to MPI-1.x.
- Focused on process creation and management, one-sided communications, extended collective communications, external interfaces and parallel IO.
- Version 2.0 published in 1997.

MPI-3.0:

- Major extensions to MPI, including nonblocking collectives, new one-sided communication operations and Fortran 2008 bindings.
- Published in 2012.



Evolution of MPI

Focus of this tutorial

MPI-1.x:

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Different MPI Implementations

- Open-source Implementations (free to download):
 - MPICH www.mpich.org
 - MPICH, MPICH2
 - MVAPICH mvapich.cse.ohio-state.edu
 - MVAPICH, MVAPICH2
 - OpenMPI www.open-mpi.org
- Vendor-specific Implementations (usually not free):
 - Intel MPI
 - HP MPI
 - ...
- You can compile your code with different MPI implementations, and compare the performance between them.



Syntax of MPI Functions

- MPI functions, data types and predefined constants all begin with MPI_
- MPI functions begin with a capital letter, followed by lowercase letters. Examples:
 - MPI_Init(int *argc, char **argv[]),
 - MPI_Finalize()
 - MPI_Comm_rank(MPI_Comm comm, int *rank)
- Predefined MPI constant names are all capitalized. Examples:
 - MPI_COMM_WORLD
 - MPI_DOUBLE



General MPI Program Structure

```
#include <mpi.h>
/* other include files */
#include ...
int main(int argc, char *argv[]){
        /*serial code*/
        /* parallel MPI code begins*/
        MPI_Init(&argc, &argv);
        MPI_Finalize()
        /* parallel MPI code ends here */
        return 0;
```

MPI Communicators

- A communicator is a collection of processes that can send messages to each other.
- MPI_COMM_WORLD is a predefined communicator which consists of all the processes running when the program begins execution.
- For this tutorial, we will only use MPI_COMM_WORLD.



Basic MPI Functions

- int MPI_Init(int *argc, char ***argv)
 - Initializes the MPI execution environment. This function must be called in every MPI program, must be called before any other MPI functions and must be called only once in an MPI program.
- int MPI_Finalize(void)
 - Terminates the MPI execution environment. It must be the last MPI routine called in an MPI program. No other MPI routines may be called after it.
- int MPI_Comm_size(MPI_Comm comm, int *size)
 - Determines the total number of processes in the specified communicator, such as MPI COMM WORLD.
- int MPI_Comm_rank(MPI_Comm comm, int *rank)
 - Returns the rank of the calling MPI process with the specified communicator. Each MPI process is assigned a unique integer value between 0 and (number of processes – 1)
- int MPI_Abort(MPI_Comm comm, int code)
 - Terminates the MPI processes associated with the communicator *comm*, and returns the error code specified in *code*.



Hello World

- A sample hello world program with MPI
- Note: no communications yet.

```
#include <stdio.h>
#include <mpi.h>
int main(int argc, char *argv[])
 int rank;
 int numtasks;
 MPI Init(&argc, &argv); /*Initializes MPI calls*/
 MPI Comm rank(MPI COMM WORLD, &rank); /* obtains the rank of current MPI process */
 MPI Comm size(MPI COMM WORLD, &numtasks); /* obtains the total number of MPI processes */
 if (rank == 0)
   printf("hello world. I am MASTER\n");
  else
   printf("hello world from process %d of %d\n", rank, numtasks);
 MPI Finalize();
                       /*Finalizes MPI calls */
 return 0:
```



SPMD Parallel Programming

- Note that in the previous Hello World example, while we do not send different programs to different processes, the code segments different processes execute are actually slightly different.
- We differentiate the data with the process ranks.
- This technique is called Single Program Multiple Data (SPMD) parallel programming.
- It is a common parallel programming technique in MIMD (Multiple Instruction Multiple Data) systems.



Compiling and Running MPI Programs

- mpicc is a shell script that sets the environment for compiling an MPI program using GNU-C compiler
- mpirun or mpiexec executes the MPI program
- On hpc set environment variables using module
 - module avail (modules available on the system)
 - module list (modules currently loaded for you)
 - module load <module name> (load a new module)
- We will use mvapich2 implementation. At terminal prompt, run
 - module load mvapich2
- Check we have the mpicc and mpirun in the path:
 - which mpicc
 - which mpirun



Compiling and Running MPI Programs

- To compile an MPI program program.c
 - mpicc program.c -o program.x
- To run an MPI program
 - mpirun -np 8 program.x
 - This will run program.x with 8 processes on the head node.
- Note: different systems may be configured differently. Be sure to check the system documentation or user guide for MPI commands and options in your own work.



Exercise 1: Hello World

- Obtain the source code helloWorld.c, Makefile and PBS batch script from GitHub:
 - On hpc, run
 - > git clone https://github.com/meifeng/MPI.git
 - This will create a directory MPI in your current work directory. You should have 1_HelloWorld subdirectory as well.
- Compile the HelloWorld program using the provided Makefile
 - > make
- Run the executable:
 - > mpirun -np <number of nodes> helloWorld.x



Running Batch Jobs

- Executing "mpirun -np 8 program.x" directly from your terminal will run the program on the host node.
- PBS scheduler can automatically distribute the jobs to the available nodes.
- PBS batch jobs are controlled by PBS scripts:
- Example:

```
→ Notify when job ends (optional)
#PBS -m e
                              → Email address to get the notifications (optional)
#PBS -M mlin@bnl.gov
#PBS -S /bin/bash
                              → Default shell
#PBS -1 nodes=2:ppn=8
                              → Number of nodes and processors per node requested
#PBS -1 walltime=00:05:00
                              → Wall-clock time requested
                              → Joining stdout and stderr in the output (optional)
#PBS -j oe
                              → Name of the job
#PBS -N mpi
                              → Name of the output file
#PBS -o $PBS JOBID.out
```

```
NODECOUNT=`sort -u ${PBS_NODEFILE} | wc -l`
PROCCOUNT=`sort ${PBS_NODEFILE} | wc -w`
WORK=${PBS_O_WORKDIR}
EXE=${WORK}/helloWorld.x
mpirun -np ${PROCCOUNT} $EXE
```



Running Batch Jobs

- Now use batch.example in the directory.
- Change the scripts to suit your needs
- Run
 - qsub batch.example
- This will submit a job to the PBS queue. Your job will be executed when there are sufficient resources available.
- You can check the status of your jobs by running
 - qstat
- Running "qstat –n" will show you the nodes you are currently running on.



```
Number of nodes is: 2
Number of processors is: 16
The hostnames of the nodes:
node15
The executable is: /home/mlin/MPI/HelloWorld/helloWorld.x
hello world. I am MASTER
hello world from process 2 of 16
hello world from process 3 of 16
hello world from process 4 of 16
hello world from process 5 of 16
hello world from process 6 of 16
hello world from process 7 of 16
hello world from process 1 of 16
hello world from process 8 of 16
hello world from process 9 of 16
hello world from process 10 of 16
                                             System bugs. Please ignore
hello world from process 11 of 16
hello world from process 12 of 16
hello world from process 13 of 16
hello world from process 14 of 16
hello world from process 15 of 16
[mpiexec@node15] HYDT_bscd_pbs_wait_for_completion (./tools/bootstrap/external/pbs
wait.c:68): tm poll(obit ev
ent) failed with TM error 17002
[mpiexec@node15] HYDT bsci wait for completion (./tools/bootstrap/src/bsci wait.c:
23): launcher returned error
waiting for completion
[mpiexec@node15] HYD pmci wait for completion (./pm/pmiserv/pmiserv pmci.c:216): 1
auncher returned error waiti
ng for completion
[mpiexec@node15] main (./ui/mpich/mpiexec.c:325): process manager error waiting fo
r completion
```

Point-to-Point Communications



Point-to-Point Communications

- MPI point-to-point operations typically involve message passing between two, and only two, different MPI processes. One process is performing a send operation, and the other process is performing a matching receive operation.
- There are different types of send and receive routines used for different purposes. For example:
 - Synchronous send
 - Blocking send/blocking receive
 - Non-blocking send/non-blocking receive
 - Buffered send
 - "Ready" send



Basic Blocking Point-to-Point Message Passing

```
int MPI Send (void *
                              buffer,
                                              /* pointer to data sent
                                              /* length of data
              int
                              count.
              MPI Datatype
                              datatype,
                                             /* message data type
                                            /* destination rank
                              destination.
              int
                                              /* non-negative integer
              int
                              tag,
                                                                         */
              MPI Comm
                              communicator) /* communicator involved
```

Routine returns only after the application buffer in the sending process is free for reuse.

```
int MPI Recv (void *
                               buffer.
                                              /* pointer to data received
                                              /* length of data
               int
                               count.
                                                                          */
               MPI Datatype
                               datatype,
                                              /* data type
                                                                          */
               int
                                              /* source rank
                               source,
                                              /* non-negative integer
               int
                               tag,
               MPI_Comm
                               communicator, /* communicator involved
                                              /* status of receive */
               MPI Status *
                               status)
```

Receive a message and block until the requested data is available in the application buffer in the receiving process.

MPI Datatypes

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

Note: MPI also allows user-defined data types.



Exercise 2: Greetings

- Let's modify the Hello World program so that Process i > 0 sends its rank to Process 0.
- Use MPI_Send and MPI_Recv.
- Compile and run on hpc.csc.bnl.gov.



Exercise 2: Example Code

- Obtain the example code 2_Greetings from GitHub
 - From your MPI directory, run
 - > git pull
 - Or point your browser to <u>http://github.com/meifeng/MPI</u>
- Compile and run the code either in interactive mode, or in batch mode.

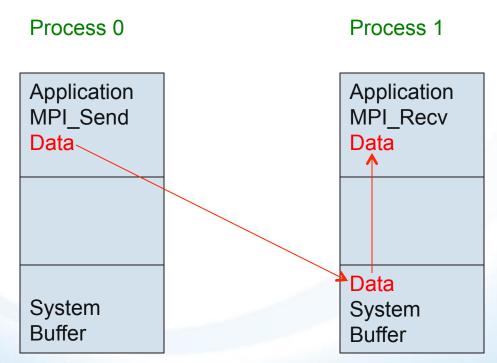


Message Passing in Greetings

```
#include <stdio.h>
#include <mpi.h>
int main(int argc, char *argv[])
  const int ROOT = 0;
  int my rank;
  int recv rank;
  int numtasks;
  int p;
 MPI Init(&argc, &argv); /*Initializes MPI calls*/
 MPI Status status;
 MPI Comm rank(MPI COMM WORLD, &my rank); /* obtains the rank of current MPI process */
 MPI Comm size(MPI COMM WORLD, &numtasks); /* obtains the total number of MPI processes */
 if (my rank != ROOT ) {
   MPI Send(&my rank, 1, MPI_INT, ROOT, 0, MPI_COMM_WORLD);
  else
   for (p = 1; p < numtasks; p++) {
     MPI Recv(&recv rank, 1, MPI INT, p, 0, MPI COMM WORLD, &status);
     printf("Greetings from Process %d\n", recv rank);
                   /*Finalizes MPI calls */
 MPI Finalize();
 return 0:
```

Buffering

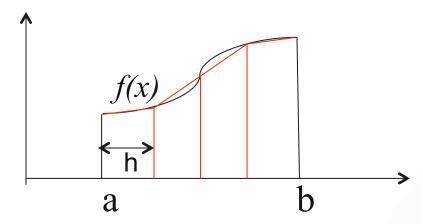
- While every process is sending, there is no one receiving. Where do the data go? (Think ball throwing).
- Typically a chunk of memory is reserved as system buffer.
- The message resides in the system buffer while waiting for the receiving node to retrieve.





Numerical Integration: Trapezoidal Rule

• A finite integral in the region [a,b] $\int_a^b f(x)dx$ is essentially the area enclosed by the function curve and the boundaries.



It can be approximated by calculating the areas of the trapezoids that evenly divide the whole area.

$$\int_{a}^{b} f(x)dx \approx \frac{h}{2} (f(a) + f(a+h)) + \frac{h}{2} (f(a+h) + f(a+2h)) + \dots + \frac{h}{2} (f(a+(N-1)h) + f(b))$$

$$= \left[\frac{1}{2} (f(a) + f(b)) + \sum_{i=1}^{N-1} f(a+jh) \right] \cdot h$$

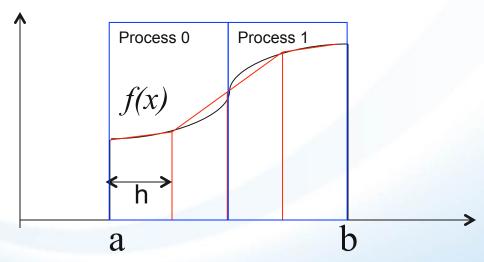
Serial Trapezoidal Rule

```
#include <stdio.h>
       #include <math.h>
       double f(double x){
         return exp(x*x);
       int main(){
         double integral; /*definite integral result*/
         const double a=0.0; /*left end point*/
         const double b=1.0; /*right end point*/
         const int N=100000; /*number of subdivisions*/
         double h;
                              /*base width of subdivision*/
         double x;
         int i;
         h = (b-a)/N;
         integral = (f(a)+f(b))/2.0;
         x = a;
         for(i = 1; i \le N-1; i++){
             x = x+h;
             integral = integral + f(x);
         }
         integral = integral*h;
         printf("%s%d%s%f\n", "WITH N=", N, " TRAPEZOIDS, INTEGRAL=", integral);
         return 0;
Brookhaven S
```



Parallel Trapezoidal Rule

- Before we can write a parallel version of the trapezoidal rule, we need to decide how we want to share the workload among different processes. → Data mapping.
- The simplest approach is perhaps to distribute the data evenly among the processes, and each process runs essentially the same program on its share of the data. → Data-parallel programming.
- We can
 - Assign a subinterval of [a, b] to each process.
 - Have that process estimate the integral of f over the subinterval.
 - Add up the local processes' calculations to get the final integral.





Exercise 3: Trapezoid

- Parallelize the Trapezoidal rule program using MPI_Send and MPI_Recv, assuming N can be divided by the number of processes evenly.
- Send the final result to Process 0 and print out the result at stdout.
- Compile and run the program on hpc.csc.bnl.gov
- Hint:
 - Each process is essentially calculating its own integral, with different integration lower and upper bounds
 - Your main job is to use the process ranks to determine the bounds and integration steps for each process.



Exercise 3: Example Code

- Obtain the example code 3_Trapezoid from GitHub
 - From your MPI directory, run
 - > git pull
 - Or point your browser to <u>http://github.com/meifeng/MPI</u>
- Compile and run the code either in interactive mode, or in batch mode.
 - You can compile the serial version of the code using
 - > make serial



Parallel Trapezoidal Rule

```
/* MPI Trapezoid Rule Program
/* [f(x0)/2 + f(xn)/2 + f(x1) + ... + f(xn-1)]*h */
#include <stdio.h>
#include <math.h>
#include <mpi.h>
double f(double x)
 return exp(x*x);
int main(int argc, char *argv[])
  double integral;
                                      /*definite integral result*/
  const double a=0.0;
                                      /*left end point*/
  const double b=1.0;
                                     /*right end point*/
  const int N=100000;
                                     /*number of subdivisions*/
                                      /*base width of subdivision*
  double h;
  double x;
  int i;
  int my rank;
  int numprocs;
  /* we will need some local variables */
  double local a, local b;
  int local N;
  double 1cl integral;
  int dest = 0;
  double recv;
                                      /* a variable to receive res
  h = (b-a)/N;
                                      /* we assume we use the same
```

```
/* MPI programming begins */
MPI Init(&argc, &argv);
MPI Status status;
MPI_Comm_size(MPI_COMM_WORLD, &numprocs);
MPI Comm rank(MPI COMM WORLD, &my rank);
/* Find out what the local values are on each process */
local N = N/numprocs;
local a = a + my rank * local N * h;
local b = local a + local N * h;
/* begins local integration */
x = local a;
lcl integral = (f(local a)+f(local b))/2.0;
for(i = 1; i <= local_N-1; i++)
    x = x+h;
    lcl integral = lcl integral + f(x);
lcl integral = lcl integral*h;
/* send the local results to Process 0 */
if ( my rank != dest ) {
   MPI_Send(&lcl_integral, 1, MPI_DOUBLE, dest, 0, MPI_COMM_WORLD);
/* Process 0 receives and sums up the results */
   integral = lcl integral;
   for (i = 1; i < numprocs; i++) {
      MPI_Recv(&recv, 1, MPI_DOUBLE, i, 0, MPI_COMM_WORLD, &status);
      integral = integral + recv;
    printf("%s%d%s%f\n", "WITH N=", N, " TRAPEZOIDS, INTEGRAL=", integral);
/* MPI programming ends */
MPI Finalize();
return 0:
```

Other Blocking Message Passing Routines

MPI_Ssend(...)

- Synchronous blocking send.
- In synchronous blocking mode, a send won't complete until a matching receive has been posted and the matching receive has begun reception of the data.

MPI_Bsend(...)

Buffered blocking send, with user-provided buffering.

MPI_Rsend(...)

- Blocking ready send.
- Send may be started only if the matching receive has begun.

MPI_Sendrecv(...)

 Combines sending of a message to one destination, and receiving of a message from another process.



Non-Blocking Message Passing

- Non-blocking message passing returns immediately, regardless of the state of the message sending or retrieval.
- It merely sends a request to the MPI library to perform the operation when it is able to.
- It is unsafe to modify the user variable space (the application buffer) until you are sure that MPI has completed the requested operation. Can use MPI_Wait or MPI_Test to check.
- Non-blocking message passing is very useful in applications with overlapping communication and computation to enhance the program performance.



Non-Blocking Message Passing

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

Starts a nonblocking send and returns immediately.

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

Starts a nonblocking receive and returns immediately.

MPI_Wait(MPI_Request *request, MPI_Status *status)

- Completes any nonblocking operation.
- The *request* parameter corresponds to the *request* parameter in MPI_Isend or MPI_Irecv.
- It blocks until the operation identified by request completes.



Collective Communications



Collective Communications

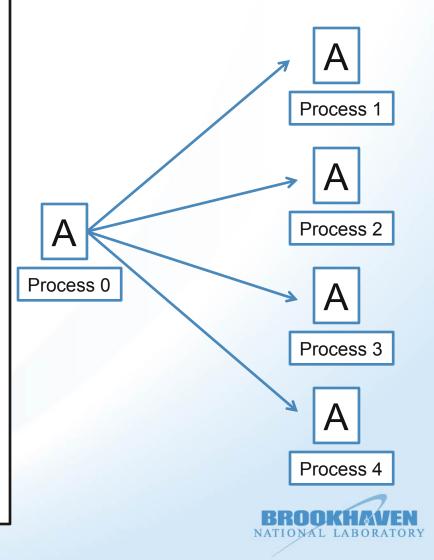
- A communication pattern that involves all the processes in a communicator is a collective communication.
- A collective communication usually involves more than two processes.
- Types of collective communications
 - Broadcast
 - Reduce
 - Allreduce
 - Gather and Scatter
 - Allgather



Broadcast

int MPI_Bcast (void* message, int count, MPI_Datatype type, int root, MPI_Comm comm)

- Sends message from root to all the processes in communicator comm.
- Must be called by all processes in the communicator comm with the same root.
- count and type should be the same on all processes in the communicator.
- A sequence of collective communications on distinct processes will be matched in the order in which they're executed.



Reduce

int MPI_Reduce(void* operand, void* result, int count, MPI_Datatype type,

MPI_Op operator,

int root,

MPI_Comm comm)

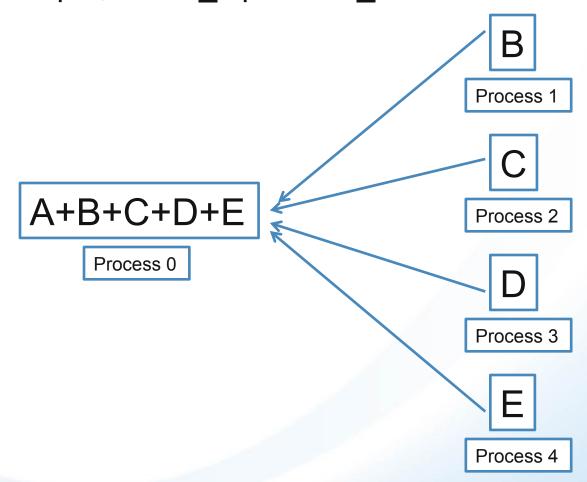
- Performs binary operation with operator on operand, and sends the result to root.
- It is run on all processes in the communicator comm.
- Count, type, operator and root must be the same on each process.

MPI_Op	Meaning
MPI_MAX	Maximum
MPI_MIN	Minimum
MPI_SUM	Sum
MPI_PROD	Product
MPI_LAND	Logical and
MPI_BAND	Bitwise and
MPI_LOR	Logical or
MPI_BOR	Bitwise or
MPI_LXOR	Logical exclusive or
MPI_BXOR	Bitwise exclusive or
MPI_MAXLOC	Maximum and its location
MPI_MINLOC	Minimum and its location



Reduce

For example, if MPI_Op is MPI_SUM





Example 4: Vector Dot Product

The dot product of two vectors x and y is defined as

$$x \cdot y = \sum_{i} x_{i} y_{i}$$

- On the right is the serial version.
- How do we parallelize it?

4_DotProduct available on GitHub: http://github.com/meifeng/MPI

```
/* Serial dot product program */
#include <stdio.h>
const int N=20000;
double dotProduct(double *x, double *y, int n) {
  int i:
  double prod = 0.0;
  for (i = 0; i < n; i++) {
    prod += x[i]*y[i];
  return prod;
int main(int argc, char *argv[]) {
  double x[N];
  double y[N];
  int i:
  for(i = 0; i < N; i++) {
    x[i] = 0.01 * i;
   y[i] = 0.03 * i;
  double prod;
  prod = dotProduct(x,y,N);
  printf("dotProduct = %f\n", prod);
  return 0;
```

Parallel Vector Dot Product

- First we need to consider how to map the vectors onto different processors.
- It is natural to divide the vectors into **blocks** of data, with each process taking one block

X	у
X ₀ X ₁	y ₀ y ₁
X ₂ X ₃	y ₂ y ₃
X _{n-2} X _{n-1}	y _{n-2} y _{n-1}
	X ₀ X ₁ X ₂ X ₃

 $local_x[i] = 0.01 * (i + my_rank * local_N);$ $local_y[i] = 0.03 * (i + my_rank * local N);$ double local prod; local_prod = dotProduct(local_x,local_y,local_N); $if (my rank == 0) {$ printf("dotProduct = %f\n", prod); MPI Finalize(); **Brookhaven Science Associates** return 0;

```
/* Parallel dot product */
#include <mpi.h>
#include <stdio.h>
const int N=20000;
double dotProduct(double *x, double *y, int n) {
  int i;
  double prod = 0.0;
  for (i = 0; i < n; i++) {
    prod += x[i]*y[i];
  return prod;
int main(int argc, char *argv[]) {
  int i;
  double prod;
  int my rank;
  int num procs;
  MPI Init(&argc, &argv);
  MPI Comm size(MPI COMM WORLD, &num procs);
  MPI Comm rank(MPI COMM WORLD, &my rank);
  int local N = N / num procs; //assuming N is totally divisible by num procs
  double local x[local N];
  double local y[local N];
  for(i = 0; i < local_N; i++) {</pre>
  MPI Reduce(&local prod, &prod, 1, MPI DOUBLE, MPI SUM, 0, MPI COMM WORLD);
```

Dealing with extras

```
/* Parallel dot product */
#include <mpi.h>
#include <stdio.h>
const int N=2000;
double dotProduct(double *x, double *y, int n) {
  int i:
 double prod = 0.0;
 for (i = 0; i < n; i++) {
    prod += x[i]*y[i];
  return prod;
int main(int argc, char *argv[]) {
  int i;
 double prod;
  int my rank;
  int num procs;
 MPI Init(&argc, &argv);
 MPI Comm size(MPI COMM WORLD, &num procs);
 MPI Comm rank(MPI COMM WORLD, &my rank);
  int local N = N / num procs;
  int extra = N % num procs;
  double local prod;
```

Some processes have to do extra work if N is not divisible by the number of processes

```
if (my rank == (num procs - 1)) {
  int new N = local N + extra;
  double local x[new N];
  double local y[new N];
  for(i = 0; i < new N; i++) {
    local x[i] = 0.01 * (i + my rank * local N);
    local y[i] = 0.03 * (i + my rank * local N);
  local prod = dotProduct(local x,local y,new N);
else {
  double local x[local N];
  double local v[local N];
  for(i = 0; i < local N; i++) {
    local x[i] = 0.01 * (i + my rank * local N);
    local y[i] = 0.03 * (i + my rank * local N);
  local prod = dotProduct(local x,local y,local N);
MPI_Reduce(&local_prod, &prod, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
if (my rank == 0) {
  printf("dotProduct = %f\n", prod);
MPI Finalize();
return 0:
```



Exercise 5: TrapezoidCollective

- Rewrite the parallel trapezoidal rule program so that
 - Process 0 takes the input values for a, b and N, and propagates these values to all processes using MPI_Bcast.
 - Use MPI_Reduce to sum up the local results from different processes to Process 0
 - Print the final result on stdout from all processes.



Exercise 5: Example Code

- Obtain the example code 5_TrapezoidCollective from GitHub
 - From your MPI directory, run
 - > git pull
 - Or point your browser to <u>http://github.com/meifeng/MPI</u>
- Compile and run the code in interactive mode (since you need to input the parameters).



Output

Enter integral lower bound, upper bound and total integration steps:

0 1 10000

Process 0, WITH N=10000 TRAPEZOIDS, INTEGRAL=1.462651

Process 1, WITH N=10000 TRAPEZOIDS, INTEGRAL=0.000000

Process 2, WITH N=10000 TRAPEZOIDS, INTEGRAL=0.000000

Process 3, WITH N=10000 TRAPEZOIDS, INTEGRAL=0.000000

Process 4, WITH N=10000 TRAPEZOIDS, INTEGRAL =0.000000

Process 5, WITH N=10000 TRAPEZOIDS, INTEGRAL=0.000000

Process 6, WITH N=10000 TRAPEZOIDS, INTEGRAL =0.000000

Process 7, WITH N=10000 TRAPEZOIDS, INTEGRAL=0.000000

Notice that only process 0 gives a non-zero value.

```
#include <stdio.h>
#include <math.h>
#include <mpi.h>
double f(double x){
 return exp(x*x);
int main(int argc, char *argv[]){
  const int ROOT = 0;
  double integral;
                           /*definite integral result*/
  double a;
                           /*left end point*/
  double b;
                          /*right end point*/
                          /*number of subdivisions*/
  int N;
  double h;
                          /*base width of subdivision*/
  double x;
  int i;
  int my rank;
  int numprocs;
  /* we will need some local variables */
  double local a, local b;
  int local N;
  double lcl integral;
  /* MPI programming begins */
  MPI Init(&argc, &argv);
  MPI Status status;
  MPI_Comm_size(MPI_COMM_WORLD, &numprocs);
  MPI Comm rank(MPI COMM WORLD, &my rank);
  if(my rank == ROOT) {
   printf("Enter integral lower bound, upper bound and total integration steps: \n");
   scanf("%lf %lf %d", &a, &b, &N);
  MPI Bcast(&a, 1, MPI DOUBLE, ROOT, MPI COMM WORLD);
  MPI_Bcast(&b, 1, MPI_DOUBLE, ROOT, MPI_COMM_WORLD);
  MPI Bcast(&N, 1, MPI INT, ROOT, MPI COMM WORLD);
  h = (b-a)/N; /* we assume we use the same integration step on all processes */
  /* Find out what the local values are on each process */
  local N = N / numprocs;
  local_a = a + my_rank * local_N * h;
  local b = local a + local N * h;
  /* begins local integration */
  x = local a;
  lcl_integral = (f(local_a)+f(local_b))/2.0;
  for(i = 1; i <= local N-1; i++) {
     x = local a+i*h;
     lcl_integral = lcl_integral + f(x);
  lcl integral = lcl integral*h;
  /* Reduce and send result to ROOT */
  MPI Reduce(&lcl integral, &integral, 1, MPI DOUBLE, MPI SUM, ROOT, MPI COMM WORLD);
  //MPI Allreduce(&lcl integral, &integral, 1, MPI DOUBLE, MPI SUM, MPI COMM WORLD);
  printf("Process %d, WITH N=%d TRAPEZOIDS, INTEGRAL=%f\n", my rank, N, integral);
  /* MPI programming ends */
  MPI Finalize();
  return 0;
```

Allreduce

```
int MPI_Allreduce ( void* operand, void* result, int count, MPI_Datatype type, MPI_Op operator, MPI_Comm comm)
```

- Similar to MPI_Reduce.
- But all the processes get the reduced result, hence there is no parameter for a root process.
- This is necessary if the calculation requires the reduced result to proceed.



Exercise:

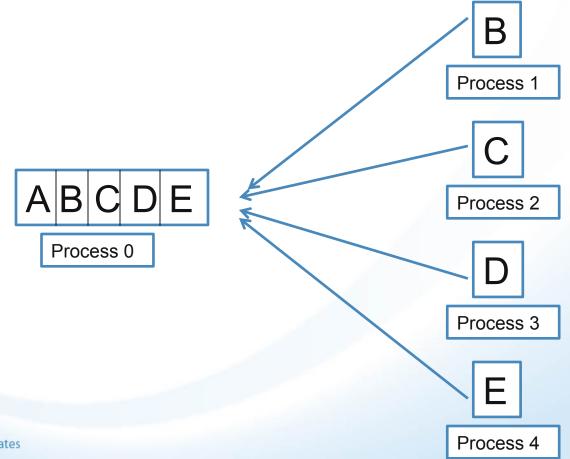
- Rewrite the parallel trapezoidal rule program so that
 - Process 0 takes the input values for a, b and N, and propagates these values to all processes.
 - Use MPI_Allreduce to sum up the local results from different processes and print the final result on stdout from all processes.
 - Login to hpc.csc.bnl.gov
 - Compile and run the new program, and see how the output is different.



Gather

Collects values from a group of processes in a communicator to root

int MPI_Gather (void *sendbuf, int sendcount, MPI_Datatype sendtype, void *recvbuf, int recvcount, MPI_Datatype recvtype, int root, MPI_Comm comm)





Allgather

Collects data from all processes and makes them available on each process

int MPI_Allgather (void *sendbuf, int sendcount, MPI_Datatype sendtype, void *recvbuf, int recvcount, MPI_Datatype recvtype, MPI_Comm comm)

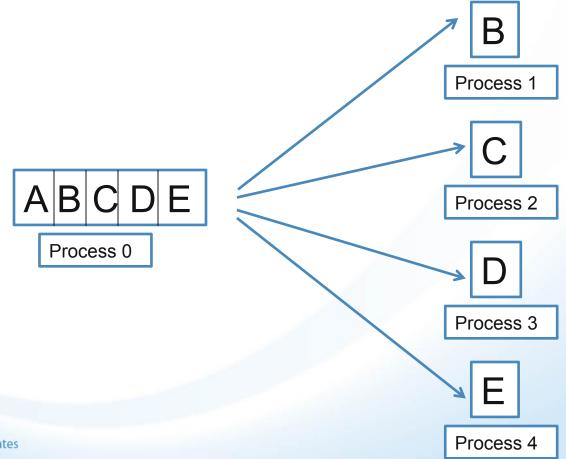
- Similar to MPI_Gather, but now all the processes get the collected data.
- Note in both MPI_Gather and MPI_Allgather, both sendcount and recvcount refer to the number of data blocks per process.



Scatter

Sends data from one process to other processes in a communicator

int MPI_Scatter (void *sendbuf, int sendcount, MPI_Datatype sendtype, void *recvbuf, int recvcount, MPI_Datatype recvtype, int root, MPI_Comm comm)





Example: Matrix-Vector Multiplication

Multiplication of a matrix A of dimensions N x M and a vector x of size
 N is computed as

$$y_i = (\mathbf{A}\mathbf{x})_i = \sum_{j=0}^{N-1} A_{ij} x_j$$

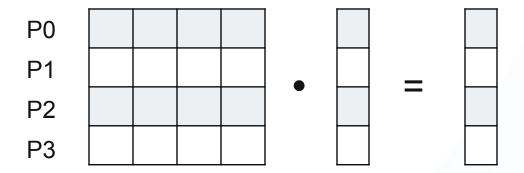
Matvec function implementation:

```
void matvec (int M, int N, int ** mat, int * vec, int * result) {
  int i, j;
  for ( i = 0; i < M; i++ ) {
    result[i] = 0.0;
    for ( j = 0; j < N; j++ ) {
      result[i] += mat[i][j] * vec[j];
    }
  }
}</pre>
```

```
int main (int argc, char * argv[]) {
 int nrows = 8;
 int ncols = 16;
 int i,j;
 int **A = (int **)malloc(nrows*sizeof(int*));
 for(i = 0; i < nrows; i++) {
   A[i] = (int *) malloc(ncols*sizeof(int));
 printf("A = \n");
 for (i = 0; i < nrows; i++ ) {
    for (j = 0; j < ncols; j++) {
     A[i][j] = i + j;
     printf("%2d ", A[i][j]);
    printf("\n");
 int x[ncols];
 printf("x = \n");
 for (j = 0; j < ncols; j++) {
   x[j] = j;
   printf("%d\n",x[j]);
 int result[nrows];
 matvec(nrows, ncols, A, x, result);
 printf("A x = \n");
 for (i = 0; i < nrows; i++) {
    printf("%d\n", result[i]);
  for(i = 0; i < nrows; i++) {</pre>
    free(A[i]);
 free(A);
```

Parallelizing Matrix-Vector Multiplication

- In order to parallelize the Matrix-Vector multiplication, again we need to decide how the data will be mapped onto different processors.
- We could use "block-row" or "panel" mapping.



- We need to either gather different elements of the vectors, or scatter the corresponding rows of the matrix in order to do the multiplication.
- You can get the example code at GitHub either by running "git pull" from your MPI directory, or point your browser to

http://github.com/meifeng/MPI



Gather in Matrix-Vector Multiplication

```
#include <stdio.h>
#include <stdlib.h>
#include <mpi.h>
void matvec (int M, int N, int ** mat, int * vec, int * result) {
 int i, j;
 for ( i = 0; i < M; i++ ) {
    result[i] = 0.0;
   for (j = 0; j < N; j++) {
     result[i] += mat[i][j] * vec[j];
int main (int argc, char * argv[]) {
 int nrows = 8;
 int ncols = 16;
 int i,j;
 int my rank;
 int nprocs;
 MPI Init(&argc, &argv);
 MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
  MPI Comm rank(MPI COMM WORLD, &my rank);
  //assuming nrows and ncols are divisible by nprocs
  int local nrows = nrows / nprocs;
  int vsize = ncols;
  int local vsize = vsize / nprocs;
  int **localA = (int **)malloc(local nrows*sizeof(int*));
  for(i = 0; i < local nrows; i++) {</pre>
    localA[i] = (int *) malloc(ncols*sizeof(int));
  for (i = 0; i < local nrows; i++ ) {
    for (j = 0; j < ncols; j++) {
      localA[i][j] = i + (j+my rank*local nrows);
```

```
int x[vsize]; //global vector
 int local x[local vsize]; //local vector
 for (j = 0; j < local vsize; j++) {
   local_x[j] = j + my_rank * local_vsize;
 //Gather the local vectors into a full vector
 //and make it available on all processes
MPI Allgather(local x, local vsize, MPI INT,
            x, local vsize, MPI INT, MPI COMM WORLD);
 int result[nrows];
int local result[local nrows];
//Do the local multiplication
matvec(local nrows, ncols, localA, x, local result);
 //Gather the final result to Process 0
MPI Gather(local result, local nrows, MPI INT,
            result, local nrows, MPI INT,
            0, MPI COMM WORLD);
if (my rank == 0) {
  printf("A x = \n");
   for (i = 0; i < nrows; i++) {
     printf("%d\n", result[i]);
for(i = 0; i < local nrows; i++) {</pre>
   free(localA[i]);
free(localA);
MPI Finalize();
```



Exercise 7: Matrix Multiplication

 Multiplication of two square matrices A and B of dimensions N x N is computed as

$$(\mathbf{AB})_{ij} = \sum_{k=0}^{N-1} A_{ik} B_{kj}$$

Use "block-row" mapping to parallelize.

P0							P0		
P1			•			=	P1		
P2							P2		
P3							P3		

- Use MPI Gather to collect the final result and print on Process 0.
- Hint: use one-dimensional array to represent the matrices.



Exercise 7: Example Code

- Obtain the example code 7_MatMult from GitHub
 - From your MPI directory, run
 - git pull
 - Or point your browser to <u>http://github.com/meifeng/MPI</u>
- Compile and run the code either in interactive mode, or in batch mode.
 - You can compile the serial version of the code using
 - make serial



```
#include <stdio.h>
#include <mpi.h>
void printMat(int R, int C, double *A) {
 int i,j;
 for (i = 0; i < R; i++) {
   for (j = 0; j < C; j++) {
      printf("%8.1f ",A[i*C+j]);
    printf("\n");
                                                                              if (my rank == 0) {
int main(int argc, char *argv[]) {
                                                                                printf("localA=\n"); printMat(local_nrows, N, localA);
 int N = 8;
                                                                                printf("localB=\n"); printMat(local_nrows, N, localB);
 int i,j,k;
 int my rank;
 int nprocs;
                                                                              for (j = 0; j < N; j++) {
                                                                                for (i = 0; i < local vsize; i++) {
 MPI_Init(&argc, &argv);
                                                                                  local_v[i] = localB[i*N+j];
 MPI Comm size(MPI COMM WORLD, &nprocs);
 MPI Comm rank(MPI_COMM_WORLD, &my_rank);
                                                                                MPI Allgather(local v, local vsize, MPI DOUBLE,
  int local nrows = N / nprocs;
                                                                                              v,
                                                                                                       local_vsize, MPI_DOUBLE,
  if (N % nprocs != 0) {
                                                                                              MPI COMM WORLD);
    printf("Matrix size is not divisible by the number of processes\n");
                                                                                for (i = 0; i < local nrows; i++) {
   MPI Abort(MPI COMM WORLD, 10);
                                                                                  localC[i*N+j] = 0.0;
                                                                                  for (k = 0; k < N; k++) {
                                                                                    localC[i*N+j] += localA[i*N+k] * v[k];
  int local vsize = local nrows;
 double *localA, *localB, *localC;
  double *local v, *v;
 double *globalC;
                                                                              if (my rank == 0) {
                                                                                printf("localA=\n"); printMat(local nrows, N, localA);
  localA = (double *) malloc(local nrows * N * sizeof(double));
                                                                                printf("localB=\n"); printMat(local_nrows, N, localB);
  localB = (double *) malloc(local_nrows * N * sizeof(double));
 localC = (double *) malloc(local nrows * N * sizeof(double));
                                                                              if (my_rank==0) {
                                                                                printf("localC=\n"); printMat(local_nrows,N,localC);
 globalC = (double *) malloc(N * N * sizeof(double));
 for (i = 0; i < N; i++) {
                                                                              MPI_Gather(localC , N*local_nrows, MPI_DOUBLE,
   for (j = 0; j < N; j++) {
                                                                                         globalC, N*local nrows, MPI DOUBLE, 0, MPI COMM WORLD);
      globalC[i*N+j] = 0.0;
                                                                              if (my rank == 0) {
                                                                                printf("globalC = \n"); printMat(N, N, globalC);
  local_v = (double *) malloc(local_vsize * sizeof(double));
          = (double *) malloc(N * sizeof(double));
                                                                              free(v);
                                                                              free(local_v);
 for (i = 0; i < local_nrows; i++) {
                                                                              free(globalC);
   for (j = 0; j < N; j++) {
                                                                              free(localC);
     localA[i*N+j] = (i + my rank * local nrows) + j;
                                                                              free(localB);
      localB[i*N+j] = (i + my rank * local nrows) - j;
                                                                              free(localA);
                                                                              MPI Finalize();
```

#include <stdlib.h>

Other Topics in MPI



Other Topics

- Grouping data for communications
- Parallel program performance
- MPI topologies



Grouping Data for Communication

- Since communication is substantially slower than local computation, we will want to minimize the use of communication routines.
- We can achieve this by grouping data into a single message.
- One way to do this is to pack the data before communication, and unpack after.

```
MPI_Pack (void *data, int count, MPI_Datatype datatype, void *buffer, int buffer_size, int *position, MPI_Comm comm)
```

```
MPI_Unpack (void *buffer, int buffer_size, int *position, void *data, int count, MPI_Datatype datatype, MPI_Comm comm)
```

Note: here buffer_size is the number of bytes in buffer.



Example 8: TrapezoidPack

 In the Trapezoidal rule example, when we take inputs for a, b and N, we send three messages. We can pack them into one message.

```
char buffer[50];
int position = 0;
if(my rank == ROOT) {
  printf("Enter integral lower bound, upper bound and total integration steps: \n");
  scanf("%lf %lf %d", &a, &b, &N);
 // Pack the data. position is increased after each call.
 MPI Pack(&a, 1, MPI DOUBLE, buffer, 50, &position, MPI COMM WORLD);
 MPI Pack(&b, 1, MPI DOUBLE, buffer, 50, &position, MPI COMM WORLD);
 MPI Pack(&N, 1, MPI INT, buffer, 50, &position, MPI COMM WORLD);
 // Now broadcast the packed data, with datatype MPI PACKED
 MPI Bcast(buffer, 50, MPI PACKED, 0, MPI COMM WORLD);
else {
 // Recall that all the processes need to call Bcast.
 MPI Bcast(buffer, 50, MPI PACKED, 0, MPI COMM WORLD);
  // Now unpack the data
  position = 0;
 MPI Unpack(buffer, 50, &position, &a, 1, MPI DOUBLE, MPI COMM WORLD);
 MPI Unpack(buffer, 50, &position, &b, 1, MPI DOUBLE, MPI COMM WORLD);
 MPI_Unpack(buffer, 50, &position, &N, 1, MPI_INT, MPI_COMM_WORLD);
```

Parallel Program Performance

- It is obviously important to be able to measure the performance of the parallel problems.
- MPI provides some functions to do this.

int MPI_Barrier(MPI_Comm comm)

- It blocks until all the processes have successfully executed it.
- It essentially synchronizes the processes in the communicator.

double MPI_Wtime(void)

- It returns a double precision value that represents the number of seconds that have elapsed since some point in the past.
- Needs matching function calls at the start and finish of the code segment being timed.



Timing

```
double start, finish;
/* some calculations */
MPI Barrier(MPI COMM WORLD);
start = MPI_Wtime();
/* some more calculations */
MPI Barrier(MPI COMM WORLD);
finish = MPI_Wtime();
if(my rank == 0)
  printf("Time elapsed = %e seconds\n", finish-start);
```



Exercise 9: Timing

- Put in some timings in your existing trapezoidal rule programs with point-to-point communications, collective communications and with MPI_Pack.
- Compare timings in different versions.
- How does the timing change with different numbers of processes?



Strong and Weak Scaling

- Ideally, as we increase the number of processors while keeping the problem fixed, the time it takes should decrease proportionally.
- Equivalently, if we keep the local problem size fixed, increasing the number of processors should allow us to solve a bigger problem within a given time.
- In reality, communication and I/O latency will cause some performance loss. And such loss is usually bigger as we spread the problem over a larger number of processors.
- We measure the "scalability" of our program using strong scaling and weak scaling.
- Strong scaling is defined as how the solution time changes with the number of processors for a fixed total problem size.
- Weak scaling is defined as how the solution time changes with the number of processors for a fixed problem size per processor.



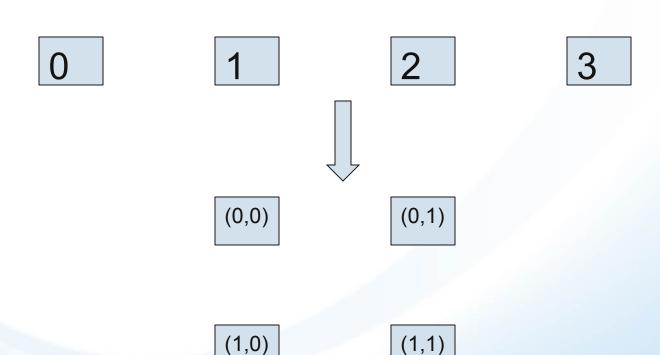
Homework

- 1. With the TrapezoidCollective example, measure the timing with 1, 2, 4, and 8 processes while keeping N fixed. [Strong Scaling]
- Choose a starting value for N, then with 1, 2, 4 and 8 processes, increase the value of N by 1, 2, 4 and 8 respectively. Measure the timings in this scenario. [Weak Scaling]



Communicators and Topologies

- So far we have been using the MPI ranks of the processes to identify the source and destination of the communication.
- Sometimes it is more convenient to define a virtual topology of the processes.





Create an MPI Topology

- There are two types of virtual topologies that can be created in MPI: a Cartesian or grid topology, and a graph topology.
- Cartesian topology is the most widely used. We will need to specify
 - The number of dimensions in the grid.
 - The size of each dimension.
 - Periodicity of each dimension.
 - Whether to allow the system to optimize the mapping of the grid to the underlying physical processors by reordering.
- The mapping will define a new communicator.



Cartesian Topology Example

```
MPI Comm new comm;
int dim_sizes[2];
int wrap_around[2];
int reorder = 1;
\dim \operatorname{sizes}[0] = \dim \operatorname{sizes}[1] = 2;
wrap around [0] = wrap around [1] = 1;
MPI Cart create(MPI_COMM_WORLD, 2, dim_sizes,
                   wrap around, reorder, &new comm);
```

Using the new MPI Topology

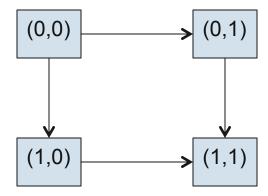
 After the new grid topology is created, we can determine the coordinates of each process by calling

- Given the coordinates, we can obtain the rank of the process
 MPI_Cart_rank (MPI_Comm new_comm, int coords[], int *rank)
- Example:



Exercise 10: Greetings2D

 Rewrite the Greetings program so that a greeting is sent to the nearest neighbors in the plus directions within a two-dimensional Cartesian topology.



 You will need to know the ranks of your four neighbors in the new Cartesian topology.



Cheat Sheet

```
int neighbor_rank;
int neighbor_coords[2];
MPI_Cart_rank(new_comm, neighbor_coords, & neighbor_rank);
```



Exercise 10: Example Code

Get the code from GitHub:

pgit pull or http://github.com/meifeng/MPI

```
#include <stdio.h>
#include <mpi.h>
#include <math.h>
int main(int argc, char *argv[])
 const int ROOT = 0;
 int my rank;
 int recv rank;
 int numtasks;
 int p;
 MPI Init(&argc, &argv); /*Initializes MPI calls*/
 MPI Status status;
 MPI Comm rank(MPI COMM WORLD, &my rank); /* obtains the rank of current MPI process */
 MPI Comm size(MPI COMM WORLD, &numtasks); /* obtains the total number of MPI processes */
 int size = (int)sgrt(numtasks);
 MPI Comm new comm;
 int dim sizes[2];
 int wrap_around[2] = {1,1};
 int reorder = 1;
 dim sizes[0] = size;
 dim sizes[1] = numtasks/size;
 MPI Cart create (MPI COMM WORLD, 2, dim sizes, wrap around, reorder, &new comm);
 int coords[2];
 int my grid rank;
 MPI Comm rank(new comm, &my grid rank);
 MPI Cart coords(new comm, my grid rank, 2, coords);
 char message[100];
 sprintf(message, "Greetings from process (%d, %d)",coords[0], coords[1]);
```

```
int xp neighbor rank, xm neighbor rank;
int yp_neighbor_rank, ym_neighbor_rank;
int xp_neighbor_coords[2], xm_neighbor_coords[2];
int yp neighbor coords[2], ym neighbor coords[2];
xp_neighbor_coords[0] = (coords[0] + 1)%dim_sizes[0];
xp neighbor coords[1] = coords[1];
xm neighbor coords[0] = (coords[0] - 1 + dim sizes[0]) * dim sizes[0];
xm neighbor coords[1] = coords[1];
yp neighbor coords[0] = coords[0];
yp neighbor coords[1] = (coords[1] + 1)%dim sizes[1];
ym_neighbor_coords[0] = coords[0];
ym_neighbor_coords[1] = (coords[1] - 1 + dim_sizes[1])%dim_sizes[1];
MPI Cart rank(new_comm, xp_neighbor_coords, &xp_neighbor_rank);
MPI Cart rank(new comm, xm neighbor coords, &xm neighbor rank);
MPI Cart rank(new_comm, yp_neighbor_coords, &yp_neighbor_rank);
MPI Cart rank(new comm, ym neighbor coords, &ym neighbor rank);
MPI Send(message, 100, MPI CHAR, xp neighbor rank, 0, new comm);
MPI Send(message, 100, MPI CHAR, yp neighbor rank, 1, new comm);
char recv messagex[100];
char recv_messagey[100];
MPI Recv(recv messagex, 100, MPI CHAR, xm neighbor rank, 0, new comm, &status);
MPI Recv(recv messagey, 100, MPI CHAR, ym neighbor rank, 1, new comm, &status);
  printf("My Cartesian coordinates: (%d, %d)\n", coords[0], coords[1]);
  printf("Message received:\n %s \n %s\n", recv_messagex, recv_messagey);
MPI Finalize();
                       /*Finalizes MPI calls */
return 0;
```

Wrapping Up...

- There are still many features in MPI that haven't been covered.
 - User-defined data types.
 - MPI groups, contexts and user-defined communicators.
 - MPI I/O.
 - MPI/OpenMP hybrid programming.
 - ...
- But what you learn today will allow you to write basic MPI programs.



References for further reading

- "Parallel Programming with MPI", Peter S. Pacheco, Morgan Kaufmann Publishers, 1997. [Pedagogical]
- "Introduction to Parallel Computing" (2nd Ed.), Ananth Grama, Anshul Gupta, George Karypis and Vipin Kumar, Pearson Education, 2003. [Technical]
- "The Art of Multiprocessor Programming", Maurice Herlihy and Nir Shavit, Morgan Kaufmann Publishers, 2008.
 [Technical]

